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**Prof. Dr. Ismail Hakki Tavman (Dokuz Eylul University, Izmir – Turkey)**

Full Professor in Mechanical Engineering Department of Dokuz Eylul University, Izmir – Turkey, and Head of Energy Section in the same department. He graduated from Mechanical Engineering Department of Bosphorus University - Istanbul in 1973. He obtained his M.Sc. and PhD degrees in Mechanical Engineering, respectively in 1983 and 1987 from ENSAM- Paris (Ecole Nationale Supérieure d'Arts et Métiers- Paris, France). His PhD thesis is on “thermal anisotropy of polymers as a function of their molecular orientation”.

He was visiting professor and researcher in several universities in different countries: Ulm University – Germany; Department of Mechanical Engineering COPPE/Escola Politécnica – Federal University of Rio de Janeiro, UFRJ Rio De Janeiro – Brazil; University of Reims Champagne-Ardenne, Laboratoire GRESPI – Thermomécanique Faculté des Sciences, Reims, France; University of Florence Mechanical Engineering Department – Florence – Italy; Polymer Institute, SAS, Dubravska - Bratislava, Slovakia.

Prof. Ismail Hakki Tavman has been invited as keynote speaker in many International Conferences.

Presently his fields of research are: Thermal and mechanical properties of conductive polymer Nano-composites; Nanofluids- Characterization; 3-omega method for measuring thermal diffusivity and conductivity; Measurement of thermal diffusivity by Laser Flash Technique; Thermal analysis of TFT-LCD TV Panels.

He has: 45 papers publications in SCI indexed journals; 11 book chapters, 88 papers published in the proceedings of international conferences and 50 papers published in the proceedings of national conferences. He was director or co-director in different international (3) or national research projects (12). He was advisor in 25 MSc and 4 PhD thesis.



**Prof. Dr.-Ing. habil. Dipl. Phys. Dr. h.c. Egon Hassel (University of Rostock, Germany)**

He was born in 1955 in Germany, near Bad Kreuznach, Rheinland Pfalz. 1962-74 Mathematical-Natural-Science High-school, Degree earned: Allgemeine Hochschulreife. 1974-76 German Army service. 1976-82 Physics study at RWTH Aachen University, Germany, Degree earned: Diplom Physiker. 1982-86 PhD work at RWTH Aachen University, Germany, Faculty of Mechanical Engineering, Institute of Technical Thermodynamics, Prof. Dr.-Ing. K. F. Knoche, theses: “Coherent anti-Stokes-Raman spectroscopy for study of IC engine knock”. 1982-89 Research assistant at RWTH Aachen University, Germany, Faculty of Mechanical Engineering, Institute of Technical Thermodynamics, Prof. Dr.-Ing. K. F. Knoche. 1989-96 Habilitation about “Laser optical measurements for combustion studies” at TU Darmstadt, Germany, Faculty of Mechanical Engineering, Institute of Energy- and Power Plant Technology, Prof. Dr.-Ing. J. Janicka. 1989-99 Research assistant at TU Darmstadt, Germany, Faculty of Mechanical Engineering, Institute of Energy- and Power Plant Technology, Prof. Dr.-Ing. J. Janicka. 1999- Full professor, chair, Institute of Technical Thermodynamics, Faculty of Mechanical Engineering and Ship Building, University of Rostock, Germany. November 2012 honorary doctorate from Azerbaijan Technical University in Baku.



**Prof. Astan Shahverdiyev (Azerbaijan Technical University, Baku, Azerbaijan)**

Prof. Astan Shahverdiyev was born on 15 February 1947 year in Fizuli city of Azerbaijan Republic. He graduated from Azerbaijan Oil and Chemistry Institute on 1970 year. A.N. Shahverdiyev was post-graduated student of Azerbaijan Technical University on 1978-1981 years. On 1981, he defended his PhD thesis and got the candidate of technical sciences degree. On 1982 year, he was elected to the assistant position of Department "Heat techniques and heat installations" of Azerbaijan Technical University. On 1992 year, he defended his doctor of science thesis at the Moscow Energy Institute and got the doctor of technical sciences degree. On 1994 year, A.N. Shahverdiyev got Professor degree. On 1995 year, he was elected member of New-York Academy of Sciences. On 2001 year, Prof. Shahverdiyev was elected to the position - head of the department: "Heat and Refrigeration Techniques".



Prof. A.N. Shahverdiyev published more than 400 scientific publications, monographs, patents and lecture book. On 1998-2002 year A.N. Shahverdiyev was co-ordinator of Ozone Centre in Azerbaijan office of UN. He is member of Renewable Energy working group of EURONETRES of UNESCO.

Prof. A.N. Shahverdiyev participated with the scientific presentations in the international conferences and symposiums held in USA, Canada, India, Egypt, Swiss, Germany, UK, Italy, The Netherlands, Portugal, China, Turkey, Slovak Republic, Greece, Uzbekistan, Belorussia, Ukraine, France, Russia etc. He was member of Azerbaijan Republic in the various congresses organized by UN and UNESCO. Prof. A.N. Shahverdiyev is honor of Z. Tagiyev scientific medal. He can speak English and Russian languages. Prof. A.N. Shahverdiyev member of Parliament of Azerbaijan Republic from 2005 year. Married, has 2 daughters.

**Assist. Prof. Dr. Javid Safarov (University of Rostock, Germany)**

Assist. Prof. Dr. Javid Safarov was born on 10 December 1965 in Urkmezli village of Qazax region of Azerbaijan. He graduated from the Azerbaijan Technical University with honours and began to work at the department of "Heat and Refrigeration Techniques" of this university. He worked on 2005-2006 years as research co-worker at the University of Erlangen-Nürnberg of Germany. He is research co-worker at the department "Technical Thermodynamics" of University of Rostock from 2006 and has permanent position in this University from year 2011. Javid Safarov is member of the German group of the International Association for the Properties of Water and Steam (IAPWS). He has honoured the DAAD (2002 and 2006), Alexander von Humboldt (2003-2004, 2007) and JSPS-Japan (2004) fellowships.



Dr. Javid Safarov is the co-author of 1 book, 1 monograph, 4 lecture book and more than 250 publications in the journals and conferences.

He is leader of the research group of "Thermophysical properties of fluids" at the department "Technical Thermodynamics" of University of Rostock. He is one of leading person in the research field of investigations of the thermophysical properties of fluids at high pressures and temperatures in the world.

Research field: Thermophysical properties of substances.

Married, has 3 daughters.

**Assist. Prof. Dr. Alpaslan Turgut (Dokuz Eylul University, Izmir – Turkey)**

Assistant Professor in Mechanical Engineering Department of Dokuz Eylul University, Izmir – Turkey. He obtained his PhD degree in Mechanical Engineering from Dokuz Eylul University, in 2010. He was visiting researcher in Multiscale Thermophysics Lab. and Thermomechanic Lab. in University of Reims, France; RAPSODEE Centre – CNRS 5302 Ecole de Mines Albi, University of Toulouse, France; Slovak Academy of Sciences Polymer Institute, Bratislava, Slovakia. His current research topics are thermophysical characterization of materials, mainly nanofluids, phase change materials with graphene additions, polymer composites, electronics cooling. He has authored or co-authored more than 40 papers in indexed journals and conference proceeding. He has participated in more than 10 scientific research projects as a director or researcher.



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## PREFACE

### **International Conference on Thermophysical and Mechanical Properties of Advanced Materials**

Thermodynamics is a very fascinating scientific field which has to do with many different phenomena in nature and technique. As an interesting example we can regard climate change which at the moment is on the agenda of many political decision makers and scientists. Climate change is partly caused by the emission of the carbon dioxide molecule to the atmosphere from farming, from technical combustion in energy technique and transport and from many other human related processes. The heat transfer processes in the atmosphere clearly have to do with thermodynamics. on the other hand, measures to reduce human impact on the environment, like CCS, carbon capture and storage, from combustion also involve thermodynamics processes. To solve and handle thermodynamics problems one needs “Thermophysical and Mechanical Properties of Advanced Materials”. One example is the possible capture of carbon dioxide from atmosphere or exhaust gases in ionic liquids. To make this technically feasible data for the thermophysical property of solution of carbon dioxide in the advanced material of an ionic liquid are needed.

Within this conference we want to bring together international scientists and engineers who work in the very broad field of “Thermophysical and Mechanical Properties of Advanced Materials”. This is a very interesting and modern research field. It covers experimental and theoretical new results for thermophysical properties, new measurement techniques and the their applications, molecular modeling with new theoretical insights, applications which show the improvement done with the described research for thermophysical properties and mechanical properties all for materials like nanofluids, nanocomposites, alternative solvents, metals, alloys, ceramics, composites, etc. These subjects cover fundamental and applied research and engineering aspects.

We want to foster lively discussions and future international collaborations on this important and stimulating field with this conference.

We choose the venue of the conference as a holiday resort with all the amenities of such a place in a very nice surrounding and with the possibility to excursions to historically interesting tourist sites like Ephesus.

We wish you a very pleasant, joyful, interesting and stimulating conference “THERMAM 2014” at the Boyalik Beach Hotel, Cesme - Izmir, Turkey.

**The Organizing Committee.**

# CONTENTS

|                                   |             |
|-----------------------------------|-------------|
| <b>ORGANIZING COMMITTEE .....</b> | <b>II</b>   |
| <b>SCIENTIFIC COMMITTEE .....</b> | <b>VI</b>   |
| <b>PREFACE .....</b>              | <b>VIII</b> |
| <b>KEYNOTE ABSTRACTS .....</b>    | <b>1</b>    |

|   |    |
|---|----|
| Microscale Frequency and Spatial Domain Photothermal Reflectance Measurement of Thermal Conductivity and Diffusivity .....                          | 1  |
| Contribution of Inverse Methods For the Thermal Characterization of Orthotropic Composite Materials.....  | 2  |
| Characterization of Heat Transport at Interfaces in Multilayers, Nanocomposites and Nanofluids .....  | 3  |
| Laser-Based Linear and Nonlinear Elastic Bulk (3D), Surface (2D), and Wedge (1D) Waves in Materials Science .....                                   | 4  |
| Deformation of Super Alloys at Elevated Temperatures .....  | 6  |
| Heat Transfer Properties of Complex Porous Media .....  | 8  |
| Experimental Determination of Thermo-Physical Properties of Metal-Organic Compounds (with Respect to Thin Film Deposition and Nanotechnology) ..... | 9  |
| Thermodynamics For Energy Engineering .....   | 10 |
| Time Resolved Measurements of Thermodynamic Properties During Chemical Reactions of Bio-Molecules .....   | 11 |
| Photoluminescence Enhancement In Metamaterial Nanostructures .....  | 13 |
| Ion Beam Assisted Enhanced Thermoelectric Properties (with figure of Merit above 2.0) ....  | 14 |

|                        |           |
|------------------------|-----------|
| <b>ABSTRACTS .....</b> | <b>15</b> |
|------------------------|-----------|

|  |    |
|--|----|
| Effective Ultrasonic Duration for Better Dispersion of Nanofluid.....  | 15 |
| The Effect of Thermal Cycles on the Mechanical Properties of High Density Polyethylene (HDPE) and Graphite/HDPE composites ..... | 16 |
| Influence of Thermal Cycling on Tensile Properties of Expanded Graphite/High Density Polyethylene Nanocomposites .....           | 16 |
| Effect of Inclination Angle on Nanofluid Based Single Phase Natural Circulation Mini Loops.....                                  | 18 |

|  |    |
|--|----|
| X-ray Computed Tomography of Gas Diffusion Layers of PEM Fuel Cells: Determination of the Effective Thermal Conductivity .....                     | 19 |
| An Experimental Study on the Dispersion Stability of Alumina-Water Nanofluids via Particle Size Distribution and Zeta Potential Measurements ..... | 20 |
| Large Deflection Behavior of Functionally Graded Beams Under Temperature Rising .....  | 21 |
| Static Behavior of Functionally Graded Structures at Elevated Temperature with Temperature-Dependent Physical Properties .....                     | 21 |
| Application of Nano-Refrigerants and Nano-Lubricants to the Domestic Refrigerators .....   | 22 |
| Measurement of Physical Properties of Nanofluids .....   | 23 |
| Shape Memory Behavior of Precipitation Hardened NiTi Shape Memory Alloys .....   | 24 |
| Effect of Base Fluid Types on Thermal Properties of Different Nanofluids .....   | 24 |
| Magneto-thermo-mechanical Characterization of Polycrystalline NiMnCoGa Meta-magnetic Shape Memory Alloys .....                                     | 25 |
| Breaching CNT Nanofluids Thermal Conductivity Modelling Uncertainties .....  | 26 |
| Thermophysical Properties of industrial Ni -based Superalloys .....  | 27 |
| Modeling of Nanofluid Thermodynamic Properties .....   | 28 |
| Photon Switching in Waveguide Fabricated From Metallic Nanorod Slab .....  | 29 |
| Numerical Simulation of Mixed Convection of Nanofluids in a Square Cavity with an Adiabatic Block at the Center .....                              | 30 |
| Characterization of Hardening Properties and Fracture Criterion for Mg Alloy Plates at Elevated Temperature .....                                  | 31 |
| Effect of Stamp Forming Pressure and Temperature on Polypropylene Sheets .....   | 31 |
| the Thermal Conductivity Measurement With DC+AC Driven Nanothermal Probe .....   | 32 |
| Numerical Simulations and Experimental Results of Quantitative SThM Measurements for Thin Layer Samples .....                                      | 33 |
| Electronic Transport in molecular materials .....  | 33 |
| Investigations of Thermal Diffusivity of Mixed $Zn_{1-x}Se_x$ Crystals and its Correlation With Optical and Electric Properties .....              | 34 |
| Development of Cellular Ceramics Bricks Starting From Clays .....  | 35 |
| Improvement of Thermal and Electrical Properties of Silicon-Ni Composites Using a Magnetic Field Process .....                                     | 36 |
| Progress in Phosphorus-Containing Polymers: Design, Structure and Properties. ....   | 37 |
| Finite Element Analysis of Damping and Vibration Response of Epoxy Resin Reinforced with Nitrile Butadiene Rubber .....                            | 37 |

|  |    |
|--|----|
| Measurement of Rock Materials By Pulse Transient Technique – Uncertainty Analysis of Two Models for Cylinder and Cuboid Shape of Samples.....              | 38 |
| Time Dependent Stability Analysis of Nanofluids.....   | 39 |
| Transverse Flexural Free Vibration Analysis of Rotating Euler–Bernoulli FGM Beams by the p-FEM .....   | 39 |
| The Effect of Synthetic Fibres on the Mechanical Behaviour of Reinforced Concrete Beams  | 40 |
| The Effect of Filler Type on the Properties of In-Situ Polymerized PP Nanocomposites .....   | 40 |
| Recycling High Performances Concrete .....   | 41 |
| A premature Failure of a Super-heater Tubing in a Power utility Unit.....  | 42 |
| Characterization of Sintered %50 Ni-%48 Cr-%2 Ti Powder Mixtures Containing Intermetallics.....  | 43 |
| Mechanical Properties of a Composite Produced From Electroless Ni Plated Cr and Ti Powders .....   | 43 |
| Experimental and Analysis of the Uniaxial Behavior of High Density Polyethylene Pipes (HDPE-100) .....   | 44 |
| Mechanical and Microstructural Study of Photo-Aged Low Density Polyethylene (LDPE) Films.....  | 45 |
| Calculation of Thermodynamic Properties of CO <sub>2</sub> Using the Combined Thermal Equation of State with a Small Number of Adjustable Parameters ..... | 46 |
| Study on the Thermal Degradation of St-MMA Copolymers with Different Compositions Using Isoconversional Method.....  | 48 |
| Study By A Genetic Algorithm the Effect of Heat Stress on the Shear Damage of the Fiber Matrix Interface of A Nanocomposite Material (Graphite/Epoxy)..... | 49 |
| Synthesis of Conductive Polymers - Metal Nanocomposites and Investigation of Their Optical Properties.....   | 50 |
| CO <sub>2</sub> Solubility in Ionic Liquids at High Pressures and Wide Range of Temperatures.....  | 51 |
| Changes in the Thermal and Other Properties of Polylactide by Blending with Thermoplastic Polyurethane.....  | 52 |
| Thermophysical Properties of Butanol-1 at Pressures up to 200 MPa.....   | 53 |
| Thermophysical Properties of Azerbaijan and Turkish Water Resources .....  | 54 |
| Numerical Contribution to Heat Treatment of Wood .....   | 55 |
| Effect of Surface Pretreatment of Aluminum Substrate on Properties of Ni Electrodeposited Coating .....  | 56 |

|  |    |
|--|----|
| Effects of Co Alloying Element on Chemical Composition, Morphology, Hardness and Corrosion Behavior of Electrodeposited Cr-Co Coatings.....                                    | 57 |
| The Investigation of the Density of Binary Methanol + Chlorobenzene Mixtures at High Pressures.....  | 58 |
| Finite Element Analysis of Out-of-plane Compressive Properties of a Novel Concept of Honeycomb Structures with Hexagonal and Auxetic (negative Poisson's ratio) topology ..... | 58 |
| A Thermal and Chemical Characterization of Limestone From Kellal Mountain (North-East Constantine, Algeria) .....  | 59 |
| Effect of A Turbulent Plane Wall Jet Impinging a Hot Obstacle.....   | 59 |
| Experimental and Analysis of the Uniaxial Behavior of High Density Polyethylene Pipes (HDPE-100) .....   | 60 |
| Study of the Shear Modulus O of Wood-Based Layered Composites Under Static Load Using Finite Element Method.....   | 61 |
| Standard Enthalpy of Combustion of Biodiesel From Hydroxylated Oils.....   | 63 |
| The Investigation of the Hydrocracking Process of Tar With Heavy Gas Oil of Catalytic Cracking In the Presence of High-Dispersed Halloysite.....                               | 64 |
| Catalytic Oxidation of Dearomatized Diesel Fraction in Liquid Phase By Extraction Method.....  | 65 |
| Effect of Activation Temperature on Properties of Activated Carbon From Orange Peel By Zinc Chloride.....  | 66 |
| Horizontal and Vertical Optical Misura® Dilatometers .....   | 66 |
| Scratch test of Silica and PVB coatings deposited on sandblasted glass .....   | 67 |
| Fundamental Equations of State for Fluorobenzene and for Mixture of Benzene With Fluorobenzene ( $C_6H_6 - C_6H_5F$ ).....   | 68 |
| Determination of the Solid-Liquid Equilibrium of Mixtures of Sugar Alcohols for Their Use as Phase Change Materials.....   | 69 |
| Research of the Level of Hydration of the Low-Main Cements and Phase Composition of the Stone on Their Basis .....   | 70 |
| Manufacturing of the Additional Cements with Using Local Rocks and Wastes of Asbestos-Cement Production.....   | 70 |
| Influence of Composition on the Thermal and Mechanical Properties of Elastomeric Polyamide Blends for Industrial Applications .....  | 71 |
| Rheological Characterization of the Modified Crude Oil of the Field of Tin Fouyetabankort (Illizi, Southern Algeria) .....   | 72 |
| Heat Flow Meter-Fox 50 .....   | 73 |

|  |    |
|--|----|
| New Flame Retardant Phosphorus-Containing Polymers with Liquid Crystalline Properties.<br>Synthesis and Characterization .....   | 73 |
| A New Generalized Correlation of Viscosity Coefficient of Complex Hydrocarbon Mixtures<br>In a Wide Range of Temperatures and Pressures.....                             | 74 |
| A New Generalized Correlation of Thermal Conductivity Coefficient of Complex<br>Hydrocarbon Mixtures in a Wide Range of Temperatures and Pressures .....                 | 75 |
| Hexavalent Chromium (Cr (VI)) Adsorption Behavior Onto Poly(Pyrrole-Co-Ortho-<br>Anisidine) Nanocomposite: Thermodynamics and Kinetics Study .....                       | 76 |
| the Assessment of Curing Parameters and Mechanical Properties of Epoxy Resins Modified<br>with Polyurethane based on Polycarbonate Diol.....                             | 77 |
| Morphology and Thermal Properties of Chitosan/Bentonite Beads Prepared for Dye<br>Removal .....  | 78 |
| Thermophysical Properties of Date Palm Fiber Reinforced Thermoset Matrix .....   | 78 |
| Property Libraries and Software for Seawater, Steam, Water, Ice, Humid Air, and other<br>Working Fluids for Calculating Desalination and Related Processes.....          | 79 |
| Performance Evaluation of Peanut Roasting Process at Continuous Type Infrared System ...   | 80 |
| Electrochemical Detection of Uric Acid Based on Polypyrrole/Iron Hexacyanoferrate Film<br>Modified Iron Electrode.....   | 80 |
| Scanning Micro and Nano-Thermal Expansion Microscopy of Polymers : Application to the<br>Determination of Surface Glass Transition Temperature in a Wood Cell Wall ..... | 81 |
| Solid State Synthesis of Spirothia(Selena) Pyranes Containing Condensed Pyrazole Rings ..  | 82 |
| Study of Thermophysical and Mechanical Properties for New Composites Based on the<br>Mortar and the Date Palm Wood to Use for Thermal Insulation in Buildings .....      | 83 |
| Synthesis of New Derivatives of Morpholinium With Acrylic and Metakrilovy Acids.....   | 84 |
| Models and Numerical Study of Thermal Conductivity for Conductive Particle Filled Polymer<br>Composite.....  | 85 |
| Thermophysical Properties of Ionic Liquids With [NTf <sub>2</sub> ] <sup>-</sup> Anions .....  | 86 |
| Simulation of Convection Heat Transport in Open-Cell Metal Foam .....  | 87 |
| The Density-Salinity Relation of Standard Seawater.....  | 87 |
| Characterization of Oscillating Water Transport in Metal Foam.....   | 88 |
| Thermophysical Characterization of a Urea Based Eutectic Mixture for Thermal Energy<br>Storage.....  | 89 |
| Modeling of the Bubble Growth Dynamics in PS/CO <sub>2</sub> Foaming System.....   | 90 |
| The IAPWS Industrial Formulation for the Thermodynamic Properties of Seawater .....  | 91 |

|  |     |
|--|-----|
| Enhancement of Compression Performances of Foam Core Sandwich Composites.....  | 92  |
| Molecular Simulation of Nano-Dispersed Fluid Phases .....  | 93  |
| Mechanical Properties, Microstructure and Density of Rigid Crosslinked PVC/Organoclay<br>Nanocomposite Foams .....   | 94  |
| Experimental and Theoretical Analysis of Heat Transfer In Micro-Models of Porous Media   | 95  |
| Solubility and Diffusivity of Normal Pentane and Supercritical CO <sub>2</sub> in St-MMA Copolymer<br>with Different Compositions .....                            | 96  |
| Simulation Under Uncertainty of Heat Conduction in Heterogeneous Media Combining<br>Integral Transformation and Polynomial Chaos .....                             | 98  |
| Thermal Degradation and Burning Behavior of a Commercial Epoxy Resin Blended with an<br>Organophosphate.....   | 99  |
| Effect of Stamp Forming Pressure and Temperature on Polyvinylchloride Sheets.....  | 99  |
| Calibration of Moisture Sensor for the Monitoring of Temperature-Moisture Regime in<br>Volcanic Tuffs (Natural Rock Dwellings) in Brhlavce Village (Slovakia)..... | 100 |
| Dilatometry- Theory, Instrumentation and Applications .....  | 100 |
| Optimum Design of the Vehicle Energy Absorber .....  | 101 |
| Adaptive Nanomechanical Response and Elastic Property Analysis of Polymer Brushes by<br>AFM Nanoscale Probing.....   | 102 |
| Low Velocity Impact Response of Sandwich Composites with Different Core Thicknesses  | 103 |
| Nature and Surface of Steel Effects on Coatings Obtained By Galvanization at Various<br>Immersion Times.....   | 104 |
| Investigation of the Ribs Effects on Dynamic Response of Grid Composite Structures Under<br>Impact Loading .....   | 105 |
| The Modelling of Solar Air Collector with Thermal Efficiency Analysis and Artificial Neural<br>Networks .....  | 106 |
| A New Fatigue Damage Model for Mechanic Parts Subjected to High-Cycle Fatigue<br>Loadings.....   | 107 |
| Preparation of Dense and Interconnected Porous Cordierite Ceramics .....   | 108 |
| Density of Bosporus Seawater .....   | 111 |
| SAC305 vs. SnPb Solder Joint Electrical and Mechanical Properties Measurements as<br>Function of Working Temperature and Soldering Thermal Profile.....            | 112 |
| Residual Stresses in the Precipitation Layer of Gas Nitrided Alloy Steels.....   | 113 |
| The Influence of Silica Nanoparticles on Thermal Properties of Poly(lactide) Based Hybrid<br>Materials.....  | 113 |

|   |     |
|---|-----|
| Thermodynamic and Thermo-Physical Properties of Liquid Li-Zn Alloys. Molecular Dynamics and CFM Study vs. Experiment.....   | 114 |
| A New Class of Maraging Steel with Increase Heat Working Stability .....  | 115 |
| Dielectric Properties of <i>PZT-PBC-ZTIS</i> Piezoelectric Ceramics .....   | 116 |
| Simulation of the Process of an Electro-Thermal Interaction in the Diode Laser System.....  | 116 |
| Cooling Condition Effects on Phase Transformation, Crystal Structure and Microstructure of Cu-Al-Co Shape Memory Alloy .....  | 117 |
| Status and Perspective of Production of Cement with Use Non-traditional Raw materials - Volcanic rocks of Uzbekistan .....  | 117 |
| Formation and Physical Properties of $Sb_2O_3$ -PbO-MnO Glasses .....   | 118 |
| Influence of the Magnetic Field on the Morphology of the Wear of the Cutting Tool.....  | 119 |
| Investigation of the Temperature Stability of Perovskite Phase Formation and the Electromechanical Properties of $Pb(Zr_{1-x}Ti_x)O_3$ Ceramics Modified with Certain Additives | 119 |
| Study of Glass Formation In the $Sb_2O_3$ - $Li_2O$ - $MoO_3$ Ternary System .....  | 120 |
| Fatigue Damage Modelling of Polymeric Matierials: Case of HDPE .....  | 120 |
| Study of Thermal Conductivity and Morphology of Bio-Polymer Based Nanocomposites with Expanded Graphite and Montmorillonite.....  | 121 |
| Structural and Optical Properties of Tin Oxide Thin Films Prepared by Spray Ultrasonic Technique.....   | 122 |
| Fatigue Life Calculation by Cycle Counting Method and Spectra Methods Under Random Loading.....   | 122 |
| Influence of Fatigue on Mechanical Properties of Kevlar Fibers Epoxy Composite and Characterized Damage By Acoustic Emission Technique (AE).....                                | 123 |
| Molarity Effect on the Optical and Structural Properties of Sprayed Indium Oxide Thin Films   | 124 |
| Simulation of carbon ion implantation in mono-crystalline silicon substrates .....  | 124 |
| Perovskite Formation and Dielectric Responses in PZN Modified PMF-PZT Ceramics.....   | 125 |
| Thermophysical Properties of Nitrous Oxide ( $N_2O$ ) from a New Highly Precise ab Initiopair Potential.....  | 125 |
| The Investigation of Usability of Wasted Cross-Linked Polyethylene in Production of Insulation Materials.....   | 126 |
| Mechanical and Thermodynamic Properties of $Zr_{21}Al$ Under High Temperature and Pressure From First-Principles Calculations.....  | 127 |
| Proposal to Reduce GUM's Recommendations to Practice in Thermophysics.....  | 127 |

|  |     |
|--|-----|
| Production Technology of Clinker and Cement Raw Mix Bicomponent Using Gabbro From Akchinsk Field .....                     | 128 |
| Heat Treatment of Wood.....  | 130 |
| Synthesis and Characterization of Ni Containing LaAlO <sub>3</sub> Perovskite.....   | 130 |
| Mössbauer Study of Feco-8nb-30b Nanocomposite Prepared By Mechanical Alloying .....  | 131 |
| Numerical Study of Two Phase Laminar Convection Nanofluid .....  | 131 |
| In Microchannel .....  | 131 |
| Development and Characterization of Triaxial Porcelain System .....  | 132 |
| Buoyancy Effect on Laminar Mixed Convection In A Horizontal Tube.....  | 132 |
| Deposition of ZnO Thin Films on Glass, Ito and ZnO:Al Coated Glass Substrates.....   | 133 |
| Optical properties and Raman investigations of CuInSe <sub>2</sub> thin film prepared from CuInSe <sub>2</sub> powder..... | 134 |
| Structural, Optical and Magnetic Characterisations of Mndoped MgO Nanoparticles .....                                      | 135 |
| Surface Properties of Activated Carbon From Different Raw Materials .....  | 136 |
| How To Optimize Data Quality of Thermophysical Properties of Nickel Based Superalloys.....                                 | 136 |
| Investigation of Polyethylene/Graphite Composites and their Electrical, Thermal and Mechanical properties .....            | 137 |
| Thermal Conductivity of Epoxy Resin Cross-linking.....   | 137 |
| Thermal Analysis of Bipolar Microelectronic Devices.....   | 138 |
| <b>INDEX</b> .....   | 139 |

# KEYNOTE ABSTRACTS

## Microscale Frequency and Spatial Domain Photothermal Reflectance Measurement of Thermal Conductivity and Diffusivity

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A photothermal technique capable of measuring thermal conductivity and thermal diffusivity with micrometer resolution is introduced. This technique involves the measurement of thermal diffusivity and thermal effusivity to extract the thermal conductivity. The experimental approach uses the same hardware to achieve measurements using two photothermal techniques: frequency domain photothermal reflectance method for thermal effusivity, and spatial domain photothermal reflectance method for thermal diffusivity. A thin film is applied to the sample to ensure strong optical absorption and to introduce a thermal boundary condition that explicitly contains an expression for the thermal effusivity. A proof of principle experiment was conducted using two surrogate samples: SiO<sub>2</sub> is a material with thermal properties representative of high burn-up nuclear fuel, and CaF<sub>2</sub> is a material with thermal properties representative of fresh nuclear fuel. To generalize this approach, sensitivity analysis is conducted for materials having a range of thermal conductivities. The measured conductivities compare favorably with published values. As a potential post irradiation examination tool, this new experimental approach has important technological applications to advance nuclear fuel development.

**Keywords:** Photothermal reflectance, Thermal conductivity, Thermal diffusivity

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## Contribution of Inverse Methods for the Thermal Characterization of Orthotropic Composite Materials

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The need for specific thermal characterization methods is often driven by the sample, according to both the structure and geometry. For instance, in the case of highly anisotropic composite materials, the samples may be quite thin, which prevents to make use of the widespread transient characterization methods designed to be used with some electro-resistive probe heating the sample with a semi-infinite thickness assumption. In that case, it is still possible to implement the same kind of methods with a convenient finite sample model. Unfortunately, the thermal parameters to be retrieved may result to be correlated and/or have a low sensitivity coefficient, which yields a quite poor expectation for their simultaneous estimation.

In this lecture we propose an estimation method for the simultaneous estimation of both the in-plane and in-depth thermal conductivities of thin highly orthotropic composite materials. Both the thermal resistance between the sample and the electrical resistance and the probe's heat capacity must also be estimated. These thermal parameters are estimated within a bayesian frame by a Monte Carlo Markov Chain (MCMC) method, implemented with a Metropolis Hastings algorithm.

The Bayesian approach offers the possibility to obtain the posterior probability distribution for each estimated parameter through adding some prior information. In this work, we include a sequential Gaussian prior for the thermal resistance, probe heat capacity and even in-plane thermal conductivity. Different kind of samples are analysed in this lecture, from fiber layers to carbon nanotubes composites, which aim to present some different in-plane/transverse ratio, correlation and sensitivity levels.

**Keywords:** Thermal conductivity, Orthotropic materials, Hot Disk, Metropolis Hastings, Bayesian methods

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**Olivier Fudym** is a Professor in Heat Transfer, Ecole des Mines d'Albi, Toulouse-University. He is the head of the program "Inverse Methods and Energy Efficiency" at the Research Center RAPSODEE (Mines Albi & CNRS) and head of the Master program "Eco-Activities and Energy". His research interests include heat transfer, inverse method in heat transfer, thermal characterization in heterogeneous media, Infrared thermography, thermal images processing, analytical methods in heat transfer, integral transforms and thermal quadrupoles, optimization and statistical inference.

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## Characterization of Heat Transport at Interfaces in Multilayers, Nanocomposites and Nanofluids

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Despite recent progress in modeling heat transfer across interfaces, numerical values of interfacial thermal resistance  $R_{th}$  in various systems show great deviations from theoretical predictions as well as large variability with the condition of the interface at micro- and nano-scale. Therefore, such data are necessary for the validation of theoretical models and computations. Measuring  $R_{th}$  is often a challenge for the experimentalist. The available methods have to be adapted to the features of the sample.

This work presents several experimental approaches to evaluate  $R_{th}$  and thermal properties in solid/solid and solid/liquid systems having planar, cylindrical, spherical or random configurations. For simple configurations,  $R_{th}$  is obtained directly from the experiment and then it can be compared to theoretical prediction. For instance, for Cu/diamond the value  $R_{th}=2.71 \times 10^{-8} \text{ m}^2 \cdot \text{K} \cdot \text{W}^{-1}$ . Based on the acoustic mismatch model, is consistent with the experiment, while for Cu/glassy Carbon the estimation  $R_{th}=0.84 \times 10^{-8} \text{ m}^2 \cdot \text{K} \cdot \text{W}^{-1}$  is more than one order of magnitude lower than the experimental value. On the other hand, in the case of nanocomposites and nanofluids  $R_{th}$  is determined as a fit parameter in the frame of effective medium models.

**Keywords:** Interfacial thermal resistance, Photothermal radiometry, Nanocomposites.

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**Nicolas Horny** is an Associate Professor of Université de Reims Champagne Ardenne URCA, Reims, France. His research interests include micro- and nano-scale heat transfer (modelling and measuring effective thermal conductivity of nanocomposites, interface thermal resistance, depth profiling of thermophysical properties in multilayers), thermophysical characterization of materials at micro- and nano-scale by scanning thermal microscopy (SThM), photothermal radiometry (PTR) and 3omega hot wire (HW) techniques, instrumentation development of mentioned techniques. Prior to working at Reims Champagne University, he was Assistant Professor at Université de Valenciennes et du Hainaut-Cambrésis at Maubeuge in France.

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## **Laser-Based Linear and Nonlinear Elastic Bulk (3D), Surface (2D), and Wedge (1D) Waves in Materials Science**

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Nondestructive evaluation (NDE) and structural health monitoring (SHM) to evaluate materials properties without causing damage and the determination of critical fracture stresses or strengths of materials to avoid catastrophic structural failure play an ever increasing role in materials science and technology. One of the important experimental tools is laser ultrasonics, suitable for pulsed excitation and continuous detection of guided one-, two, and three-dimensional (1-3D) elastic waves. While for nondestructive evaluation the easy scanning of excitation and probe laser beams and the high spatial resolution obtainable by focusing are the most important features, destructive testing is based on the high laser power, allowing the generation of nonlinear elastic pulses with shocks leading to fracture.

Even in well-established conventional applications of conventional ultrasonics with 3D waves to macroscopic objects such as rails or tubes, there is a tendency to use guided waves for industrial inspection, which is connected with reduced cost, less inspection time, and greater coverage. These guided ultrasonic waves are constrained by the boundaries of the particular geometric structure and include, for example, torsional waves in a tube or Lamb waves in a plate but also longitudinal or shear modes. Permanent sensor installation for long distance diagnostics by conventional transducers, e.g. in rails, is a new approach in SHM. A serious challenge of guided modes in complex geometries is their dispersive and multimode nature. In NDE applications, substantial computational effort is needed for data analysis under these conditions. 3D applications by laser ultrasonics are under development.

Surface acoustic waves (SAWs), first discovered in 1885, can be characterized by a two-dimensional (2D) wave vector. The planar surface of an elastic half space is a 2D waveguide for these particular waves. Their displacement field decays to zero in the direction normal to the surface, e.g. exponentially within about one wavelength depth. SAWs or Rayleigh waves are non-dispersive in homogeneous media. In recent years laser photoacoustics has been used for the determination of elastic coefficients of advances materials (e.g. nanodiamond), or in nondestructive evaluation (NDE) of surface-breaking cracks. Real partially closed surface cracks of micrometer size have been analyzed with this method. Furthermore, the excitation of short nonlinear SAW pulses with steep shock fronts is possible that fracture brittle materials such as silicon. With the laser method it is possible to measure the fracture strength and compare the critical failure stress with ab initio calculations of the theoretical strength of the corresponding single crystal, giving an upper limit of the mechanical strength.

The acoustic edge or “wedge waves” were discovered in 1972 by numerical calculations. The displacement field decays exponentially away from the tip in the plane normal to the edge. The selective excitation of these guided waves was performed with an optically-pumped angle-tunable transducer. The characteristic features of the non-dispersive linear wedge waves in ideal systems such as their small phase velocity below the Rayleigh velocity and the very high degree of localization of the displacement field at the wedge tip could be clearly verified. Several applications have been discussed and feasibility studies were carried out already but no commercial devices are on the market yet. Future applications of dispersive wedge waves in real systems include monitoring of defects of cutting tools or turbine blades, sensor applications by measuring the velocity change upon tip and surface modifications. Owing to the large displacements involved in the excited flexural mode, ultrasonic motors, stirring and acoustic streaming in fluidics, and aquatic propulsion can be realized.

**Keywords:** Laser ultrasonics, Guided bulk, Surface, and Wedge waves, NDE, Fracture.

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**Peter Hess** is professor (retired) of Physical Chemistry at the University of Heidelberg. He has been active in different research fields such as surface spectroscopy and chemistry of semiconductors and laser ultrasonics. In gas phase photoacoustics chemical relaxation and trace gas detection have been studied. In solids laser-based guided surface acoustic waves and wedge waves have been applied in all-optical nondestructive evaluation, measurement of linear elastic coefficients and mechanical properties of superhard materials such as diamond, generation and detection of solitary surface waves, and measurement of the fracture strength of solids such as silicon using elastic shock waves.

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## Deformation of Super Alloys at Elevated Temperatures

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Material parameters affecting the material structures can be used for modeling the deformation behavior of super alloys. Thermo-mechanical processes are applied to P/M super alloys for consolidation. Stress-strain relationship can be established by the factors such as strain, strain rate, grain size, temperature and structural parameters. A new deformation model is suggested in this work by means of searching the compatibility of experimental results and analytical studies. In this study, P/M Rene' 95 super alloy was used as experimental material and micro-thermo-mechanical behaviors were investigated.

The changes in microstructure induced by plastic deformation in hot isostatically pressed (HIPed) P/M Rene 95 under isothermal conditions are discussed. Results of the constant true strain rate compression tests are presented for initially fine (7 µm) and coarse (50 µm) grained compacts deformed at temperatures of 1050 °C, 1075 °C and 1100 °C and at strain rates in the range from  $10^{-4} \text{ s}^{-1}$  to  $1 \text{ s}^{-1}$ . Under these test conditions, both the fine and coarse-grained compacts recrystallize and their grain size are refined during flow. This grain refinement gives rise to softening in both materials. Ultimately, their microstructures transform into the same equiaxed fine-grained microduplex structure at which point their flow strength becomes identical. Continued deformation at that point produces no further change in grain size or flow strength. Under this steady state regime of deformation, the microduplex grain size and flow strength are independent of the original microstructure but are conditioned by the strain rate at a given temperature. The steady state grain size increases whereas the steady flow strength decreases with a decrease in strain rate and/or an increase in temperature.

Material parameters affecting the material structures can be used for modeling the deformation behavior of super alloys. Thermo-mechanical processes are applied to P/M super alloys for consolidation. Stress-strain relationship can be established by the factors such as strain, strain rate, grain size, temperature and structural parameters. A new deformation model is suggested in this work by means of searching the compatibility of experimental results and analytical studies. In this study, P/M Rene' 95 super-alloy was used as experimental material and micro-thermo-mechanical behaviors were investigated.

Modeling of deformation mechanisms of engineering materials can be expressed by constitutive equations. These are useful for calculation and estimation of strength of material subjected to hot or cold deformation or extrusion operations. Some factors affecting materials' yield stress could be grouped as direct or indirect. While direct factors are said to be as deformation, deformation rate, and temperature; indirect factors may be chemical and metallurgical composition of the material, grain size, and history of the material.

Recently completed researches dealing with high temperature effects on deformation of materials also reviewed by this study. Ongoing studies suggest new methods to be applied to gain new features for aeronautical applications. Some comparisons are made between test results. Weakening of strength of materials is observed by the effects of elevated temperatures. Temperature, grain size, diffusion mechanisms are also found as the effects of influencing deformation mechanisms and strength as well as the constant strain rates.

**Keywords:** P/M Rene' 95, Super alloy, Modeling, Strain rate, Modeling of constitutive equation.

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**M. Oktay Alniak** graduated from Military Academy in 1962. He completed academic education between 1966-1990. He has BS degree in mechanical engineering from Aegean University, MSc. Degree from Bosphorous University, CSE from İstanbul University in managerial economics, and Ph.D degree from Gazi University in mechanical engineering. He worked for NRC laboratories about superalloys in Canada between 1986-1988. He worked in military service for 39 years as officer. ALNIAK has been working in Universities since 2001. He has academic experience in Military Academy, Gazi University, Süleyman Demirel University, Cyprus International University, and Bahçeşehir University. He has been giving lectures in Bahçeşehir University since 2004

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## Heat Transfer Properties of Complex Porous Media

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Porous materials such as cellular foams are known to have interesting combinations physical properties (low density, mechanical and thermal properties). These properties depend on the microstructures, relative density and properties of base materials (solid matrix). Depending on the domain of application, the solid matrix could be made of carbon, metal, ceramic or polymer. Metal and ceramic open-cell foams can be applied for high temperature in advanced energy and combustion systems such as low-NO<sub>x</sub> combustion burners. The solar thermal energy systems for fuel and chemical processing can be cited as other applications where ceramic foams are envisioned to exchange absorbed radiative energy. For applications requiring lightness and high insulating efficiencies at ambient temperatures, some polymer foams such as polyurethane (PU) or polystyrene (XPS and EPS) foams are often. Aerogel materials can be used as super insulating materials.

The improvement of the thermal performances of such porous media used in these applications requires two capabilities: modelling coupled conduction and radiation heat transfer inside these media and assessment of the thermal properties involved in the models. The most common assumption in predicting heat transfer in such complex materials is treating the disperse media as continuous and homogeneous media and using the so-called “effective thermal properties”.

The knowledge of the effective radiative properties is crucial. Theoretical prediction permits to analyze and understand the influence of morphology and optical constants of the particle and matrix materials on the radiative properties of the medium. Obviously, the experimental identification provides the knowledge of real material properties. This paper deals with the theoretical prediction and experimental determination of porous media thermal properties (especially radiative properties). After a brief review of the properties of interest, the emphasis will be placed on methods of investigation, both predictive and experimental. Following the book by Dombrovsky and Baillis (2010) and other recent studies, some examples will be presented showing recent advances and remaining challenges.

**Keywords:** Porous media, Cellular materials, Foams, Thermal properties, Modeling.

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**Dominique Baillis** is a Professor of the INSA Lyon Thermal Science Centre (CETHIL). She received the PhD degree in 1995 from INSA (National Institute of Applied Sciences) Lyon, France and the Professor degree in 2007 from the same institution. Her research interests have been focused on experimental identification and theoretical modeling of thermal radiative and conductive properties of diverse disperse systems such as advanced thermal insulations, fibrous materials, porous ceramics, foams, and nanoporous materials.

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## Experimental Determination of Thermo-Physical Properties of Metal-Organic Compounds (with Respect to Thin Film Deposition and Nanotechnology)

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Metal-organic compounds are precursors in different gas phase thin film deposition or nano-particle synthesis processes, like Chemical Vapor Deposition (CVD) or Chemical Vapor Synthesis (CVS). The metals, which shall be included into the solid phase, shall be present in the precursor, which is evaporated and transformed in a chemical reaction to the material desired. Thus, the vapor pressure of such substances, which is often between 0.1 and 100 Pa at temperatures between 70 and 150°C, have to be determined carefully in order to use them in reproducible deposition processes. Also, for the evaporator design transport properties like the diffusion coefficient has to be known, together with information regarding long term stability within the evaporator. A combination of isothermal thermo-gravimetry at ambient pressure with a specially designed Knudsen cell with in-situ mass measurement using a magnetic suspension balance is used to determine such thermo-physical properties. Since, many of the metal-organic compounds are sensitive against air and water vapor; parts of these set-ups are within glove-boxes. Further methods like the usage of a quartz microbalance for the determination of diffusion coefficients and the determination of activity coefficients for solutions of metal-organic compounds for liquid injection systems will be presented and discussed. Data for well-known metal-organic compounds like metal acetyl-acetonates are presented as well as data for newly synthesized chemicals from cooperation partners from inorganic chemistry.

**Keywords:** Metal-organic compounds, Vapor-pressure, Sublimation, Diffusion coefficients, Experimental methods.

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**Burak Atakan** is a full professor and chair of engineering thermodynamics at the University of Duisburg-Essen since 2002. He studied chemistry at the University of Heidelberg after finishing his Dr. rer.-nat. in physical chemistry in 1992 on gas phase reaction kinetics, he worked for the German aerospace center (DLR) on laser diagnostics in combustion and from 1995 on at the University of Bielefeld, where he finished his habilitation in 2000 on fuel-rich flames and chemical vapor deposition (CVD) mechanisms. His research interests are thermodynamical properties of metal-organic substances, thin film deposition by CVD and sol-gel techniques, energy conversion and storage as well as combustion mechanisms."



## Thermodynamics For Energy Engineering

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The sea change of German energy policy provokes a lot of research in systems, based on renewable energy. In the German state of Bavaria, a new center for research (Nuremberg Energy Campus) and several initiatives (like Bavarian Hydrogen center) were started to make possible the phase-out of nuclear energy in the year 2022.

The main problem is to make renewable energy like photovoltaics (PV) or wind able to replace the base load of electricity supply as it was done by nuclear power stations. This leads to energy storage. The authors are convinced that medium to long term storage of large amounts of electrical energy is only possible by chemical storage. Hydrogen is suited but not in its pure state. One option is to use LOHC's, chemical compounds that exist in an energy-lean state (not hydrogenated) and in an energy-rich state (hydrogenated). To find such a pair of chemicals is a challenge for thermodynamics and chemistry.

The lecture highlights the basic research and the application in decentralized local storage of electricity and in mobility. Demonstration units should be available end of 2014. Because the electrical energy is partly converted to heat during storage, the authors follow the goal of storage-heat-coupling (SHC), thus making the heat available for house heating or cooling.

**Keywords:** Thermodynamics, Energy, Hydrogen, Transport

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**Wolfgang Arlt** is professor and chair at the University of Erlangen-Nuremberg in Bavaria/Germany. The chair is called Separation Science & Technology. His research interest includes: thermodynamics of mixtures, thermodynamical models including those stemming from quantum chemistry (COSMO-RS), application to thermodynamics to energy engineering, separation processes like chromatography and distillation, tomography of separation equipment. Prof. Arlt is founder and director of the Energy Campus Nuremberg and advisor to the Bavarian government."

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## Time Resolved Measurements of Thermodynamic Properties During Chemical Reactions of Bio-Molecules

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After photoexcitation to the electronic excited states of any molecules in condensed phases, the photon energy should be converted to the translational energy of the solvent (heating). The heating time is related with the speed of the relaxation process. Using a femtosecond pulsed laser, heat induced structural change in ultrafast time scale can be obtained. There are several techniques to detect such photo-induced heating process, such as the transient lens, transient grating and photoacoustic methods. Here, we mainly used the transient grating (TG) and transient lens (TrL) method for the detection of the thermodynamical properties in time-domain. Because these methods are sensitive to the refractive index change around the photoexcited region, the time dependence of the density, pressure, and temperature changes, which accompany refractive index change, can be monitored over a broad range of timescales. By fitting the signal with thermal diffusion equations, the temporal evolutions of the temperature distribution and molecular volume changes were determined.

We applied this technique to a time-resolved detection of enthalpy change of biomolecules during the chemical reactions in solution. For example, we studied the reaction intermediate species of phototropin (phot) on the basis of their thermodynamic properties, such as changes in enthalpy, thermal expansion, and heat capacity. Phototropins are blue light sensor proteins that regulate phototropism, chloroplast relocation, and stomatal opening. It contains LOV (Light-Oxygen-Voltage) domains and a linker region. For the first intermediate of the reaction, the values of these thermodynamical properties were similar to those of the ground state for both LOV2 and LOV2-linker. A relatively large thermal expansion volume ( $0.09 \text{ cm}^3 \cdot \text{mol}^{-1} \cdot \text{K}^{-1}$ ) and a positive heat capacity change ( $4.7 \text{ kJ mol}^{-1} \cdot \text{K}^{-1}$ ) were detected for the intermediates. These characteristic features were interpreted in terms of structural fluctuation and exposure of hydrophobic residues in the linker domain, respectively. The enthalpy change of the intermediate was significantly greater. The results demonstrate clear picture of photo-reactions of the protein.

We have also applied the time-resolved technique to study another protein, TePixD. TePixD is a blue light sensor protein with BLUF domain and forms a unique decamer in crystal. Furthermore, in solution, TePixD is in equilibrium between the decamer and pentamer. The TG signal of TePixD at 1 atm pressure has revealed that TePixD shows volume expansion and diffusion change of the decamer during the photoreaction. Furthermore there is a surprising feature about this photo-induced conformational change; the conformational change of TePixD decamer is suppressed under strong excitation laser power, and this inhibition is thought to be caused by multi-excitation in a TePixD decamer. We used a high pressure instrument for detecting the TG signal. Interestingly, the diffusion signal intensity and the time profile of TePixD were found to depend on pressure dramatically. This dependence is considered to be pressure effect on the flexibility of the protein. We quantitatively measured the flexibility using the time-resolved compressibility and found that the flexibility is drastically enhanced during the reaction.

**Keywords:** Thermodynamics, Reaction, Protein.

**Masahide Terazima** is a professor of Physical Chemistry at Kyoto University of Japan. He received the PhD degree in 1987 from Kyoto University. He became an associate professor in 1993, and currently a professor at Kyoto University from 2001. His research interests have been focused on developing new techniques of time-resolved spectroscopy for elucidating photochemical reactions in solution phase. In particular, recently, he has been studying reaction dynamics of proteins and molecular mechanisms of biological functions. By using these techniques, he found that thermodynamics that can detect structural fluctuation is a key to understand the reactions leading to the bio-functions, and has been studying the reactions by the time-resolved thermodynamics.



## Photoluminescence Enhancement In Metamaterial Nanostructures

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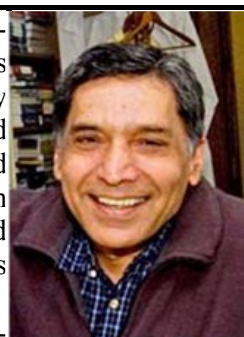
We study the photoluminescence (PL) and spontaneous emission of semiconductor nanoparticles doped in a metamaterial heterostructure. Metamaterials are a new class of artificial materials with optical properties determined by their classical atomic composition and nanoscale organization of their structural components. Metamaterials have unique electromagnetic properties which cannot be obtained from naturally occurring materials. Recently, metamaterials based on periodic arrangements of metallic nanocomposites have received special attention. They possess simultaneously negative effective dielectric permittivity and magnetic permeability for a range of frequencies in the electromagnetic spectrum. It is well known that the negative electric permittivity in noble metals leads to the formation of surface plasmon which may generate exceptionally strong localized electromagnetic fields. Heterostructures studies here are formed by fabricating a split-ring resonator and metallic rod metamaterial on a dielectric substrate. An ensemble of quantum dots (QDs) are doped near the interface in the heterostructure. The QDs interact with surface plasmon polaritons of the heterostructure. PL spectrum and spontaneous decay of excitons in the QD are studied. Our results indicate that the PL and spontaneous emission of the QDs are enhanced in the presence of the metamaterial when the exciton and surface plasmon frequencies are resonant. These findings are consistent with recent experimental studies. The present study can be used to make new types of nanoscale optical devices for sensing, switching and imaging applications based on metamaterials.

**Keywords:** Photoluminescence, Metamaterials, Surface plasmon polaritons, Density matrix, Nanooptics, Plasmonics.

**Mahi R. Singh** received both M.Sc. (1970) and PhD (1976) degrees from Banaras Hindu University, Varanasi in condensed matter physics. After that he was awarded an Alexander von Humboldt Fellow in Stuttgart University, Germany from 1979 to 1981. Between 1981 and 1985 he was a Research Associate and Lecture at McGill University, Montreal, Canada. From 1982 to 1983 he worked in INSA, Toulouse, France as a visiting scientist. He also worked as Research Associate at University of North Carolina, Chapel Hill, USA. After that he joined the University of Western Ontario as associate professor in 1985. Currently he is professor in this university.

He was the director of the Centre of Chemical Physics at the University of Western Ontario, Canada. He also served as the director of Theoretical Physics Program for many years at the University of Western Ontario, Canada. He is a senator at the university of Western Ontario.

Dr. Singh has worked in many research areas of science and technology including nanoscience, nanotechnology, nanophotonics, plasmonics, optoelectronics, photonic crystals, Metamaterials, semiconductor heterostructures, high temperature superconductors, positron annihilation, Josephson Junctions, many body theories, condensed matter physics, semiconductor devices, Thermal Transport, DNA Molecules and DNA wires and so on. He has published more than 300 papers in International journals. He has written several books which are used as text books at UWO, Canada. He has organized several International conferences. He has been invited as a plenary and an invited speaker in several international conferences throughout the world.



## Ion Beam Assisted Enhanced Thermoelectric Properties (with figure of Merit above 2.0)

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The reason behind why thermoelectric generators (TEG) have not been used to generate electricity or as to charge batteries, extensively, can be summarized by their low efficiencies, high temperature operation, and non-conformal. Recent TEGs can operate starting at room temperature as the heat or the cold source, that is, as long as there is a temperature difference ( $\Delta T$ ), of few degrees of Kelvin, is available, then there is a potential difference and there is current generated by the recently produced thermoelectric materials. Thus enabling us capturing the power generated, per few square centimeters, from human body, while the ambient temperature is at or below 300 K, in order to charge a cellphone battery, to charge the batteries for the jogging LED indicators and more. In fact, few off the shelf TEGs can provide enough power to achieve the above goals, despite their bulkiness, despite the lack of flexibility and despite their low efficiency. In this presentation, we will present our work on production of thin films of thermoelectric materials which has higher figure of merit, conformal, and can operate at lower temperature difference ( $\Delta T$ ) than existing off the shelf TEG\*.

Our work stem from the properties of regimented quantum dot quasi-lattices, consisting of nanocrystals of gold and/or silver separated at one to few angstroms from each other creating new electric and thermal properties as well as interesting optical properties. We will discuss how ion beam have been used by our team in order to achieve properties similar to what is predicted theoretically by regimented quantum dot quasi-lattices. We will, also, review a series of materials resulted from our investigation, some operating at temperatures around 300K and some at about 400K. Such ultra-thin thermoelectric materials, 0.1 to 1 micrometer thickness, operating at room temperature will allow integration to the existing devices for continuous charging the low power required portable unites such as cell phones, tablets, heart-pacemakers, and more.

\* One patent awarded & one patent pending.

**Keywords:** Thermoelectric, Ion Beam, Figure of Merit.

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**Daryush Ila** is an expert in ion-matter interactions and nanoscale materials/device fabrication and has authored or coauthored over 300 publications, over eleven books, two book chapters, over 55 invited & plenary talks and three patents. As the founder of Center for Irradiation of Materials and the cofounder of an Institute, ILA built partnerships that won more than \$125 million in grants and contracts – more than \$40 million of which were from the Department of Defense alone. ILA as a faculty member supervised and co-supervised over 35 MS Theses and PhD Dissertations and provided summer trainee for few hundred students. ILA's filed four patents, three on highly efficient thermoelectric materials and one on production of nanopores for filtration, with the potential for DNA sequencing and as a nano-filter for air and water purification, in addition to few more patent applications filed recently.

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# ABSTRACTS

## Effective Ultrasonic Duration for Better Dispersion of Nanofluid

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Nanofluids are promising fluids for heat transfer application. Lower stability and higher viscosity are two important drawbacks for practical application of nanofluids. Aggregation and sedimentation of nanoparticles are related to the colloidal structure of nanofluids, which directly affects the stability and other properties of nanofluids. Different types of ultrasonication process are used to breakdown the aggregation of particles. The aim of this work was to study the effects of ultrasonic duration on the colloidal stability of nanofluid. 0.5 vol.% of Al<sub>2</sub>O<sub>3</sub> nanoparticles were dispersed in water by using a horn type ultrasonic homogenizer with the duration from 30 min to 300 min. Microstructure, cluster size, precipitation and zeta potential were analyzed to check the aggregation and sedimentation. TEM microstructures show that nanoparticles started dispersion in water with the starting of ultrasonication and within 60 min, it found to be better dispersed until 90 min. After that, the nanoparticles started partially coalesced again until 150 min of sonication and found to be well dispersed for 180 min of sonication. Furthermore, from 210 min of sonication it started again partially coalesced until 240 min of sonication and further sonication until 270 min it found better dispersion and the best dispersion for 300 min of sonication. However, the nanoparticle cluster size found to be decreased with the increase of ultrasonic duration until 180 min and further sonication could not reduce the cluster size. Similarly, zeta potential found to be increased with the increase of sonication time until 150 min of sonication and further sonication could not increase the zeta potential value. In addition, lower precipitation amount was found to be for higher duration of sonication. In brief, better particle dispersion, lower particle and colloid size and precipitation, and higher zeta potential have been observed with the increase of ultrasonic duration. Therefore, more stable (less aggregation and sedimentation) nanofluids can be obtained by applying 150 min or higher ultrasonication time.

**Keywords:** Nanofluid, Ultrasonication, Colloid; Stability.

## **The Effect of Thermal Cycles on the Mechanical Properties of High Density Polyethylene (HDPE) and Graphite/HDPE composites**

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In this study, the Graphite/HDPE composites having different graphite content were prepared by melt blending. The graphite content was in the range of 2 to 30 wt%. To investigate the effect of thermal cycles on the mechanical properties of HDPE and graphite/HDPE composites, HDPE and each composite samples were subjected to the thermal cycle processes for 100, 200 and 400 times between temperatures of 85°C and -25 °C. The moduli of HDPE and HDPE/GR composites at the end of each thermal cycle at 100, 200 and 400°C increased.

**Keywords:** Polymer Composites, Thermal Cycles, Mechanical Properties

## **Influence of Thermal Cycling on Tensile Properties of Expanded Graphite/High Density Polyethylene Nanocomposites**

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In this study, expanded graphite (EG) /high density polyethylene (HDPE) nanocomposites having concentrations of 2–20 wt.% were prepared by the melt-mixing process. EG5 and EG50 flakes have 5–7 µm in diameter and 40–55 µm in diameter, respectively. HDPE matrix and the nanocomposites were subjected to the thermal cycle for 200 times between temperatures of -30 °C and 90 °C. After thermal cycling, the tensile properties of HDPE matrix and the nanocomposites were investigated. The tensile strengths and Young moduli of HDPE and EG/HDPE nanocomposites after thermal cycling of 200 times increased. It was found that HDPE showed the best modulus enhancement after thermal cycling.

**Keywords:** Polymer composite, Tensile properties, Thermal cycling.

## Effect of Ultrasonic Duration on Thermal Conductivity and Viscosity of Alumina-Water Nanofluid

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Nanofluids are colloidal suspension of nanometer size particles in a base fluid that are promising fluids for heat transfer application. Lower stability and higher viscosity are two important drawbacks for practical application of nanofluids. Aggregation and sedimentation of nanoparticles are related to the colloidal structure of nanofluids, which directly affects the stability and thermophysical properties of nanofluid. Different types of the ultrasonication process could break the aggregation of particles. The aim of this work was to study the effects of ultrasonic duration on the colloid, thermal conductivity and viscosity of nanofluid. 0.5 vol % of Al<sub>2</sub>O<sub>3</sub>-water nanofluid was prepared by using ultrasonic homogenizer with the duration from 1 to 5 h. Microstructure, cluster size, and zeta potential was analyzed to check the colloid. Thermal conductivity and viscosity were measured for each ultrasonic duration with temperature ranging from 10 °C to 50 °C. Better particle dispersion, lower cluster size, and higher zeta potential have been observed with the increase of ultrasonication time. There was no strong variation on thermal conductivity for the change of sonication time. However, viscosity of nanofluid decreased with the increase of ultrasonic duration. Therefore, higher ultrasonic time could give better thermal performance of nanofluids.

**Keywords:** Nanofluid, Ultrasonication, Thermal conductivity, Viscosity.

## Effect of Inclination Angle on Nanofluid Based Single Phase Natural Circulation Mini Loops

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This study presents a numerical analysis, to investigate the effect inclination angle on nanofluid based single phase natural circulation mini loop. An experimental study which consists of a mini loop working with Al<sub>2</sub>O<sub>3</sub> – distilled water (DIW) nanofluid from the existing literature was selected for the comparison of the numerical results. Nanofluids having different filler contents were used as the working fluid and different heater power values were applied to the mini loop to better validate the numerical study. The results show that, proposed numerical model can predict the reaction of the mini loop to inclination angle sufficiently.

A full buoyancy model was used for modeling the laminar natural convection flow. Furthermore, viscosity, thermal expansivity, and thermal conductivity were taken as functions of temperature in the numerical calculations. Table values were used to define the dependency of properties on temperature when water is the working fluid. The effective specific heat values have been taken as constant at the average loop temperature for every fluid. However, for Al<sub>2</sub>O<sub>3</sub>-DIW nanofluid, models adopted from the literature for determining the effective density and effective thermal expansivity for different filler ratios. Experimental values from the literature were used as thermal conductivity and viscosity data. Second order polynomials were fitted to the property data to obtain polynomial functions and these functions were used as inputs to the numerical model. A 3D CFD model was built in this study. Although the CFD results can not totally predict the unsteady chaotic behavior of the SPNCLs, we can better predict the steady behavior of the SPNCmLs numerically because of the increased stability of the system as a result of miniaturization. Therefore, steady flow results are given in this study.

$T_{max}$  (maximum temperature in the loop),  $\Delta T_{heater}$  (temperature difference between the two sides of the heater) and effectiveness (represent the ratio between actual heat transfer and maximum possible heat transfer) values obtained from the numerical simulations were compared with the experimental data. Results showed that, for the upright position (0° inclination angle) the deviation from the experimental results increases as the heater power and filler content increases. Possible reasons for this deviation are un-modelled heat loss from the experimental setup, improper models for determining heat transfer and flow of nanofluids and imprecise thermo-physical property determination. Deviation from the experimental results is similar for the 30° and 60° inclination angles. Moreover, the increase in the performance of the mini loop as the inclination angle increases for all the criteria ( $T_{max}$ ,  $\Delta T_{heater}$ , and effectiveness) is modelled well with the numerical study. However, the unexpected behavior of the DIW filled mini loop for 50 W heater power and 75° inclination angle, which is thought to be the result of the boiling inside the heater part, could not be represented by the numerical model. Because phase change is not included in the numerical study. Although there is a deviation from the experimental results, the presented numerical model is still a powerful tool for comparative parametric studies about the performance of SPNCmLs. Phase change effects and the effect of different geometrical parameters on the SPNCmL performance may be investigated in the further studies.

**Keywords:** Nanofluid, Single phase flow, Natural convection.

## **X-ray Computed Tomography of Gas Diffusion Layers of PEM Fuel Cells: Determination of the Effective Thermal Conductivity**

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Gas diffusion layers (GDL) are critical part of the proton exchange membrane fuel cells (PEMFCs) for diffusion of the reactant gases and the removal of byproduct water. Another function of GDL is to provide electrical and thermal conductivity between the catalyst layer and bipolar plate of PEMFCs. Therefore, the thermal conductivity of the GDL should be known accurately as input for the fuel cell modeling studies. In this study, commercially available gas diffusion layer was investigated by 3D X-ray computed tomography (CT). By using this technique, the orientation of the carbon fibers inside the gas diffusion layers was analyzed. The 3D structural data obtained from CT was converted and used in order to calculate the effective (saturation-dependent) thermal conductivity of the structure. The thermal conductivity and the effective (saturation-dependent) thermal conductivity values were calculated by using SatuDict module of Geodict program. SatuDict calculates the relative thermal conductivity as in ConductoDict which is another module calculates the thermal conductivity of materials in the absence of liquid water. The thermal conductivity of structure constituent materials and the thermal conductivity of the fluid phases were introduced in Satudict. The effective thermal conductivities were calculated in three directions (in plane and through plane) by using GeoDict. The effective thermal conductivities of GDL were investigated at different operating temperature conditions of PEM fuel cells: 65 °C, 75 °C and 85 °C. The effective thermal conductivities with respect to saturation were presented in graphically for these three different temperature values. The results showed that the effect of GDL anisotropy and of the liquid water on the effective thermal conductivity values cannot be neglected.

**Keywords:** Effective thermal conductivity, Gas diffusion layer, X-ray computed tomography, PEM Fuel cell, Numerical simulation.

## **An Experimental Study on the Dispersion Stability of Alumina-Water Nanofluids via Particle Size Distribution and Zeta Potential Measurements**

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Nanofluids as the dispersions of nanoparticles and industrial liquids have gained significant attention due to their improved thermophysical properties. The industry worldwide is leaning towards sustaining of the improvements in process variables. Since the nanofluids' applicability in applications is determined by their improved properties, sustaining of their improvements is essential. Colloidal behavior of the nanoparticles is temporal and can dramatically change when affected by the external conditions. If the nanoparticles form big and heavy aggregates, those aggregates are then prone to settle down due to the gravity forces. Nanoparticle settlement (sedimentation) reduces the nanoparticle fraction within the nanofluids, and at the maximum sedimentation condition, the amount of nanoparticles contributing to the dispersion can approach to zero, leaving the primary nanofluid as the base liquid, alone. In such condition, one cannot take benefit from the improvements in the thermophysical properties, not to mention the damages that settled nanoparticle layer could cause on the system components. Therefore, a fairly "stable" nanofluid is needed for industrial applications. Alumina ( $\text{Al}_2\text{O}_3$ ) nanoparticles are not soluble in water, thus addition of surfactants is required to properly disperse them within water, as the base liquid. In the current study, stability  $\text{Al}_2\text{O}_3$ -water nanofluids were investigated in terms of particle size distribution (PSD) and zeta potential measurements. The nanofluids were supplied from NanoAmor, Inc. in USA, one year before the stability measurements. The manufacturer reported the particle size of the nanoparticles as  $30 \pm 10$  nm, and the nanofluids are containing Acetic Acid as a surfactant (0.1–0.3% by weight). The PSD and zeta potential analyses were done using ALV/CGS-3 compact goniometer system (Malvern Instruments, Inc, UK) and Malvern Nano ZS, respectively. For the experiments, nanofluids of 0.125, 0.25 and 0.5 vol. % nanoparticle fraction were prepared using the stock material (nanofluid of 6.33 vol. %) and water de-ionized for two times. The zeta potential of the 0.125 vol. % sample was measured as 47.5 mV, indicating high electrodynamic stability. on the other hand, the PSD results showed that, the nanoparticles were agglomerated and had 75-85 nm average sizes. Since the PSD is a very dynamic parameter, the experiments were done in a weekly manner. After the PSD of each sample were measured and the nanoparticle aggregation was observed in all the samples, it was tried to re-develop the mono-dispersed condition of nanoparticles via ultrasonication up to 5 hours. The samples were ultrasonicated for different ultrasonication durations via Bandelin SONOREX<sup>TM</sup> Digital 10 P Ultrasonic Bath. Decrements in the particle sizes were obtained at initial, but the average particle size never approached to  $30 \pm 10$  nm as a result of ultrasonication. Further, the ultrasonicated 0.5 vol. % nanofluid was let to relax for up to 30 minutes. After the PSD's were measured following subsequent relaxations, it was seen that they were disposed to approach the before-ultrasonication values. The particle size was very close to the one-week before value after relaxation for 30 minutes. In conclusion, the mono-dispersed condition of nanoparticles ( $30 \pm 10$  nm average particle size) could not be re-established via the tried ultrasonications. However no color change of the solution and nanoparticle sedimentation were evident to eye, the particles were agglomerated over a year. Considering the significant daily changes in the particle sizes reported in literature, the changes observed in the current study over one year could be considered as not very critical. The study emphasizes that, the stability of nanofluids should be investigated in terms of the quantitative parameters, e.g. zeta potential and PSD, since visual inspection may not be sufficient for nanofluids containing particles like  $\text{Al}_2\text{O}_3$  with white to light gray color dispersed within water. The authors would like to highlight the requirement of performing the stability experiments periodically on the nanofluids, and in a simultaneous manner to the other experiments, if decided. Such approach may diminish the biases resulting from the changes in the PSD on the measured properties/ behaviors.

**Keywords:** Nanofluids, Particle size distribution, Zeta potential, Dispersion stability.

**Acknowledgements:** Prof. Dr. Vural Bütün (the head) and Res. Asst. Cansel Tuncer (research associate) at the Polymer Research Laboratory, Eskisehir Osmangazi University is acknowledged on performing the experiments. The nanofluids have been purchased with the first author's own sources.

## **Large Deflection Behavior of Functionally Graded Beams Under Temperature Rising**

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In this study, large deflections of a cantilever beam made of functionally graded material under temperature rising is investigated by using the total Lagrangian Timoshenko beam element approximation. Material properties of the beam change in the thickness direction according to a power-law function. It is known that large deflection problems are geometrically nonlinear problems. The considered highly non-linear problem is solved considering full geometric non-linearity by using incremental displacement-based finite element method in conjunction with Newton-Raphson iteration method. In this study, the effect of material gradient property and temperature rising on the large deflection behavior of the beam is investigated in detail. The relationships between deflections, thermal configuration, stresses of the beams and temperature rising are illustrated in detail. Also, the difference between linear and non-linear analysis of functionally graded beams is studied under high temperature rising.

**Keywords:** Functionally graded materials, Temperature rising, Large deflection behavior, Non-linear analysis.

## **Static Behavior of Functionally Graded Structures at Elevated Temperature with Temperature-Dependent Physical Properties**

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This study focuses on static analysis of functionally graded three-dimensional (3-D) structures subjected to temperature rising with temperature-dependent physical properties. Material properties of the beam are both temperature-dependent and position-dependent. In the mathematical solution of the problem, finite element model of three-dimensional continuum approximations is used. Finite element equations of three dimensional continuums for an eight-node quadratic element are used. In this study, the difference between temperature dependent and independent physical properties is investigated for functionally graded 3-D structures. The relationships between deflections and thermal configuration of the 3-D structures and temperature rising are illustrated.

**Keywords:** Temperature-dependent physical properties, Functionally Graded Materials, Three-Dimensional Continuum, Temperature Rising.

## Application of Nano-Refrigerants and Nano-Lubricants to the Domestic Refrigerators

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Due to the global warming and ozone depletion, the standards of the refrigeration industry force the manufacturers to find out not only new thermodynamic cycles but also innovative working fluids to improve. Several studies have been performed on different parameters of cycles in order to improve the performance of a mechanical refrigeration system. As a new idea in recent years, the new refrigerant fluids for improving of the performance take attention of researchers.

R134a and R600a are the most widely used refrigerants in the refrigeration industry. These kinds of refrigerants have higher global warming potential than hydrocarbons mixture (HCM). Many studies showed that HCM refrigerants are found to energy efficient and eco-friendly when compared with the R134a and R600a refrigerants. Besides be the refrigerant, the lubricant oil is used by the compressors to remove the heat from the system. Refrigeration oil lubricates parts for reduction of frictions, thus helps oil-sealing function of bearing and consequently reduces the energy consumption. The lubricant must be well-matched with a refrigerant used by the compressor to remove heat from the system.

Nowadays, nano technology is considered one of the most important technological areas. Nanoparticles can be used to improve the working fluid properties due to their special properties. That's why, the refrigeration sector deals with the nano additive refrigerants and lubricant oils. Using nano particle technology in the refrigerators has many advantages such as enhancing the solubility between the refrigerant and lubricant, reducing the friction coefficient of the lubricant, and improving the heat transfer characteristics and thermal conductivity of the refrigerant. Due to these advantages, many researchers studied nano technology on refrigerators. The study of Bi et al. concluded that using 0.1% mass fraction TiO<sub>2</sub> Nanoparticles compared to the HFC134a and Polyol-ester oil system causes 26.1% energy consumption reduction for a domestic refrigerator. In another study of Bi et al., the 0.1 and 0.5 g/L concentrations of TiO<sub>2</sub>-R600a can save 5.94% and 9.60% energy consumption when compared with the pure R600a system. Application of TiO<sub>2</sub> nanoparticles as a lubricant-additive for vapor compression refrigeration systems is studied in the study of Sabareesh et al.. Based on their experimental results, 0.01% volume fraction increased the average heat transfer rate by about 3.6%, and reduced the average compressor work by about 11%, and increased the COP 17% due to the addition of nanoparticles in the lubricating oil.

In spite of many researchers have studied on the nano refrigerants and/or nano lubricants for the domestic type refrigerators, many significant questions should be investigated and answered; the mixing method (diffuser mixing, laser ablation etc.) of the nano particles in an explosive refrigerant at the room conditions, the sedimentation rate of the nanoparticles in the refrigerant or the lubricant, the corrosion rate of the components used in the system, and the thermodynamically changes of the two phase refrigerant in the vapor compression cycle.

**Keywords:** Nano refrigerant, Nano lubricant, Refrigerator, Vapor compression.

## Measurement of Physical Properties of Nanofluids

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This work presents the results obtained in the Heat Transfer Laboratory – LTTC of PEM/COPPE/UFRJ for the measurement of the physical properties of selected nanofluids. The physical properties of interest here are: thermal conductivity, specific heat and viscosity.

For the measurement of the thermal conductivity, we have used the line heat source probes commercially available by Hukseflux, models TP-02 and TP-08, as well as the Flash method (Netzsch LFA-447). The specific heat was measured with the Differential Scanning Calorimeter DSC 204 F1 Phoenix, made by Netzsch, while the viscosity was measured with the rotational rheometer LVDV-IIIU made by Brookfield. The equipment utilized for the Flash method, DSC and rheometer allowed for the temperature variation/control through their own temperature controllers. On the other hand, an experimental apparatus was developed in this work in order to measure the thermal conductivity with the line heat source probe, at temperatures above the room temperature. Such apparatus consists of a chemical reactor, in which the probe was installed along its center-line. The temperature of the nanofluid under analysis is controlled through by the control system of the chemical reactor, which also allows for pressurization of the fluid with an inert gas; 99.998% pure Argon was used in this work.

Water-based commercial nanofluids were utilized for the analyses conducted in this work, with nanoparticles of Al<sub>2</sub>O<sub>3</sub>, ZnO and SiO<sub>2</sub> in different volumetric concentrations. Special focus is given for the nanofluids with SiO<sub>2</sub> nanoparticles, because they presented the best stability among those nanofluids tested, without any apparent deposition of nanoparticles, even after more than one year of tests and stock.

The physical properties measured in this work are compared to other measured values available in the literature, as well as to theoretical predictions and to the correlations proposed by Khanafer and Vafai (A critical synthesis of thermophysical characteristics of nanofluids, *International Journal of Heat and Mass Transfer*, 54, 2011, 4410–44, 2011).

A comparison between the thermal conductivity measured with the Flash and the line heat source methods reveals that the last one provides more consistent results. Such is the case because of heat conduction through the lateral walls of the sample holder used in the Flash method, which was provided by the equipment manufacturer, as demonstrated by numerical computations developed in the work.

**Keywords:** Flash method, Line Heat Source Probe, Differential Scanning Calorimeter, Rheometer, Nanofluids.

## Shape Memory Behavior of Precipitation Hardened NiTi Shape Memory Alloys

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Nickel rich NiTi shape memory alloy (SMA) has been widely used for bio-medical, electrical and mechanical applications due to their distinct superelasticity and shape memory properties as compared to near equi-atomic NiTi SMAs. In this study, the effects of composition, aging and orientation of Ni-rich NiTi alloys on their shape memory (transformation strain, hysteresis and cyclic stability) and mechanical properties are investigated.

Polycrystalline NiTi alloys were prepared by conventional induction melting method while single crystalline NiTi alloys were grown by using the Bridgeman technique. Compression specimens, with a 16 mm<sup>2</sup> cross section and a 8 mm length, were cut by electro discharge machining. Transformation temperatures are determined by differential scanning calorimetry. The thermo-mechanical experiments were conducted on compression samples by a servohydraulic test frame. Transmission electron microscopy observations were conducted at room temperature to reveal precipitation characteristics and martensite morphology.

Effects of heat treatments (between 400 to 600 °C for 15 minutes to 24 hours) were investigated on Ni-rich Ni-Ti alloys. Precipitation formation is found to be an effective method to improve the strength of material and also control the shape memory properties. It was revealed heat treatments and applied stress could significantly alter the transformation temperatures and shape memory effect response. High Ni-rich NiTi alloys has the ability to exhibit shape memory effect under high stress levels of 1 GPa and superelasticity when up to 2 GPa was applied without any significant plastic deformation after selected heat treatments in compression. The shape memory behavior of NiTi alloys was found to be highly orientation dependent. [100]-oriented NiTi single crystals have high strength and show perfect superelasticity for a wide temperature range.

**Keywords:** Shape memory, High strength, Superelasticity.

## Effect of Base Fluid Types on Thermal Properties of Different Nanofluids

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The aim of this study is to determine the effect of base fluid type on thermophysical properties of nanofluids. Three different base liquids were used. The base liquids were de-ionized water, ethylene glycol and de-ionized water and ethylene glycol mixture (50%-50% volumetric). Four different nano particles Al<sub>2</sub>O<sub>3</sub>, CuO, TiO<sub>2</sub> and SiO<sub>2</sub> were suspended in to the base fluids. There existed 0.25%, 0.5%, 1.0%, 2.0% and 4.0% nanoparticles in the base liquids as volumetrically. The measurements were made with respect to thermal conductivity, viscosity and specific heat capacity. The thermo physical properties of the base fluids were also made for the calculation of effective thermal conductivity and to see the effect of suspended particles into the base fluids. Correlations obtained from the measurements were also presented for viscosity and thermal conductivity.

**Keywords:** Al<sub>2</sub>O<sub>3</sub>, CuO, TiO<sub>2</sub>, SiO<sub>2</sub>.

## **Magneto-thermo-mechanical Characterization of Polycrystalline NiMnCoGa Meta-magnetic Shape Memory Alloys**

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Magnetic shape memory alloys (MSMAs) have attracted considerable attention recently as an alternative to the long-existing magnetostrictives and piezoelectrics in actuator applications. MSMAs exhibits large reversible strains (up to 10%) compare with magnetostrictives and piezoelectrics (~0.2%) and they can operate much higher frequencies (up to kHz range) than conventional SMAs such as NiTi (~1Hz). Single crystalline of NiMnGa alloys are the most well-known MSMAs due to large transformation strain and high thermal stability. Magnetic actuation occurs by variant reorientation of ferromagnetic martensite phase in NiMnGa alloys. Brittleness, low actuation stress (due to limited magnetic energy), limited operation temperature, and high orientation dependence are the disadvantages of NiMnGa alloys.

Additional element is one of the most efficient method to alter mechanical, physical and shape memory properties. Co addition to NiMnGa alloys increase the ductility of the alloy through the formation of ductile second phases. Doping Co element also provides an opportunity to tailor the Curie temperatures of transforming phases where ferromagnetic austenite can transform to paramagnetic-like martensite. Thus, NiMnCoGa alloys can be classified as meta-magnetic SMAs where magnetic field-induced phase transformation can be one order of higher actuation stress than that of variant reorientation in NiMnGa alloys. Meta-magnetic SMAs, e.g., NiMn(In,Sn,Sb) alloys, can be utilized in polycrystalline form since Zeeman Energy does not depend on orientation in contrast to Magnetocrystalline Anisotropy Energy (MAE) in NiMnGa alloys.

In this study, the effects of Co addition to polycrystalline NiMnCoGa alloys on shape memory behavior and mechanical properties under compressive stress investigated in order to determine of potential of NiMnCoGa alloys as meta-magnetic SMAs.

Polycrystalline NiMnCoGa alloys were prepared by conventional arc melting method in an argon atmosphere using high-purity elements. Transformation temperatures are determined by differential scanning calorimetry and magnetization properties are measured by superconducting quantum interference device magnetometer. The magneto-thermo-mechanical experiments were conducted on compression samples by a superconducting magnet attached to the servohydraulic test frame.

NiMnCoGa alloys exhibits good shape memory behavior under stress levels up to 200 MPa in polycrystalline form and can also be classified as high temperature SMAs with perfect superelasticity at temperatures above 150 °C. They can also be trained easily to show good two-way shape memory effect that might result in high strain upon field-induced transformations. Applied magnetic field decreases transformation temperatures due to magnetization differences between transforming phases where martensite start temperature decrease around 5 °C under 50 MPa compressive stress under 9 Tesla.

**Keywords:** Meta-magnetic, Shape Memory, Superelasticity, Phase transformation.

## Breaching CNT Nanofluids Thermal Conductivity Modelling Uncertainties

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The continuous advances on electronic devices and industrial processes increased the demand for new technological solutions to improve the effectiveness of heat transfer, mainly in what concerns compact or miniaturised systems. A novel strategy for heat transfer improvement is, therefore through the improvement of the thermo-physical properties of available thermal fluids. In the past years, a great deal of research work was undertaken and considerable progresses have been reported mainly through the incorporation of nanomaterials in conventional fluids, the so called nanofluids.

Among the several thermo-physical properties of nanofluids, the thermal conductivity is the one gathering more attention as it appears to present an anomalous and unpredictable behaviour. Within the various nanoparticles suitable for nanofluids tailoring, it appears that carbon nanotubes (CNT) present the higher enhancements on the thermal conductivity. The production of CNTs nanofluids may be achieved through the use of surfactants or covalent functionalization of the CNTs surface. The latter seems the most promising dispersion technique.

Inconsistency in the experimental data from various research groups, due to a huge variety in the sample production and measuring approaches, resulted in the formulation of distinct theories, and so far no predictive model was assertively validated. Since nanofluids are a mixture of nanoparticles with conventional fluids, perhaps the best approach to ensure correct thermo-physical property definition lies upon the fluid colloidal stability. The literature agrees that it is essential to ensure long-term stability for the development of reference nanofluids with improved heat transfer capability, preferably without dispersing agents or stabilizers. Recently, Lamas et al. suggested that the dispersion of covalent functionalized multiwalled carbon nanotubes (MWCNT) through a short period of sonication, enables the production of reliable long term nanofluids. In this study it is reported the work undertaken to identify the heat transfer mechanisms responsible for the thermal conductivity enhancement of CNTs nanofluid. With this purpose, a full factorial design of experiment arrangement of 6 MWCNTs geometries, dispersed in 2 distinct aqueous solutions of ethylene glycol at 5 volume fractions is envisaged, performing 60 different nanofluids. All nanofluids were tested at 6 temperatures, ranging from 283.15 to 323.15 K, in a total of 360 experimental points. To ensure the accuracy of this data base, noise factors were identified and kept to a minimum through monitoring of each test conditions and repeatability analysis.

The nanofluids colloidal stability was assessed according to Lamas et al.. The results seem to highlight the long term stability of the nanofluids, with shelf life up to several decades. The thermal conductivity was assessed for all nanofluids and was found to increase with particle concentration and aspect ratio, as well as temperature independent behaviour, as expected by the classical theory. Moreover, the thermal conductivity results are in good agreement with the effective medium theory, developed for high aspect ratio particles with an adjusted interfacial thermal resistance. It is expected that this methodology and extensive data-base may significantly contribute to proper tailoring of long term nanofluids with engineered thermo-physical properties.

**Keywords:** Nanofluids, Thermal conductivity, Carbon nanotube, Colloidal stability, Effective medium theory.

## Thermophysical Properties of industrial Ni -based Superalloys

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In the production of materials with high performances concerning the mechanical properties and the use at high temperatures, the solidification processing has to be controlled with ever-increasing precision. In order to improve casting quality and reproducibility, yield strength, creep resistance and other properties, predictive quantitative numerical simulations of grain-structure formation using sophisticated integrated software are needed. The application of such numerical tools is generally hampered by the lack of reliable thermophysical property values, such as surface tension and density, which are input parameters for the computational models. In the framework of the ESA-MAP International THERMOPROP Project, the containerless processing using non-contact diagnostic tools has been applied to measure the thermophysical properties of several industrial metallic systems, included the Ni-based super-alloys. However, benchmark experiments in space require, wherever possible, comparison with the values obtained by other or similar techniques under 1-g conditions.

In this work, the results of the on ground measurements of the surface tension of a group of commercial Ni-based superalloys are presented.

The surface tension and density of six Ni-based superalloys, namely RENE N90, RENE N5; TMS 75; LEK 94; CMSX 10 and MC 2, have been measured by a variant of the large drop method called pinned drop method. In this case, the solid support was a special circular crucible with sharp edges made in Al<sub>2</sub>O<sub>3</sub> single crystal. The design of the edges of the crucible blocks the triple line at an “apparent” contact angle that is much higher than the real one. A further advantage of the pinned drop method is that the axi-symmetry of the drop can be imposed. The experiments were performed using an apparatus built expressly for this purpose. A dedicated software acquired images of droplets at high resolution and calculated geometric parameters (e.g. drop height, drop diameters, contact angles, drop area, drop volume), surface tension and contact angles. All the measurements have been carried out under a constant flow of Ar-5%H<sub>2</sub> mixture. In addition a Zr-getter was used to further lower the oxygen content close to the sample. The surface tension and density measurements were made by decreasing the temperature step by step. The properties were measured with an uncertainty of about 3%. The measured values of both the density and surface tension are well described by linear relationships and show negative temperature coefficients over the temperature ranges. The density as a function of the Al concentration increases with the decrease of the Al content in the alloys. The experimental densities are in good agreement with the Al-Ni density calculated taking into account a negative excess volume. The surface tension of the Ni-based super-alloys investigated shows linear behavior as a function of the temperature and increases with the decrease of the Al-content in the alloy.

The results obtained in the present work will be used within the project THERMOPROP to be compared both with the results of containerless measurements on ground (1-g) and during parabolic flights ( $\mu$ -g) and then the reference values could be selected and made available for computational models of the relevant industrial processes, thus filling the gap on the data of thermophysical properties of liquid Ni-based superalloys selected.

**Keywords:** Liquid metals, Surface tension, Density, Large drop method.

## Modeling of Nanofluid Thermodynamic Properties

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Nanofluids have recently become a subject of growing scientific interest due to reports of greatly enhanced thermal properties. The nanostructured materials have specific properties and their adding can change a landscape of thermodynamic surface of classic fluids. The key value that defines thermodynamic and phase behavior of fluids is the critical point. These singular properties of nanofluids have not been studied yet. at present time neither experimental data nor theoretical assessments about changes in the singularities of conventional fluids after nanoparticle doping are available in literature. The presence of nanoparticles should displace the singularity allocation and change the phase behavior of mixtures due to critical point shift of components.

The principal aim of this work is to study the effect of nanoparticle doping on thermodynamic properties of classic working fluids. We suggest the fluids with small impurities obey the corresponding state principle. It is hypothesized that the regular and singular parts of thermodynamic surface of base fluid and nanofluid with small nanoparticle volume concentration are coincided in reduced form. To predict the critical point shift of pure substances at nanostructured materials adding the thermodynamic models are used and influence of nanoparticle size and geometry is studied. The equations of state for nanofluids are presented and thermodynamic properties are calculated on the similarity theory base. The search algorithm of nanofluid critical parameters is as follows. The compressibility factor ( $Z$ ) of nanofluid is defined via scaled pure reference fluid properties. To estimate the critical parameters of reference fluid nanoparticles (e.g., CNT) system the fundamental equations of state in reduced form for industrial fluids (Lemmon and Span, 2006) are used.

Here we have considered the critical point shift for some low GWP working fluids for heat pumps and organic Rankine cycle embedded with CNT,  $\text{MnO}_2$ ,  $\text{F}_3\text{O}_4$  nanoparticles. To compute thermodynamic properties of nanofluids in the range 0... 5% volume concentrations of nanoparticles the density of nanofluid calculated via reference fluid density by standard linear relationship. The critical parameters for nanofluids also give an opportunity to calculate their thermodynamic properties from the reduced EoS. The speed of sound is most effective estimator of thermodynamic surface description since includes main thermodynamic derivatives. Also speed of sound is related with proposed mechanisms of thermal conductivity enhancement in nanofluids. Phonon transport speed is related the sound speed as function of the compressibility and the density of the fluid. We have evaluated the compressibility and speed of sound via equation of state by conventional thermodynamic relationships. The change of thermodynamic properties due to the compressibility of the fluid with nanoparticles suspended is negligible in the low volume fraction limit. A significant growth of sound speed is appeared at the higher CNT concentrations and corresponds to similar picture of sound speed increasing at pressure rising.

A general approach to the working fluid selection for organic Rankine cycle that meets a sustainable development criterion is developed. The direct assessment of the efficiency criteria for the Rankine cycle via artificial neural networks (ANN) approach is proposed. The construction of ANN includes the following sequence of actions: a choice of initial data for training; a choice of architecture of a network; dialogue selection of ANN parameters; process of training; check of adequacy of training (validation); and forecasting. The back propagation algorithm has been used for ANN training. Output values in the initial sample were calculated for various configurations of cycles based on thermodynamic properties. As input values the given  $T_C$ ,  $P_C$  and  $T_B$  are used. The various architectures of neural networks with different neuron numbers and activation functions in the first and second layers were considered. The forecast of efficiency criteria for the Rankine cycle as output parameters which describe the coefficient of performance with high accuracy and without thermodynamic property calculations is given.

**Keywords:** Nanofluids, Working media, Equation of state, Thermodynamic properties.

## **Photon Switching in Waveguide Fabricated From Metallic Nanorod Slab**

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Recently there is a considerable interest to study a new class of materials called photonic nano-fibers and nano-waveguides fabricated from metallic nanorods. This field is known as nanophotonics and it is a new emerging research area which has applications in sensing and advanced information technology. Photonic waveguides made by embedding a high index material into a low index material have been widely studied. However there is not much work done on photonic waveguides made from metallic rods slab embedded in photonic crystals. Photonic crystals are materials which have band gaps in their photonic spectra. Metallic rod lattice contains surface plasmon polaritons (SPPs). Frequencies of SPPs can lie between gigahertz to visible light. This means that SPPs lie in regime of photonics and electronics. Therefore, polaritonics bridges the gap between electronics and photonics and has a wide range of applications, including high bandwidth signal processing, THz imaging and THz spectroscopy. In this paper we have considered that energies of the SPPs lie within the band gap of photonic crystal. Due to this band engineering, metallic rod slab acts as a photonic waveguide. Numerical simulations have been performed on photon absorption and bound SPPs of the waveguide. It has been found that when the thickness of metallic slab is greater than the wavelength of the SPPs the energies of SPPs are degenerate. However, when the thickness of metallic lattice is smaller than the wavelength of the SPPs the degeneracy of SPPs is removed due to the dipole-dipole coupling between SPPs. The energies of the SPPs split into the symmetric and asymmetric states. This means that the waveguide can be switched on and off by changing the thickness of the metallic slab by applying the stress and strain. We have also investigated the nonlinearity of the photonic crystal. It is found that the absorption in the waveguide can be switched on and off by applying the pump laser. This reveals interesting results and can be applied to develop new types of nanophotonic devices such as nano-switches, nano-transistors, nano-limiters and nano-gates.

**Keywords:** Plasmonic, Photonic, Electronic, Polaritonic.

## Numerical Simulation of Mixed Convection of Nanofluids in A Square Cavity with an Adiabatic Block at the Center

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Since heat transfer fluids such as water, oil and ethylene glycol have low thermal conductivity, in recent years nanofluids, which are a suspension of nano-sized solid particles in a base fluid, with high thermal conductivity are used to enhance the heat transfer in many engineering electronic devices. In this study, a numerical simulation is carried out to investigate mixed convection of water-based nanofluids in a square cavity with insulated horizontal walls and isothermal vertical walls maintained at different temperatures and containing an adiabatic square block at the center. The top wall of cavity moves from left to right with uniform velocity  $U$ . The geometry and boundary conditions of the studied problem is given in Figure 1. The governing equations are solved using a commercial CFD code. Three different nano-particles, Cu, Ag and  $Al_2O_3$  are considered in the study. The computations are performed for solid volume fraction of 0%, 5% and 10%. The Grashof number is kept at a constant value of  $10^4$  and the Reynolds number is varied so that the Richardson number will have values of 0.1, 1 and 10. The results show that the presence of nanoparticles causes a significant increase in the heat transfer rate.

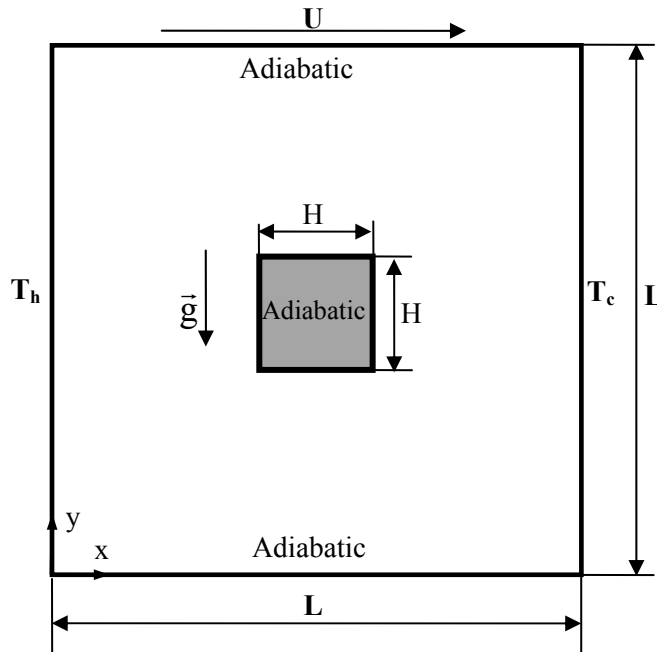


Figure 1. Physical geometry and boundary conditions

**Keywords:** Mixed Convection, Nanofluids, Square cavity.

## **Characterization of Hardening Properties and Fracture Criterion For Mg Alloy Plates at Elevated Temperature**

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The hardening properties and fracture criterion of an AZ31 Mg alloy plate with the thickness of 3mm were characterized at the elevated temperature of 250 °C in this work. In order to account for the softening behavior beyond the uniform deformation limit, the flow curves of the Mg alloy plate were obtained based on the inverse calibration method, utilizing the finite element analysis of the simple tension test, in which its strain rate sensitivity was also considered. As for the fracture criterion, triaxiality-dependent effective fracture strains, mainly covering the non-negative stress triaxiality zone, were numerically characterized utilizing experimental data based on specimens with four different shapes as well as the hardening data and deformation paths. For the comparison purposes, empirical fracture criteria such as the Cockcroft-Latham, Brozzo and Ayada models were also calibrated. For validation purposes, the four fracture criteria were applied for a real part drawing case and the result confirmed that the fracture criterion developed in this work performed best among the four tried out.

**Keywords:** Mg alloy plates, Warm forming, Fracture criterion, Softening behavior, Triaxiality.

## **Effect of Stamp Forming Pressure and Temperature on Polypropylene Sheets**

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Materials that have been used in this work were formed in stamp forming. A stamp forming mould which has a shape that has rectangular geometry was designed and manufactured to use this mould in this operation. Unreinforced polymer sheets were heated with an external heater to temperature which is close to melting limit but under melting point for each different material and formed by the mould which has been employed at room temperature to shape any parts from unreinforced PP. Some useful parameters for stamp forming of the polymer sheets such as heating time of polymer sheets, mould velocity, stamping pressure etc. were determined before the experimental operation started. These materials were formed in different temperature and pressure conditions. Some specimens were cut and taken from these sheets by machining. Tensile characteristics of these materials were investigated. According to tensile test results obtained from experimental stamp forming operations, after changing the stamp forming parameters as stamping pressure and stamping temperature PP materials showed different characteristics in (%)elongation at break and ultimate tensile strength.

**Keywords:** Compression, Temperature, Polypropylene (PP), Sheet, Strength.

## The Thermal Conductivity Measurement with DC+AC Driven Nanothermal Probe

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The scanning thermal microscopy (SThM) is a kind of scanning microscopy which allows imaging of temperature or thermal conductivity distribution at the sample surface. An idea is to combine atomic force microscopy (AFM) in contact mode with local temperature measurement. For this purpose special AFM probes with temperature sensors are used. The temperature imaging is obtained in a passive mode, when the probe measures local temperature, while the thermal conductivity imaging is realized in an active, in which the probe is used as a heated and the temperature sensor simultaneously. With nanofabricated thermal probe (NThP) spatial resolution better than 100 nm can be achieved.

In this work a possibility of use of resistive NThP for quantitative measurement is considered. The main difficulty connected with such measurement is relatively low sensitivity of probe resistance to the thermal conductivity of sample. In typical experimental setups working at normal pressure a relative change of the probe resistance caused by the change of the sample thermal conductivity does not exceed a few percent. For the NThP driven with dc current this changes are often comparable with interferences connected with instability of ambient temperature, noises of electronic equipment, etc. The sensitivity of measurement can be improved by the use of lock-in signal detection in a case of ac driven probe. However periodical probe heating causes problems with mechanical stability of a system because of thermoelastic bending.

A possible solution is probe driving with a sum of dc current and small ac current of frequency  $\omega$ . In this case the dc component and three ac components at frequencies  $\omega$ ,  $2\omega$  and  $3\omega$  of probe voltage can be measured. The theoretical analysis showed that the sensitivity of the amplitude of  $\omega$  component is 3 times higher than the one of dc voltage. Moreover, the sensitivity can be considerably increased when the amplitudes of higher harmonics are measured. An additional opportunity connected with ac measurements is a possibility of phase measurements. In general a phase signal is more immune to interferences than the amplitude one. A correctness of theoretical considerations is confirmed by results of experiments.

Finally, results of investigations of the thermal properties of selected samples by the use of the dc+ac driven NThP are presented. Qualitative and quantitative measurements were carried out for bulk and layered samples. It is shown that after proper calibration of the probe it can be used for determination of local thermal conductivity of different structures used in nowadays technology.

**Keywords:** Scanning thermal microscopy, Thermal conductivity, Thermal measurement.

## Numerical Simulations and Experimental Results of Quantitative SThM Measurements for Thin Layer Samples

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Scanning Thermal Microscopy (SThM) is a technique used to investigating local thermal properties. Application of nanofabricated thermal probes (NThP) with thin-film resistive temperature sensor ensures high spatial and thermal resolution. One of the problems associated with the use of SThM for quantitative measurements is the lack of a satisfactory model describing processes occurring in the probe – sample system. This is especially important for NThP, for which the complex geometry does not allow the creation of even approximate analytical description. In this case an interesting tool for the analysis of processes in the probe - sample system is the finite element method (FEM).

We present the probe-sample FEM model allowing accurate modeling of the basic physical processes occurring during the measurement. It enables an estimation of the dynamic range of signal changes, determining the highest sensitivity regime, and analyzing the potential sources of errors.

In this work we present the results of numerical simulations of SThM measurements of thin layer samples. Simulations mainly concern the influence of various factors, such as the type of substrate, the thickness and thermal conductivity of the layer, on the SThM signal. In the case of sub-micron layer thickness the thermal properties of the substrate influence the apparent thermal conductivity obtained directly from experimental data. Based on the results obtained from the simulation, a general procedure has been developed which allows the correction of “primitive” thermal conductivity value obtained in the experiment, taking into account the thickness of the investigated layer. Experimental results carried out for selected thin layers complement the numerical analysis.

**Keywords:** Finite Element Method, Scanning Thermal Microscopy, Thin layers, Thermal properties.

## Electronic Transport in Molecular Materials

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For evaluating the performances of devices electronics based on the junctions, the study electronic structure of interface metal-organic materials such as phthalocyanines is a key of their future application and is a present a dynamic field of research. The observed frequency dependence of AC conductivity has been found to obey the power law:  $\sigma_{ac} = A \cdot \omega^S$  where the variation of  $S$  with temperature indicates multi-hopping conduction mechanism in the  $M_eP_c$  thin films. A.C measurements have been used for identifying the charge transport phenomenon where hopping conduction mechanisms are frequency dependent process and provide information about the interior of materials in the region of low conductivity and are helpful in distinguishing the hopping conduction in the localized states from the free band conduction.

**Keywords:** Conduction, Hopping, Depletion layers, Interfacial dipoles.

## Investigations of Thermal Diffusivity of Mixed $\text{ZnS}_x\text{Se}_{1-x}$ Crystals and its Correlation with Optical and Electric Properties

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$\text{ZnS}_x\text{Se}_{1-x}$  single crystals with different content S were examined. The crystals were grown from the melt by the high pressure (150 atm of Argon) modified Bridgman method using high purity (99.995%) powders of ZnSe and ZnS put in graphite crucible in stoichiometric proportion. Thermal, optical and electric measurement for solid solution of  $\text{ZnS}_x\text{Se}_{1-x}$  crystals are presented and analyzed to determine an influence of composition on the thermal diffusivity, the electrical resistivity, the relative permittivity, and the energy gap. Thermal measurement was based on thermal wave method with detection using mirage effect. To interpretation of experimental data a thermal model of layered system was adopted. The results showed that the thermal diffusivity of samples decreases with the increase of S content x. Thermal diffusivity of ZnSe falls from  $1.62 \cdot 10^{-6} \text{ m}^2 \cdot \text{s}^{-1}$  to  $0.28 \cdot 10^{-6} \text{ m}^2 \cdot \text{s}^{-1}$  for  $\text{ZnS}_{0.3}\text{Se}_{0.7}$  crystal. The electrical resistivity of investigated samples was measured by the constant voltage method. The electrical resistivity changed from  $4.97 \cdot 10^9 \Omega \cdot \text{m}$  for ZnSe to  $10.3 \cdot 10^9 \Omega \cdot \text{m}$  for  $\text{ZnS}_{0.3}\text{Se}_{0.7}$ . The relative permittivity was determined by dielectric spectroscopy and decreased with increasing sulfur content in the ZnSe. Further, the optical band gap of  $\text{ZnS}_x\text{Se}_{1-x}$  were determined from photoluminescence spectra. The following values of energy gap were obtained: 2.71 eV, 2.76 eV, 2.84 eV and 2.89 eV for ZnSe,  $\text{ZnS}_{0.1}\text{Se}_{0.9}$ ,  $\text{ZnS}_{0.2}\text{Se}_{0.8}$  and  $\text{ZnS}_{0.3}\text{Se}_{0.7}$  crystals, respectively. Possible correlations between the thermal diffusivity, the optical band gap and electrical properties were studied. Obtained results showed clear dependence of those parameters on S concentration in the sample.

**Keywords:** Thermal diffusivity, Photothermal wave method, II-VI Semiconductors, ZnSe.

## Development of Cellular Ceramics Bricks Starting From Clays

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This study presents a method of elaboration of cellular ceramics, developed according to the principle of elaboration of cellular structure at green state; the heat treatment of sintering consolidates this green state to give the final porous material. This method facilitates the reproducibility of the manufacture of porous materials having same porous volume and an only size of cell.

The elaboration of cellular ceramics bricks is carried out by following 5 steps: **(1)** Preparation of barbotine of clay and chamotte. A deflocculating agent is added to optimise a maximal density of barbotine associated with a minimal tenor of water. Chamotte is obtained by calcination of clay at high temperature. The use of chamotte allows to decreasing the large contraction which undergo the clays during firing, and which causes deformations, and damages to the products. The optimal mixes of clays and chamotte must be optimised for avoiding the deformations and guarantee a minimal solidity at dry. **(2)** 10 cm<sup>3</sup> of commercially foamed agent is added for obtaining foamed slurry by energetic mechanical agitation. **(3)** The last solid material which is added is a mineral binder such refractory cement or Portland cement. This mineral binder allows fast drying of the cast foamed slurry without collapse, and it provides solidity to the dry sample. The optimal quantity of cement which avoids collapse is ~10 % in weight based on the weight of solids materials. **(4)** Pouring the foamed slurry into parallelepiped metallic moulds for drying at room temperature during 24- 48 hours, followed by total drying in oven at 100 °C. **(5)** Firing the specimens at high temperature for obtaining the cellular ceramics.

Cellular ceramics are elaborated in interval of density which varies from 1.0 to 0.40 g/cm<sup>3</sup> which corresponds to a porosity which varies from 60 to 90 % of total volume of material. The evolution volume of the foam slurry as a function with the addition of water shows a critical point where the volume increases abruptly, and the density decreases strongly. The corresponding porosity is around 75 - 80 % of total volume of specimen.

The same remark is observed on the flexural strength; around the critical porosity, the mechanical resistance falls brutally. Also The stress-strain curve of porous ceramics (porosity < 40 %) compared to cellular ceramics (P>60 %), shows a strong decrease of elastic modulus for over 70 % of porosity.

The cellular specimens have an interconnected cellular structure with a good pore size distribution. The size of cells varies from 1/100 mm to 1 mm.

Cellular ceramics bricks were elaborated starting from foamed slurry of water, formed of Algerian clays, and foaming agent. The consolidation is performed at room temperature, by adding mineral binder which allows the transformation of foamed slurry into a rigid and stiff body that can be machined in the green state after drying. The sintering of samples gives interconnected cellular materials with a good pore size distribution. This way of elaboration confirms well, the possibility to predict the density, the volume of voids, and the size of cells of porous specimen.

Various porosities were obtained with this novel method of elaboration of cellular materials from 60 % to 90 % of vacuum, and various sizes of cells, from 1/100 mm to 1 mm.

**Keywords:** Elaboration, Cellular ceramics, Clays, Lightweight bricks.

## Improvement of Thermal and Electrical Properties of Silicon-Ni Composites Using a Magnetic Field Process

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The research aiming at creating new materials with high performances based on polymer composites and nanocomposites is still growing. Among large investigations in this field, the production of thermally and electrically conductive polymer composites takes a special place because of the possibility to use such materials in a large variety of applications including many sectors (microelectronic devices, automotive, biomedical applications...).

The polymer matrix includes both thermosetting and thermoplastic types. Different kinds of fillers or reinforcements have been developed to process composite materials with desired thermal, mechanical and electrical properties. Reinforcement fillers have an important role to play in enhancing polymer performance and production efficiency. For electrical and thermal conductivities improvement, the use of conductive metallic particles is well adapted. However, the introduction of such filler alters the advantageous mechanical or physical characteristics of polymer matrices (high impact strength, low density). Therefore, it is of great interest to minimize the amount of added filler.

In previous works, we have shown that spatial distribution of dispersed the metallic filler (Ni and Cu) influences thermal conductivity of the PVC/Ni, PVC/Cu and PP/Cu composites. When filler distribution results in formation of a segregated structure, the thermal conductivity gets enhanced compared to a random distribution of filler in the polymeric matrix.

The use of electrical and magnetic fields during the process of the preparation of composites, is also an interesting way to enhance both electrical and thermal conductivity of composites along the aligning direction, provided that the particles are electrically or thermally conductive in nature.

In this work, composites based on silicon rubber filled with Ni particles with average size of 10 $\mu$ m were prepared. Three different spatial distributions of Ni particles (randomly orientation, // and  $\perp$  to the magnetic field) with several filler concentrations were used.

The samples of pressed silicon-rubber/Ni composites for measurements of thermophysical characteristics were produced as 25 $\times$ 25 mm plates with 1mm thickness. The samples used for electrical measurements were shaped as discs with 30 mm in diameter and thickness of 1mm.

The thermal conductivity was measured using an experimental device that represents an extension of the normalized hot guarded plate method. The specific heat measurements were performed using a microcalorimeter Perkin Elmer DSC Pyris with a -70 °C cryostat. The DC electrical specific conductivity was measured using a two-electrode method.

The experimental results were analyzed and compared with theoretical models to explain the thermal conductivity behavior of composite as a function of filler content and alignment. The results indicate the enhancement of electrical and thermal conductivities of silicon-rubber/Ni composites in case of magnetic field processing. The alignment of Ni particles to parallel magnetic field in the host-polymer system is identified as the main advantageous way for the enhancement of the electric and thermal conductivities compared to the random and/or perpendicular alignment of particles by magnetic field.

**Keywords:** Thermal and electrical conductivity, Polymer composites, Nickel particles, Thermophysical properties.

## **Progress in Phosphorus-Containing Polymers: Design, Structure and Properties.**

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The present contribution focuses on our recent research in the field of phosphorus containing macromolecular compounds, the main goals being the design, synthesis, characterization and study of the properties of new polymers containing phosphaphenanthrene heterocycle in the side chain and some polymers containing phosphorus in the main chain.

These polymers have been prepared through polycondensation reaction between aromatic dichlorides, aromatic bisphenols and a series of aliphatic diols, functional modification through polycondensation with phosphonic dichlorides etc.

The complete synthetic procedure of the monomers, intermediates and polymers will be presented. The structure of the monomers and intermediates and the basic characterization of the polymers have been performed using elemental analysis, NMR and FTIR spectroscopy, inherent viscosity and molecular weight measurements. The complete study of thermal stability, liquid crystalline, mechanical and optical properties, fire resistance was also done, by means of thermogravimetric analyses, FTIT-TGA-SEM measurements, DSC, X Ray diffraction, polarized light microscopy etc. The structure-properties correlations will be discussed.

**Keywords:** Thermal properties, Flame retardance, Liquid-crystalline polymers (LCP).

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## **Finite Element Analysis of Damping and Vibration Response of Epoxy Resin Reinforced with Nitrile Butadiene Rubber**

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A computational analysis is performed in order to investigate the vibrational behavior of epoxy resin composites reinforced with Nitrile Butadiene Rubber (NBR). Mechanical tests were conducted for concentrations of 10, 15, 20 and 25 wt% of NBR as well as pure epoxy resin which served as a reference sample. The damping ratio for each composite specimen was theoretically estimated with a proposed arithmetic model, based on the rule of mixtures and it was subsequently used to calculate the theoretical vibration modes of composite materials under study with the aid of finite element analysis (FEA). The FEA model simulated the samples with the various NBR concentrations based on the properties derived from the mechanical tests while utilizing within the model the theoretical damping ratio. The method to evaluate the vibrational behavior of the specimens was a cantilever beam excited into its fundamental mode by an impact force. The mechanical tests have shown a clear reduction of the modulus with the addition of NBR, while it was evident that the NBR composites could absorb greater amounts of strain energy. The vibrational analysis results reveal that the cantilever beam reaches the highest tip deflection for the sample with 25wt% NBR, while it demonstrates the highest rate of amplitude decrement among all tested samples. Overall, the study has shown that NBR composites could advance the state-of-art in the field of polymeric damping, helping to ensure ductility and great amounts of energy dissipation in a wide variety of structural components and systems.

**Keywords:** Polymer matrix composite, Epoxy Resin, Nitrile-Butadiene Rubber, Vibrational behavior.

## Measurement of Rock Materials by Pulse Transient Technique – Uncertainty Analysis of Two Models for Cylinder and Cuboid Shape of Samples

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The non-stationary dynamic method - the Pulse transient technique – has been used for investigation of thermophysical properties of porous rock materials. The small heat disturbance in a form of heat pulse generated inside the specimen set is used for thermal characterization of the specimen within a single measurement. From the temperature response to the heat pulse the thermal conductivity, thermal diffusivity and specific heat are calculated. Several models for pulse transient technique has been tested in regarding various effects that influence of accuracy of measured thermophysical parameters. The effect of heat losses from the sample surface in dependency on cylindrical or cuboid shape of specimen set is discussed in this paper. Discussed models are including the heat transfer coefficient from the sample surface to the surrounding. The real experimental condition considered by models is the temperature of the heat exchangers at the both ends of specimen set. Thus the both models for cylinder as well as cuboid shape accounts stabilized temperature at the both ends of specimen set.

The uncertainty analysis of models was introduced. The uncertainty in this analysis follows the influence of small disturbance on the model input. In this case it is a temperature noise at the measurement of temperature response. This noise causes certain level of uncertainty in the estimation of output parameters of the model. The analysis show under which conditions this uncertainty is acceptable and helps to set measurement conditions. It serves as the back-loop for the set of experimental parameters in measurement process.

The three dimensional model is solved for cuboid shape of samples and the two dimensional for the cylindrical one. Both models account the final geometry of the specimens. The heat transfer coefficient between the sample surface and free surrounding is accounted and discussed with regards to the measurement uncertainty. The uncertainty analysis was done to explain relations with the total time of the recording of the temperature response and the specimen geometry with respect to uncertainty and thus the final accuracy of measurement. The proposed analysis is applicable to any physical model within even outside of the class of the transient techniques.

The test of uncertainty analysis procedure has been performed on data obtained from experimental data measured on natural stones, e.g. sandstone, tuff and marble.

**Keywords:** Ttransient technique, Uncertainty analysis, Sensitivity coefficients.

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### Time Dependent Stability Analysis of Nanofluids

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Stability of nanofluids is an important issue due to their definitions. The steady state thermophysical properties of nanofluids has been well known. But, there is no enough data on time dependent thermal properties of nanofluids. In this study, the detailed time dependent thermal property variations of nanofluids were investigated. The nanofluids used in this study were water based TiO<sub>2</sub> and SiO<sub>2</sub> nanofluids. The TiO<sub>2</sub> and SiO<sub>2</sub> nano sized particles were added into the de-ionized water in five different particle volume fractions (0.25%, 0.5%, 1.0%, 2.0% and 4.0%). De-ionized water was used as base liquid in order to see only the effect of the nano particles. The analyses were made in two steps. In the first step, the measurements of thermal conductivity, viscosity and specific heat were made in every 1 hour during 24 hours. In the second step, The TEM images taken in 1<sup>st</sup>, 3<sup>rd</sup>, 5<sup>th</sup>, 10<sup>th</sup> and 15<sup>th</sup> days were evaluated by comparing the each other. Thus, time dependent thermophysical properties of water based TiO<sub>2</sub> and SiO<sub>2</sub> nanofluids were determined.

**Keywords:** Nanofluid, Thermal conductivity, Viscosity, TiO<sub>2</sub>, SiO<sub>2</sub>.

### Transverse Flexural Free Vibration Analysis of Rotating Euler–Bernoulli FGM Beams by the p-FEM

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The lifetime and operating temperatures of turbine blades, turbo-engine blades and helicopter blades could be further improved considerably by thermal barrier coatings with functionally graded concept. The functionally graded materials are inhomogeneous composite materials where the properties of the constituents vary gradually and smoothly. In this study, the transverse free flexural vibration of a rotating functionally graded beam is investigated. From Hamilton's principle, the linear partial differential equations based on Euler–Bernoulli beam theory are derived for coupled stretching and bending motion. Here we show that, by neglecting the inertia force in axial direction and the inertial coupling terms between axial and transverse displacement caused by the variation in material properties through the thickness, the uncoupled bending equations of motion can be obtained. A two node beam Fourier p-element is developed and used with 4-dof at each node (longitudinal displacement, transverse displacement, the slope and the curvature). The convergence properties of the rotating beam Fourier p-element is examined, the results are compared with those of the literature. Only one element is used to obtain good modal frequency prediction, leading to a significant decrease in computational effort compared to conventional elements. The Southwell coefficient giving a useful approach between rotating and non-rotating frequencies of rotating beam is investigated, for a given Young's modulus ratio, power-law exponent and hub ratio. Also, the influence of angular speed, Young's modulus ratio and power-law exponent on the natural frequencies and mode shapes is investigated.

**Keywords:** Rotating functionally graded beam, Fourier *p*-element, Southwell coefficients, centrifugal stiffening, natural frequencies.

## **The Effect of Synthetic Fibres on the Mechanical Behaviour of Reinforced Concrete Beams**

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The objective of the present investigation is to study the effect of the inclusion of synthetic fibres on the mechanical behaviour of reinforced concrete beams subjected to a flexural loading. The synthetic fibres used are recycled from the waste of brushes and domestic sweeps fabrications; they have lengths between 40 and 60 mm and a diameter of 0.47 mm. This present experimental work shows that the presence of the synthetic reinforcement in concrete confers it a high ductility and a better distribution of cracks along the tension zone of the loaded beams. Moreover, the beams reinforced with synthetic fibres have exhibited a significant flexural strength by comparison to those without fibres.

**Keywords:** Synthetic fibres, Reinforced concrete, Beams, Cracks, Ductility

## **The Effect of Filler Type on the Properties of In-Situ Polymerized PP Nanocomposites**

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Polypropylene/filler nanocomposites were prepared by in-situ polymerization with MAO activated metallocene catalyst without supporting the catalyst on the filler. The effect of addition of MAO treated nanofiller, at different loads, on the polymerization kinetics and consequently on PP matrix microstructure was investigated. To this end, two different fillers (Silica and Calcium carbonate) were used in this study for the preparation of the PP nanocomposites. A C<sub>2</sub> symmetric metallocene catalyst *ansa* dimethylsilylbis(2-methyl benzoindenyl) zirconium dichloride (MBI) was used as the catalyst. Results show that the kinetic of the polymerizations were profoundly affected by the presence of the filler particles, in comparison to the kinetic of homogeneous polymerizations. Therefore, the microstructure of the polymer matrix was also influenced by the presence of treated nanofillers in the polymerization media. It was also evident that the different types of the filler affect the polymerization activity and the produced PP microstructure differently.

**Keywords:** Nanocomposites, PP microstructure, In-situ polymerization.

## Recycling High Performances Concrete

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Concrete is the world's most used construction material owing to a number of factors such as the adaptability and flexibility in use, the availability of workmanship, the relatively lower cost and the longer term maintenance. The higher rate of construction development that is witnessed today throughout the world requires an ever increasing demand in natural aggregates to supply the concrete construction industry. Yet, the available stockpiles and quarries for aggregates are no more sufficient to fulfil this need. Furthermore, the search for new aggregate extraction plants is facing multiple obstacles due to severe ecological equilibrium problems of the nature and the preservation of the natural resources of our planet. In this sense, the continuous land use for aggregate extraction and the mountains devoured represent real negative environmental impacts that should seriously be taken into consideration by the concrete construction industry. Such concrete construction industry is also affecting our nature and hence having a serious negative impact on our environment through the landfills and disposals of the demolished concrete and building rubbles resulting from the increased and varied demolition activities. Reducing such negative environmental impacts goes inevitable through the search for replacing natural aggregates to make concrete. This will certainly safeguard the ecological equilibrium of our nature and relief our environment from undesired residual waste products.

In this sense, recycling the demolished concrete into construction is an ideal replacement solution. For this objective to be achieved, the first step needed is to identify the important properties of the material required to produce a stronger and highly performing concrete using recycled aggregates. Once it will be shown that these properties can be achieved and sustained with recycled aggregates, recycled aggregate concrete will become a more viable option for a sustainable development in harmony with nature.

The present work looks at the possibilities of recycling the demolished high performances concrete as aggregates to produce new concrete. The results show that the recycled aggregates produced may be particles of an original natural aggregate covered with cement paste, particles of a stronger cement paste and particles of an original natural aggregate. Different concretes were made with substitutions of 50%, 75% and 100% of recycled aggregate respectively as coarse aggregate. The resulting concrete materials had compressive strengths and tensile strengths comparable to those of the original concrete even when 100% of recycled aggregate was used. This was thought to be due to the relatively stronger cement paste by comparison to that of ordinary concrete. Indeed, in high performances concrete, the hardened cement paste is often as strong as the aggregate itself or even more; traces of crushed aggregate particles are often observed in a crushed high performances concrete specimen. The results obtained lead to the conclusion that recycling high performances concrete as aggregates leads to a new high performances concrete without any major drop in the mechanical strengths. Recycling high performances concrete appears to be a valuable resource that has a key role in meeting the challenge of a sustainable concrete construction for a sustainable development that fulfils the needs for the current generation without endangering the opportunities for future generations to meet their particular needs.

**Keywords:** Compressive strength, Tensile strength, High performances concrete, Cement paste, Aggregate, Recycling.

## **A premature Failure of a Super-heater Tubing in a Power utility Unit**

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Boiler tube failures continue to be a major cause of boiler forced outages. This paper presents the failure investigation of a superheater tubing material, and describes some mechanisms by which materials may fail at high temperature service. Samples were collected from one of the oil-fired power plants in Tripoli after five years of service. The as received super-heater tube showed considerable bulging at the fracture location. Collected failed samples were undergone several experimental examinations including visual inspection, thickness measurement, chemical analysis, and micro-structural evaluation.

Based on the results of this investigation, it is believed that the tube has failed as a result of ductile stress over-load failure caused by rapid short-term overheating. In this situation, the tube metal-temperature is extremely elevated from a lack of cooling steam flow through the tube. This has been assisted by presence of internal oxide scale deposit on inner tube surface which leads to higher than design operating temperatures. The internal oxide deposit could have been formed by the carry-over of a bad quality steam which brings suspended or dissolved solids (hardness). As a result, creep expansion thinned the tube wall and creep rupture resulted in failure by ductile stress over-load at elevated temperature.

**Keywords:** Superheater, Oil-Fired Boiler, Overheating, Rupture, Oxidation.

## **Characterization of Sintered %50 Ni-%48 Cr-%2 Ti Powder Mixtures Containing Intermetallics**

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Intermetallic materials are among advanced technology materials that have outstanding mechanical and physical properties for high temperature applications. Especially creep resistance, low density and high hardness properties stand out in such intermetallics. The microstructure, mechanical properties of %50Ni-%48Cr and %2Ti powders were investigated using specimens produced by tube furnace sintering at 1000-1400°C temperature. A composite consisting of ternary additions, a metallic phase, Ti,Cr and Ni have been prepared under Ar shroud and then tube furnace sintered. XRD, SEM (Scanning Electron Microscope), were investigated to characterize the properties of the specimens. Experimental results carried out for composition %50Ni-%48Cr and %2Ti at 1400°C suggest that the best properties as 184HV and 6,24/cm<sup>3</sup> density were obtained at 1400°C

**Keywords:** Sintering, Intermetallic, High temperature, Composite.

## **Mechanical Properties of A Composite Produced From Electroless Ni Plated Cr and Ti Powders**

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Intermetallic materials such as NiTi, Ni<sub>3</sub>Cr<sub>2</sub>, CrTi are among advanced technology materials that have outstanding mechanical and physical properties for high temperature applications. Especially creep resistance, low density and high hardness properties stand out in such intermetallics. The microstructure, mechanical properties of %64Ni plated %32Cr and %4Ti powders were investigated using specimens produced by tube furnace sintering at 1000-1400°C temperature. A composite consisting of ternary additions, a metallic phase, NiTi and Ni<sub>3</sub>Ti have been prepared under Ar shroud and then tube furnace sintered. XRD, SEM (Scanning Electron Microscope), were investigated to characterize the properties of the specimens. Experimental results carried out for composition %64Ni plated %32Cr-%4Ti at 1300°C suggest that the best properties as 208HV and 6,87/cm<sup>3</sup> density were obtained at 1400°C

**Keywords:** Sintering, Intermetallic, Electroless plating, Composite.

## Experimental and Analysis of The Uniaxial Behavior of High Density Polyethylene Pipes (HDPE-100)

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In this paper, an experimental analysis for determining the fatigue strength of PE-100, one of the most used High Density Polyethylene (HDPE) materials for pipes, under cyclic axial loadings is presented. HDPE is a thermoplastic material used for piping systems, such as natural gas distribution systems, sewer systems and cold water systems, becoming in a good alternative to metals, as cast iron or carbon steel. One of the causes for failures of HDPE pipes is fatigue, due to pipes are under cyclic loading, such as internal pressure, weight loads or external loadings on buried pipes, which generate stress in different directions: circumferential, longitudinal and radial. HDPE pipes are fabricated using an extrusion process, which generates anisotropic properties. By testing in the Laboratory a series of identical specimens obtained directly from PE-100 HDPE pipes in longitudinal directions, the relationships between amplitude stress and number of cycles (S-N curve) test frequency 2 Hz and stress ratio  $R = 0.0$  are established.

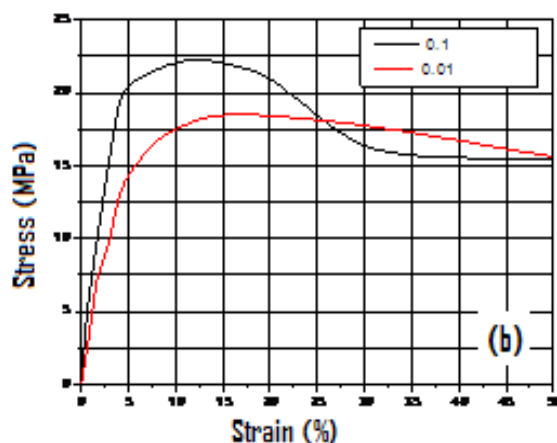


Fig. 1. Stress-strain curves for both strain rates, (a) global, (b) Small deformation zoom.

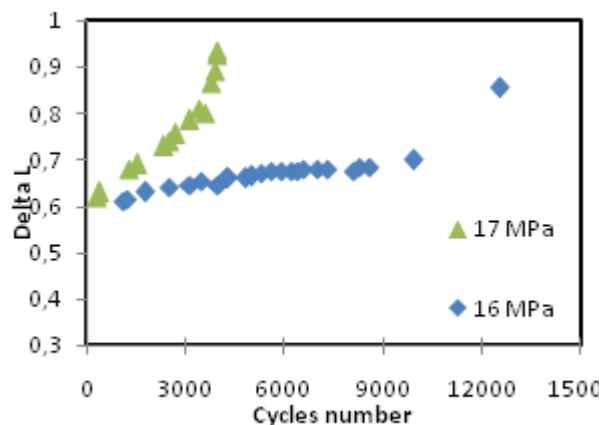


Fig. 2. Elongation changes during fatigue testing - Longitudinal direction for two levels of maximum stress 16 an 17 MPa.

**Keywords:** High Density Polyethylene, Pipes, HDPE-100; Cyclic loading.

## **Mechanical and Microstructural Study of Photo-Aged Low Density Polyethylene (LDPE) Films**

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This study deals with the aging of Blown extruded films of low-density polyethylene (LDPE), used for green house covering. The LDPE have been subjected to climatic ageing in a sub-Saharan facility at Laghouat (Algeria) with direct exposure to sun. The microstructural changes in the films were analyzed by IRFT for different states of ageing. The mechanical characterization was performed on a uniaxial tensile apparatus. The mechanical properties such as Young's modulus, strain at break, and stress at break have been followed for different states of exposure time (0 to 6 months).

The Climatic ageing of LDPE films shows the effect of ageing on the microstructural Plan which leads to: i) To an oxidation of the molecular chains. ii) To the formation of crosslinkings and breaking chains, which both of them are responsible of the mechanical behavior's modifications of the material. Crosslinks are in favor of strengthening of the mechanical properties at break (increase of  $\sigma_r$  and  $\epsilon_r$ ). In other side the chains breaking leads to a decrease of these properties. The increase in the Young's modulus also seems to be related to those structural changes since the crosslinks increase the average molecular weight. Branchings and tangles are favorable pairs for the ductile nature of the material. And in other side the chains breaking reduces the average molecular weight and therefore promotes the stiffening (following to morphological changes) so the material becomes fragile.

The post-mortem analysis of the samples shows that the mechanical stress has an effect on the molecular structure of the material. Although if quantitatively the concentrations of different chemical species exchanges, from a quantitative point of view only the unsaturations raises the polemics of a possible microstructural modification induced by mechanical stress applied during the tensile test. Also we recommend a more rigorous analysis with other means of investigation.

**Keywords:** Low-density polyethylene, Ageing, Mechanical properties, IRFT.

## Calculation of Thermodynamic Properties of CO<sub>2</sub> Using the Combined Thermal Equation of State with a Small Number of Adjustable Parameters

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The approximation  $p, \rho, T$  data of CO<sub>2</sub> was made in the intervals ( $0 < \rho/\rho_c < 2$ ,  $217 \text{ K} < T < 430 \text{ K}$ ,  $0 < p \leq 25 \text{ MPa}$ ) using the new combined equation of state (CES). In this equation, the pressure  $p$  is an explicit function of  $\rho$  and  $T$ . CES written in the form  $p/p_c = Y p_{scal}/p_c + (1-Y) p_{reg}/p_c$ . It includes a new regular part  $p_{reg}$  for the approximation of  $p, \rho, T$  data in liquid and gaseous states of areas outside the critical region, the singular part  $p_{scal}$  which is scaling equation of state for the critical region, and crossover function  $Y = \omega \operatorname{erfc}(\sqrt{\lambda} \cdot |\tau|) \exp(-\mu(\Delta\rho)^2)$  to combine these equations ( $\tau = (T-T_c)/T_c$ ,  $\omega = \rho/\rho_c$ ,  $\Delta\rho = \omega - 1$ ,  $\lambda$  и  $\mu$  - adjustable constants).

Regular contribution  $p_{reg}$  consists of the sum of 8 terms of the equation including adjustable constants  $A_1 - A_8$ , three of which are calculated through the remaining 5 adjustable constants using the conditions at the critical point.

$$p_{reg}/p_c = \frac{\omega t}{z_c} \{1 + A_1(f_1(t) - 1/t)\omega\varphi(\omega) - A_2\omega f(t) - A_3 \frac{\omega}{t} + \frac{A_4\omega}{(1-A_6\omega)} + A_5\omega^4/(1-A_6\omega)^4 + A_7\omega^5 t^3 e^{-5\omega-3t} + A_8(\omega_t - \omega)^3(3\omega - \omega_t)\omega^2(e^{5/t} - 1 - 5/t)\} \quad (1)$$

Here  $\omega_t = \rho_w/\rho_c$ ,  $\rho_{tr}$  is the liquid density at the triple point,  $t = T/T_c$ ,  $f(t) = \exp(-1/t) - 1$ ,  $f_1(t) = \exp(1/t) - 1$ ,  $z_c = p_c/\rho_c RT_c$  is the compressibility factor at the critical point,  $\varphi(\omega) = (\omega_t - \omega)^2(4\omega - \omega_t)$ .

The scale (singular) part of the equation of state  $p_{scal}$ , containing the values of  $p_c$ ,  $\rho_c$ ,  $T_c$  and adjustable constant  $q$ ,  $k$ ,  $M-a_p$ ,  $C_1$ , used in the form taking into account the expansion of the integral term  $-k \int \Delta\rho(\tau + q_p |\Delta\rho|^{1/\beta})^\gamma d\Delta\rho$  in series:

$$p_{scal}/p_c = 1 - k(q_p - q)^\gamma \Delta\rho |\Delta\rho|^{\delta-1} \left(1 + \frac{\delta}{1+\delta} \Delta\rho\right) + k(\tau + q_p |\Delta\rho|^{1/\beta})^\gamma (\Delta\rho + \Delta\rho^2) - k\tau |\tau|^{\gamma-1} \Delta\rho^2 \left(\frac{1}{2} + \frac{\gamma\beta}{1+2\beta} \frac{q_p |\Delta\rho|^{1/\beta}}{\tau}\right) + (M - a_p)\tau + C_1\tau^2/2, \quad (2)$$

where  $k$  is the compressibility coefficient in asymptotic dependence  $p_c K_T = \tau^{-\gamma}/k$  on the critical isochore. The magnitude of  $q$  in Eq.(2) is a factor in binodal dependence  $\Delta\rho = \pm (-\tau/q)^\beta + B(-\tau)^{1-\alpha}$ ,  $\gamma$ ,  $\beta$ ,  $\delta$  are critical exponents,  $\alpha$  - the index of the specific heat  $C_v$  at  $\rho = \rho_c$ ;  $M-a_p = s_c T_c/p_c - a_p$ ,  $s_c$  is critical entropy per unit volume,  $a_p$  is a constant of Pokrovsky transformations. Values  $\beta = 0.3255$ ,  $\gamma = 1.239$ ,  $\alpha = 0.11$  are taken in accordance with the 3-dimensional Ising model. For CO<sub>2</sub>, the critical parameters are taken from the paper *R. Span, W. Wagner*, J. Phys. Chem. Ref. Data (1996):  $T_c = 304.1282 \text{ K}$ ,  $\rho_c = 467.6 \text{ kg/m}^3$ ,  $p_c = 7.3773 \text{ MPa}$ ,  $\omega_t = 2.520381$ . The total number of system-specific constants - fourteen. To find them the minimization of a quadratic functional of relative deviations was used. The array of  $p, \rho, T$  data for CO<sub>2</sub> (731 points) was formed using a tabular data up to 25 MPa (*R. Span, W. Wagner*, 1996) which do not include the critical region, and in addition an experimental  $p, \rho, T$  - data of *V.G. Martynets, E.V. Matizen* (GSSSD, Physical constants and properties of substances. Issue 13, Izd. Standarty, 1979, Moscow), and *P. Nowak, Th. Tielkes, R. Kleinrahm and W. Wagner* (J. Chem. Thermod. 1997) in the wide vicinity of the critical point. Rms error on pressure is  $\pm 0.63\%$  (AAD =  $0.42\%$ ) in description of  $p, \rho, T$  CO<sub>2</sub> data over the entire region of gas and liquid states. The heat capacity  $C_v$  was calculated on isochores and isotherms including the critical region and the binodal, using defined CES constants ( $A_1 = 0.03526105$ ;  $A_2 = 1.2189927$ ;  $A_3 = 2.4763865$ ;  $A_4 = 0.789272$ ;  $A_5 = 0.0298947$ ;  $A_6 = 0.0799580$ ;  $A_7 = 69.729003$ ;  $A_8 = 0.0000733330$ ;  $M-a_p = 7.280166$ ;  $q = 0.110155$ ;  $k = 9.7211647$ ;  $\lambda = 152.318$ ;  $\mu = 10.07$ ;  $C_1 = -26.50$ ). The well-known expression

$C_v = C_{v,id} - z_c R t \int_0^\omega \left[ \frac{\partial^2 (p / p_c)}{\partial t^2} \right]_\omega \frac{d\omega}{\omega^2}$  was applied to calculate  $C_v$  using this CES constants. We obtain total expression for  $C_v$  using Eqs.(1) and (2):

$$C_v = C_{v,reg} - z_c R t \int_0^\omega \left[ \frac{\partial^2 (p_{scal} - p_{reg}) / p_c}{\partial t^2} \right]_\omega \frac{d\omega}{\omega^2} - 2 z_c R t \int_0^\omega \left[ \frac{\partial (p_{scal} - p_{reg}) / p_c}{\partial t} \right]_\omega \left( \frac{\partial Y}{\partial t} \right) \frac{d\omega}{\omega^2} - R t \int_0^\omega (p_{scal} - p_{reg}) / p_c \left( \frac{\partial^2 Y}{\partial t^2} \right) \frac{d\omega}{\omega^2} \quad (3)$$

where the integrals can not be expressed in terms of elementary functions and are calculated numerically via a simple program.  $C_{v,reg}$  has a form:  $C_{v,reg} = C_{v,id} - R t \{ A_1 e^{(1/t)} / t^3 \cdot I_1 - A_2 e^{(-1/t)} / t^3 \cdot \omega + A_7 e^{(-3/t)} 3 t^2 (4 - 8 t + 3 t^2) \cdot I_2 + 25 A_8 e^{(5/t)} / t^3 \cdot I_3 \}$ , where  $I_1 = \omega (\omega - \omega_t)^3$ ,  $I_2 = - e^{(-5\omega)} [24/5^4 + 24\omega/5^3 + 12\omega^2/25 + 4\omega^3/5 + \omega^4/5 + 24/5^5]$ ,  $I_3 = - \omega^2 (\omega_t - \omega)^4 / 2$ . The accurate expressions for derivatives of  $p_{scal}/p_c$  (2) on  $t$  were applied to calculate the  $C_v$  (3) on the near-critical isochores:

$$(\partial p_{scal} / \partial t)_\omega / p_c = k\gamma(\tau + q_p |\Delta\rho|^{1/\beta})^{\gamma-1} (\Delta\rho + \Delta\rho^2) - k\gamma \int \Delta\rho(\tau + q_p |\Delta\rho|^{1/\beta})^{\gamma-1} d\Delta\rho + (M - a) + C_1 \tau, \\ (\partial^2 (p_{scal} / p_c) / \partial t^2)_\omega = k\gamma(\gamma-1)(\tau + q_p |\Delta\rho|^{1/\beta})^{\gamma-2} (\Delta\rho + \Delta\rho^2) - k\gamma(\gamma-1) \int \Delta\rho(\tau + q_p |\Delta\rho|^{1/\beta})^{\gamma-2} d\Delta\rho + C_1, \quad (4)$$

where the integrals in (4) were replaced by convergent series. In formulas (4) the dependence of temperature on the density on the binodal was included in symmetric approximation ( $\tau = - q |\Delta\rho|^{1/\beta}$ ) to calculate  $C_v$  along binodal. In this case, the expressions (4) have the form:

$$(\partial p_{scal} / \partial t)_\omega / p_c = k\gamma(q_p - q)^{\gamma-1} [\Delta\rho + (1 - \frac{\beta}{1-\alpha}) \Delta\rho^2] |\Delta\rho|^{(\gamma-1)/\beta} + (M - a_p) + C_1 \tau, \\ (\partial^2 (p_{scal} / p_c) / \partial t^2)_\omega = k\gamma(\gamma-1)(q_p - q)^{\gamma-2} [|\Delta\rho|^{(\gamma-2)/\beta} (\Delta\rho + \Delta\rho^2) + \beta |\Delta\rho|^{-\alpha/\beta} / \alpha] + C_1$$

The curves of the specific heat  $C_v$ , calculated on the same isochores and isotherms, where experimental data on  $C_v$  are measured by the various authors (*L. Beck et al.*, J. Chem. Thermodyn. (2002); *I.M. Abdulagatov et al.*, J. Chem. Thermodyn.(1994); *J.W. Magee; J.F. Ely*, Int. J. Thermophys.(1986); *Kh.I. Amirkhanov et al.*, Teploenergetika (1970-71)) show good agreement with experiment to within  $\pm 8\%$  in different regions of the state, including the critical region. Also calculated values of  $C_v$  along binodal are in satisfactory agreement with the reference values of  $C_v$  calculated by the multiparametric equation of state *Span and Wagner* (1996) using 58 adjustable parameters and 35 different exponents only for residual part of the Helmholtz energy. The specific isobaric heat capacity  $C_p$  and sound velocity calculated along the binodal from the triple point up to the critical point using the CES constants. The calculation results shown in figures in comparison with the experimental and reference data.

We are proposed a unified description of thermal and caloric properties of CO<sub>2</sub> using a new type of thermal combined equation of state in the explicit form with a small number of adjustable parameters (only 14 coefficients). Coefficients of CES were found using the approximation  $p, \rho, T$  data without including data on  $C_v$ . In calculations the theoretical values of critical indices were used in accordance with three dimensional Ising model. The specific heats  $C_p$ ,  $C_v$  and sound velocity were calculated in a wide range of single-phase state including the critical region and the binodal. Calculated values of these properties are in satisfactory agreement with the tabulated values and describe the known experimental  $C_v$  data with an accuracy of  $\pm 8\%$ .

This work was supported by RFBR grant 12-08-00293-a and was partially supported by the Interdisciplinary Integration Project of SB RAS № 25.

**Keywords:** Equation of state, Specific heat, Carbon dioxide.

## Study on the Thermal Degradation of St-MMA Copolymers with Different Compositions Using Isoconversional Method

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Styrene-Methyl methacrylate (St-MMA) random copolymer in different compositions, polystyrene (PS) and polymethyl methacrylate (PMMA) particles were synthesized by suspension polymerization. The copolymer compositions were determined using nuclear magnetic resonance (H-NMR) method as well as their molecular weights were examined by gel permeation chromatography (GPC). The non-isothermal degradation behavior of the synthesized copolymers was studied by thermal gravimetric analysis (TGA) under nitrogen purge and the results were compared with corresponding homopolymers. Thermal gravimetric (TG) method has been extensively used for thermal degradation studies. Experiments are usually performed under non-isothermal conditions. Reaction mechanism fitting method which can provide some information on the reaction mechanism of pyrolysis is used through the determination of the apparent activation energy. In this study, the activation energies of different copolymers, PS and PMMA homopolymers have been calculated using Flynn-Wall-Ozawa method. Furthermore the isokinetic relationship (IKR) was used to estimate a model-independent pre-exponential factor for each degree of conversion. Thermal gravimetric analyses (TGA) were carried out for St-MMA, PS and PMMA particles by a Perkin Elmer Pyris Diamond, TG/DTA analyzer instrument. For thermal degradation experiments 5 mg of the particles was placed in an aluminum crucible and heated from room temperature to about 600 °C under nitrogen purge at different heating rates of 5, 10, 15 and 20°C /min and the weight loss versus temperature was recorded. The degradation process rate is dependent on the time, temperature and mass change of the sample. The kinetic parameters include;  $f(\alpha)$  that is the differential conversion function (kinetics model),  $E$  is the activation energy (J/mol) and  $A$  is the pre-exponential factor. One of the kinetic methods is an iso-conversional method in which the activation energy is estimated without the knowledge of reaction model (Flynn-Wall-Ozawa method). This method is useful for the kinetics interpretation of the TG data obtained from complex reactions. If the determined activation energy changes with increasing of conversion, the existence of a complex reaction mechanism can be concluded. Otherwise a simple-step reaction may be occurred during pyrolysis. A model-independent estimate of the pre-exponential factor can be obtained through the use of an artificial isokinetic relationship (IKR), in which a common intersection point of Arrhenius lines is defined as  $T_{iso}$  and  $k_{iso}$ . These values are isokinetic temperature and rate constant, respectively. In a general case the actual value of  $\ln A$  can be determined by this method. It is important that this approach is based on a completely artificial IKR derived from results of the model-fitting method. The complexity of the degradation reaction was shown by the iso-conversional method which the apparent activation energy was changed with degree of conversion for all samples. The results show that the iso-conversional method allows reliable prediction of kinetic scheme for all conversion ranges. Two main points could be concluded; the first one is the relationship between degradation rate and the activation energy, in which fast degradation rate means low amount of activation energy. The second one is the effect of MMA units in degradation behavior of copolymers, that higher amount of MMA means lower initiation degradation temperature and finally small value of activation energy in low conversion values. From the results of iso-conversional method, it was conclude that it is difficult to make a decision about exact thermal degradation mechanism. Furthermore the values of  $\ln A\alpha$  were determined using iso-kinetic relationships (IKR) and it was mentioned that  $\ln A\alpha$  and  $E$  have the same behavior with conversion changes. The important problem is that, the interpretation of reaction model is meaningful for a single-step process in which the  $E$  values are independent of  $\alpha$ . In this work, the activation energy values change with degree of conversion significantly indicating the presence of multiple-step reactions in thermal degradation of both foams. Therefore it seems that such reconstruction of reaction model with model-fitting method is not reliable. As a conclusion, the iso-conversional methods can be suggested as a suitable way of determining consistent kinetic parameters.

**Keywords:** St/MMA copolymer, Degradation kinetics, Isoconversional method, Flynn-Wall-Ozawa, IKR method.

**Study by a Genetic Algorithm the Effect of Heat Stress on the Shear Damage of the  
Fiber Matrix Interface of a Nanocomposite Material (Graphite/Epoxy)**

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The objective of this work is to develop an analytical model to evaluate the influence of thermal stress on the shear damage of the fiber-matrix interface nanocomposite material Graphite/Epoxy; from the properties of the fibers, matrix and interfacial bonding characteristics. This study developed by a genetic algorithm has shown the influence of heat stress beyond a critical threshold of shear damage to the interface, and also showed that damage to the interface of the composite material carbon/ epoxy is greater compared with that of the nanocomposite Graphite / Epoxy under the effect of the same thermal stress.

**Keywords:** Nanocomposite, Interface, Thermal stress, Shear damage, Genetic algorithms.

## Synthesis of Conductive Polymers - Metal Nanocomposites and Investigation of their Optical Properties

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Conducting polymers has received a great deal of attention in the last two decades. One of the remarkable features of conducting polymers is that it is possible to control the electrical conductivity of them over a wide range from insulating to metallic by proper doping with suitable dopants. These polymers have their unique electrical, optical, magnetic and chemical properties leading to the wide range of technological applications in rechargeable batteries, electrodes, electromagnetic interference shielding (EMI), sensors, corrosion protection coatings, microwave absorption, light emitting diodes, etc. In our present work we selected polyaniline among different conducting polymers because of its simple synthesis procedure, good environmental and thermal stability, low cost price, high conductivity, good electrical, optical, magnetic and chemical properties. The metal nanoparticles, such as silver and gold, have potential in technological applications because of their interesting properties. Silver nanoparticles have applications in catalysis, conductive inks, thick film pastes and adhesives for various electronic components, in photonics and in photography. In this work, we synthesized polyaniline with silver nanoparticles embedded in its matrix. Polyaniline was prepared by both chemical and electrochemical synthesis then silver nanoparticles injected in the polymers matrix. After synthesis of this nanocomposite, we investigated its characteristics by various methods such as UV/Vis analysis, Scanning Electron Microscopy, X-Ray diffraction and Ellipsometry analysis. Result showed that the electrochemically synthesized PANi (ECS-PANi) had somewhat lower conductivity, higher solubility, more benzenoid rings than quinoid rings, lower crystallinity, higher band energy, and higher particle size than that of chemically synthesized PANi (CS-PANi). This was due to the differences in synthesis method, the efficiency of oxidation or polymerization and ways of arrangement of polymer chains. The PANi obtained from both the electrochemical and chemical polymerization, had almost similar thermal stability. The presence of silver nanoparticles dispersed into porous polyaniline structures was confirmed by using X-ray diffraction (XRD) and scanning electron microscopy (SEM). From the SEM image it was observed that grains are well resolved and circular in shape and dopant nanoparticles were uniformly distributed in the polymer matrix. The XRD patterns showed that polyaniline was amorphous, but peaks present in XRD patterns in polymer nanocomposites were related to silver nanoparticles. It was well known that metal nanoparticles displayed surface plasmon resonance bands in the UV-vis region due to the excitation of electrons. A surface plasmon absorption band was obtained from the optical absorption at 380 nm, which indicated that silver nanoparticles presented in the polyaniline matrix. Optical absorption showed the shifting of plasmon peak of silver nanoparticle. Optical band gap polyaniline was decreased with increasing content of silver nanoparticles and hence optical resistivity increased. By means of ellipsometry we measured the complex refraction index of the nanocomposite. As we know the refractive index of a material is the most important property of any optical system. Since refractive index is a fundamental physical property of a substance, it is often used to identify a particular substance, confirm its purity, or measure its concentration. The real part of the refractive index 'n' indicates the phase velocity, while the imaginary part 'k' indicates the amount of absorption loss when the electromagnetic wave propagates through the material. With the ellipsometry analysis it was shown that silver nanoparticles also increased the real part of complex refraction index, and it means that the light could be trapped in the polymer matrix. By managing the refractive index of the nanocomposite with variable amount of doping nanoparticles, we could control the light route in it and also manage the light's behavior which could be very useful in many fields. By doping this polymer with the silver nanoparticles, electrical conductivity of the nanocomposite was increased and with the control of nanoparticles amount, this could be used in many fields such as touch screens. So, this is a simple way by which optical and electrical properties of other conducting polymers may be enhanced by using different nanoparticles.

**Keywords:** Conductive Polymers, Metal nanocomposites, Optical Properties, Polyaniline, Silver nanoparticles.

## CO<sub>2</sub> Solubility in Ionic Liquids at High Pressures and Wide Range of Temperatures

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Over the last 100 years a number of so called greenhouse gases have shown an increasing concentration in the atmosphere. At the end of the last century, because of the intensive development of instruments, remote methods and extensive application of isotopic methods in earth sciences, independent proofs of current climate heating were obtained. The main cause for this is attributed by common scientific belief to the continued increase of greenhouse gas concentrations in our atmosphere over the last century. One of the most important greenhouse gases at the present time is carbon dioxide. The continued burning of fossil fuels has and will continue to increase carbon dioxide (CO<sub>2</sub>) in the atmosphere.

Ionic liquids (ILs) are regarded as environmentally-benign solvents due to their immeasurably low vapor pressure. Recently, significant progress has been made in the application of ILs as alternative solvents for CO<sub>2</sub> capture due to their unique properties, a broad range of liquid temperatures, excellent thermal and chemical stabilities and selective dissolution of certain organic and inorganic materials. The prediction of gas solubility in ILs is a fundamental step toward the development of simulation tools to aid in the process calculations prior to industrial applications.

The experiments to determine the high pressure solubility of CO<sub>2</sub> in IL's at various temperatures are performed in a stainless steel measuring cell in equilibrium by using the isochoric method. The installation consists of three main parts: a) gas reservoir, b) stainless steel measuring (equilibrium) cell, c) Electronic tracking system box.

The wall of gas reservoir consists of two parallel 19 mm Kömacel (Germany) expanded plastic slab materials with a vacuum in between them. Such insulated wall system is a very high protection against heat exchange between the outside and inside of reservoir. In the inside of the gas reservoir have the aluminum heating plate and three high pressure gas balloons [two of them with 150 cm<sup>3</sup> (Swagelok, Germany) and one with 300 cm<sup>3</sup> (HPS, Germany)]. Beside the balloons, the gas reservoir consists of pressure transducers (PAA33X-V-100, Omega Engineering inc., 0-100 bar, Newport Electronics GmbH, Germany), PT100 thermometer (1/5 DIN Class B, Temperatur Messelemente Hettstedt GmbH, Germany), and an emergence (overflow) valve (R3A, Swagelok, Germany). The heating is done by eight parallel connected hot foils (100 X 200 mm 24 V ca. 20 W, Conrad Electronic SE, Germany) in the back side of the heating plate.

Experiments were carried out in four different pressure steps: in the first step, the maximum possible pressure (about 5 MPa) is created in the gas reservoir. The other steps with maximum pressure are: second - about 3 MPa, third – about 1.5 MPa, and finally – about 0.5 MPa. Experimental temperatures ranging from  $T=413.15$  K to  $T=273.15$  K in decrements of 20 K at selected pressures controlled by a PC with the LabVIEW program.

The temperature dependency of Henry's law constant was calculated and the average deviation of the Henry's law constant is always better than  $\pm 1\%$ . Thermodynamic properties of solution such as the free energy of solvation  $\Delta_{\text{sol}}G$ , enthalpy of solvation  $\Delta_{\text{sol}}H$ , entropy of solvation  $\Delta_{\text{sol}}S$  and heat capacity of solvation  $\Delta_{\text{sol}}C_p$  were calculated at various temperatures  $T$  to evaluate the solute-solvent molecular interactions.

The measured CO<sub>2</sub> solubility results in IL as a function of temperature at the various pressures are fitted to virial equation using the mole fraction dependence.

**Keywords:** Solubility, Ionic liquid, Equilibrium, Henry's constant.

## **Changes in the Thermal and Other Properties of Polylactide by Blending with Thermoplastic Polyurethane**

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Poly(lactide) (PLA) is an important biopolymer used especially for biomedical and food packaging applications. The problem to be used in other industrial applications is its rather lower mechanical and thermal properties compared to high performance engineering polymers. Therefore, the purpose of this work is to investigate mechanical and thermal properties including flow behavior of PLA when blended with thermoplastic polyurethane (TPU) elastomeric material. PLA/TPU blends with the ratios of 100/5, 100/10, 100/15, 100/20 were prepared by melt-mixing method in a laboratory scale twin-screw extruder. Specimens for testing and analysis were shaped in required dimensions by using a laboratory scale injection molder. Various mechanical tests (tensile, bending, Charpy impact,  $K_{IC}$  fracture toughness, Shore-D hardness) indicated that ductility and toughness of PLA could be increased significantly by blending with TPU, while there was certain level of expected decreases in the strength and hardness values. Thermal analyses (DSC, TGA, DMA) revealed that various transition temperatures ( $T_g$ ,  $T_c$ ,  $T_m$ ), crystallinity, thermal degradation ( $T_{10\%}$ ,  $T_{50\%}$ ) and thermomechanical properties ( $E'$ ,  $E''$ ,  $\tan \delta$ ) of PLA could be influenced by TPU blending substantially. Additionally, melt flow index (MFI) measurements showed that viscosity of PLA decreased by the incorporation of TPU.

**Keywords:** Polylactide, Thermoplastic polyurethane, Mechanical properties, Thermal properties

## Thermophysical Properties of 1-Butanol at Pressures up to 200 MPa

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The use of various alcohols as alternative to conventional gasoline and diesel fuels is increased dramatically. The successful using of 1-butanol as a fuel in an internal combustion engine is actually during the last years. 1-butanol has longer hydrocarbon chain causes and it to be fairly non-polar. In this case, 1-butanol more similar to gasoline than it is to ethanol. 1-butanol has been demonstrated to work in vehicles designed for use with gasoline without modification [1].

Today, the fuel injection systems for diesel engines reach pressures approximately up to 160 MPa for auto transport systems. Future systems are targeting even higher pressures in excess of 200-300 MPa. The one question in this filed: the possible number of injections per cycle during such extreme high pressures can be expanding and the time of one injection can be reduced. From another side, under such high pressure conditions, it is necessary to have the thermophysical properties of the fuel. Because, they can increase many times its atmospheric levels. Upon injection of the fuel in the cylinder, the large depressurization of the fuel results in a significant gradient of the viscous properties of the fluid [2]. The density, viscosity, speed of sound, heat capacity etc. are the main thermophysical properties for the study of such processes.

In this work, we present the thermophysical properties of 1-butanol at high pressures and wide range of temperature. The temperature interval was increased up to  $T=263.15$  K and pressure up to 140 MPa. The experimental  $(p, \rho, T)$  results are helpful to extrapolate the temperature up to  $T=253.15$  K and pressure up to 200 MPa using the constructed equation of state.

An equation of state for fitting of the  $(p, \rho, T)$  data has been developed as a function of pressure and temperature to calculate the various thermophysical properties of 1-butanol, such as isothermal compressibility, isobaric thermal expansibility, differences in isobaric and isochoric heat capacities, thermal pressure coefficient, internal pressure, heat capacities, speed of sound.

**Keywords:** Density, 1-butanol, Alternative fuel, Equation of state.

### Literature:

1. [http://en.wikipedia.org/wiki/Butanol\\_fuel](http://en.wikipedia.org/wiki/Butanol_fuel)
2. Duncan, A.M., Ahosseini, A., McHenry, R., Depcik, C.D., Stagg-Williams, S.M., Scurto, S.M. High-Pressure Viscosity of Biodiesel from Soybean, Canola, and Coconut Oils, Energy Fuels 2010, 24, 5708–5716.

## Thermophysical Properties of Azerbaijan and Turkish Water Resources

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Azerbaijan and Turkey possesses rich water (geothermal, mineral and river water) resources. Various thermal water resources of these countries has temperatures up to ~140 °C. Mainly, these resources potentially use for bottled water production, medicinal purposes, for spas and health clinics that utilize the waters to treat arthritis, dysfunction of the nervous system and skin diseases. But they can be also used for: thermal heat, for warming soil, hotbeds and hothouses with the aim of early and rapid growth of vegetables and fruits (40-50 °C). In this filed, Turkey have more knowledge and there are many alternative energy installations already installed in the country. There are some installed energy equipments in Azerbaijan also and this work developing speedily.

Kura river starting in north-eastern Turkey, it flows through Turkey to Georgia, then to Azerbaijan, where it receives the Aras River as a right tributary, and enters the Caspian Sea. Pollution of the river from the territory of the neighbouring states creates an environmental tension. Mineralisation of the water of the Kura river raises till 800-1200 mg in the connecting part of Araz and Kura rivers is 35-50 per cent more compared to its medium current. Density of polluted water of Kura river is max. 9 times more than sanitary norms.

To use the water resources for the alternative energy source, also in daily life requires the investigation of the chemical and thermophysical properties of a wide range of parameters. In this work, we present the chemical and thermophysical properties of geothermal, mineral and river water resources of both countries using the various installations (Spectrometer, Chromatography, Densimeter, Viscometer, DSC calorimeter etc.)

The samples were filtered and degassed slowly using the vacuum system. To stop vaporisation of pure water, the vacuum procedure was very slow (the groove of the flask valve, which held the sample, was very slightly opened). These investigations have been examined for the first time.

An empiric equation of state for fitting of the ( $p, \rho, T$ ) data of these water samples has been developed as a function of pressure and temperature. The molecular weight of thermal waters was analysed. The fitting of properties of water resources are discussing. The equation of state is used for the calculation of the thermophysical properties of IL, such as isothermal compressibility, isobaric thermal expansibility, thermal pressure coefficient, internal pressure, isobaric and isochoric heat capacities, speed of sound and isentropic expansibility.

**Keywords:** Geothermal water, River, Density, Viscosity, Speed of sound.

## Numerical Contribution to Heat Treatment of Wood

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Heat treatment of wood which is a clean process may be an alternative to chemical treatments. The temperatures used are located on a range between 180 and 280°C, The gas temperature and duration of treatment are the parameters which determine the change in physical and chemical properties of wood. These changes increase the dimensional stability, improve weather resistance and increase resistance to wood degrading agents.

Many mathematical approaches modeled this phenomenon. In this work, the Luikov model applied to a rectangular geometry with a numerical approach based on finite volumes is used. A sample of wood assumed as porous medium with  $2l \times 2h$  size is considered. This sample has an initial temperature ( $T_0$ ) and a moisture ( $M_0$ ), it is placed in an oven heated to a temperature ( $T_g$ ), and a moisture content ( $M_g$ ). Because of the symmetrical situation, the study is done on a quarter of the sample in the X, Z plane.

Heat and mass transfer are governing by the Luikov model equations given as follow.

Heat transfer:

$$\rho \cdot C_p \frac{\partial T}{\partial t} = \nabla(k_{eff} \nabla T) + \alpha \cdot Q_1 \cdot \rho \frac{\partial M}{\partial t} \quad (1)$$

Mass transfer:

$$\rho \frac{\partial M}{\partial t} = \nabla[D_{eff} \nabla M + D_{eff} \delta \nabla T] \quad (2)$$

The coupled equations of heat and mass transfer and boundary conditions are solved with the finite volume method. Uniform grids in both directions X and Z are considered.

The algebraic system is solved using the Thomas algorithm for two-dimensional problem (2D). Direct method of the Thomas algorithm (TDMA) in one direction and the iterative Gauss-Seidel in the other direction are combined.

Results show that the temperature of the wood reaches the oven temperature more quickly for the extremity of the sample than the interior parts. All the parts of the wood become at the oven temperature later. We also note that moisture decreases more rapidly at the point on the boundary as internal points. This decrease of the moisture starts at 12% corresponding to dry wood and finishes at near zero corresponding to heat treated wood. The time to reach these values is given in our results. After removing the moisture, it is important to complete the heat treatment in order to reach the needed color. This can be done by using an experimental device.

The drying speed is represented for three reference points (extremity of the sample, an internal point and the middle of the sample). For the first point drying starts with a high speed and stabilizes quickly, for the second and third point, because of the drying is late, the speed starts increasing and after a certain time it decreases due to the reduction of moisture.

Distribution of temperature and humidity in the sample during heat treatment are analyzed. We note that the temperature increases until the oven temperature is reached and the moisture content decreases with time to a value close to zero, which is the aim of the heat treatment in order to preserve the wood from the different aggressions.

**Keywords:** Wood, Moisture, Heat treatment, Temperature.

## Effect of Surface Pretreatment of Aluminum Substrate on Properties of Ni Electrodeposited Coating

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Plating on Al alloys, due to the presence of a surface oxide film, is difficult. Therefore, a pretreatment on the substrate is necessary to obtain suitable surface prior to deposition process. Zincating is extensively used for preparation of aluminum surface. In this process, the substrate surface is covered by a zinc film via displacement reaction of aluminum and zinc. In fact, zincate treatment makes the aluminum surface suitable for deposition of final coating. However, the zinc layer may be dissolved in acidic solutions such as Watts bath used for electrodeposition of Ni coating. Hence, use of an intermediate layer between Zn film and Ni coating was suggested. In this paper the effects of Cu intermediate layer on properties of Ni coating electrodeposited on 6061 Al alloys substrate was investigated. The properties of the coatings were studied by means of peel test and potentiodynamic polarization techniques. The results indicated that using of Cu intermediate layer increased the adhesion strength of the coating from  $0.85 \times 10^3$  N/m to  $4.01 \times 10^3$  N/m. Furthermore, the polarization curves shifted to less negative potentials and the corrosion current density decreased when Cu intermediate layer was applied after zincate process. Indeed, Cu film as intermediate layer suppresses the Zn dissolution in Watts bath, and so, the Ni coating applied on Cu layer shows a dense and uniform microstructure which improves the adhesion strength and corrosion resistance.

**Keywords:** Ni coating, Zincate treatment, Peel test, Potentiodynamic polarization.

## Effects of Co Alloying Element on Chemical Composition, Morphology, Hardness and Corrosion Behavior of Electrodeposited Cr-Co Coatings

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Conventional chromium coatings deposited from Cr (VI) electrolytes have been used for more than 100 years. However, Cr (VI) plating process should be replaced by other technologies, because Cr (VI) is highly hazardous and toxic. Unfortunately, few coatings could completely replace the conventional hard chromium coatings. Trivalent chromium plating process is considered as a very promising technology to replace conventional Cr (VI) coatings. These electrolytes are environmentally safe and plating is more productive and less power consuming. Nevertheless, Cr (III) based coatings have poor corrosion resistance as compared to the coatings deposited from the Cr (VI) electrolyte. Addition of Co (II) ions to a Cr (III) bath can improve the corrosion resistance of the resultant coating in comparison with that of Cr film obtained from a bath without Co (II) ions. Oxidation and thermal resistance along with cracking of chromium coatings can also be improved by electrochemically alloying of chromium with iron family metals, such as cobalt. These alloys are used in power generation, marine, aerospace, and oil and gas industries under high temperatures or corrosive environments.

In the present study, DC current was used for electrodeposition of pure Cr and Cr-Co alloy coatings on 316L SS from a chromium sulfate bath containing 0-6 g/L cobalt sulfate. Current density and temperature were 140 mA/cm<sup>2</sup> and 35 °C, respectively. Effect of Co (II) ion concentration on current efficiency, morphology, chemical composition, micro-hardness, and corrosion behavior of the resultant deposits was investigated. Pure cobalt coatings were also produced from cobalt sulfate bath for the purpose of comparison. Results revealed that the current efficiency of the pure cobalt electrodeposition is much higher than that of the Cr and the Cr-Co alloys deposition. The cathodic current efficiency was decreased by addition of up to 3 g/L of Co (II) ion to the chromium sulfate bath. However, further addition of Co (II) ion increased the current efficiency. SEM micrographs from the surface of the coatings showed that the morphology of the pure cobalt film is smooth, while the morphology of the Cr-Co alloys is lumpy containing micro-cracks. According to EDS analyses, cobalt content of the alloy deposits is increased from 0 to about 85 wt.% by the addition of 0 to 6 g/L cobalt sulfate to the bath electrolyte. Micro-hardness and polarization tests results revealed that pure Cr and the alloy containing about 70 wt.% cobalt have the highest micro-hardness (i.e. ~ 900 HV) and corrosion resistance ( $i_{\text{corr}} \approx 0.8 \mu\text{A}/\text{cm}^2$ ) between all the coatings, respectively.

**Keywords:** Co-Cr alloy, Electrodeposition, Corrosion properties, Hardness.

## **The Investigation of The Density of Binary Methanol + Chlorobenzene Mixtures at High Pressures**

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The experimental investigation of the thermal properties of substances in liquid state is one of the most important problems in modern thermophysics because the theory of liquid state has been insufficiently developed. The density of pure high hydrocarbons and their solutions attracts the attention of both the researchers engaged in different fields and design engineers of chemical, petrochemical, power and other industries. This is natural, because the information on the properties of such solutions processes. The density of pure hydrocarbons of normal and isomeric structure in the liquid state is well studied, and, the results of such measurements have been published in scientific journals. at the same time, the density of binary mixtures of high hydrocarbons is not investigated. We this performed experiments to determine PVT-dependences of binary mixtures of methanol+ chlorobenzene in liquid phase in the range of temperatures 290-560 K and pressures 0.1-60 MPa.

The measurements were carried out in facilities utilizing the method of hydrostatic weighing. The total relative error of density measurement is 0.08 percent. All experimental results were analyzed. It is found that the density of the studied hydrocarbon binary mixtures decreases as the temperature, pressure and concentration increases

The value of the density is described by the equation as function of the concentration.

The density of liquid binary mixtures of methanol+chlorobenzene was calculated.

**Keywords:** Density, Thermal properties, Binary mixtures, Hydrostatic weighing.

## **Finite Element Analysis of Out-of-plane Compressive Properties of a Novel Concept of Honeycomb Structures with Hexagonal and Auxetic (negative Poisson's ratio) topology**

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This work illustrates the manufacturing and compressive testing of a novel concept of honeycomb structures with hexagonal and auxetic (negative Poisson's ratio) topology. The cellular configuration is simulated using a series of finite element models representing fullscale. The models are benchmarked against experimental results from pure compression tests. Finite element models of the honeycomb assemblies under compressive loading have been developed using nonlinear shell elements from an ANSYS code. Good agreement is observed between numerical nonlinear simulations and the experimental results.

**Keywords:** Lattice structures, Voronoi, Finite element analysis.

## **A Thermal and Chemical Characterization of Limestone from Kellal Mountain (North-East Constantine, Algeria)**

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New building materials could be prepared from appropriate mixtures of local rocks such as white and gray limestone from Kellal Mountain (North-East Constantine, Algeria). Firing of both limestone: White Kellal Mountain Limestone (WKML) and Gray Kellal Mountain Limestone (GKML), was carried out in the temperature range 25 to 1000 °C under atmosphere and the mineralogical transformations were investigated with X-ray diffraction (XRD), Thermo Gravimetric Analysis (TGA), Differential Thermo Gravimetric Analysis (DTGA), Differential Scanning Calorimetry (DSC) and Fourier Transform Infrared spectroscopy (FTIR).

The predominant phases emerge on the spectra of X-ray diffraction (calcite, dolomite and some minor elements such as kaolinite). Thermal analyses of limestone by TGA/DTGA and DSC confirmed the presence of the same phases and the overall appearance of the DSC curves is similar to that of DTGA curves. The spectral variations of the internal modes of the carbonate ( $\nu_1$ ,  $\nu_2$ ,  $\nu_3$  and  $\nu_4$ ) and their combinations were used to study the structural phase transitions.

The effect of the annealing temperature on the phase changes is discussed: the disappearance of the substantial phases and the appearance of new phases using the previous techniques.

In fact, thermal analyses are powerful tools in determining mineral phases and their combination provide a maximum of information for qualitative study and is an unavoidable means and meet the needs of geologists, the road infrastructure and pharmaceutical industries.

**Keywords:** Limestone, TGA/DTGA, DSC, XRD, FTIR.

## **Effect of a Turbulent Plane Wall Jet Impinging a Hot Obstacle**

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The mean turbulent flow structure around an elongated hot obstacle is studied numerically. Two types of incoming flow are examined in order to show the influence of the external zone of the flow on the reattachment process. It comes about a wall jet and a boundary layer. The effects of the Reynolds number and the ratio between the width nozzle to the obstacle height are detailed simultaneously. The results show that the increasing of Reynolds number and nozzle thickness; enhances the heat transfer and modifies considerably the stagnation point location. The boundary layer case gives the greatest Nusselt number values in comparison of wall jet cases. The turbulence kinetic energy and vorticity are found great around the nozzle cross section where the shear layer attains the great deformation. This can be justified by the longitudinal direction of the main flow. The distribution of average Nusselt number is correlated according with some problem parameters.

**Keywords:** Wall jet; Heat transfer, Turbulence, Obstacle, Boundary layer.

## Experimental and analysis of the Uniaxial behavior of High Density Polyethylene Pipes (HDPE-100)

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In this paper, an experimental analysis for determining the fatigue strength of PE-100, one of the most used High Density Polyethylene (HDPE) materials for pipes, under cyclic axial loadings is presented. HDPE is a thermoplastic material used for piping systems, such as natural gas distribution systems, sewer systems and cold water systems, becoming in a good alternative to metals, as cast iron or carbon steel. One of the causes for failures of HDPE pipes is fatigue, due to pipes are under cyclic loading, such as internal pressure, weight loads or external loadings on buried pipes, which generate stress in different directions: circumferential, longitudinal and radial. HDPE pipes are fabricated using an extrusion process, which generates anisotropic properties. By testing in the Laboratory a series of identical specimens obtained directly from PE-100 HDPE pipes in longitudinal directions, the relationships between amplitude stress and number of cycles (S-N curve) test frequency 2 Hz and stress ratio  $R = 0.0$  are established.

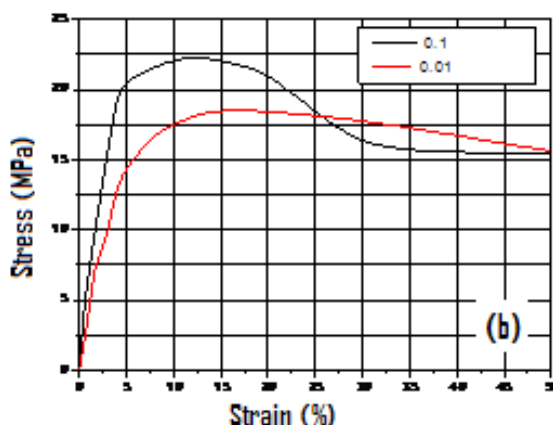


Figure 1. Stress-strain curves for both strain rates, (a) global, (b) Small deformation zoom.

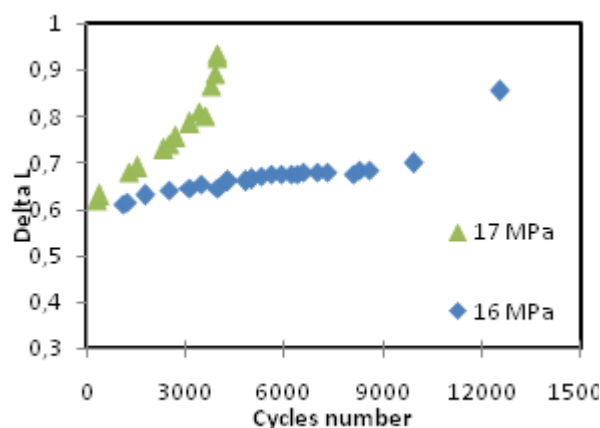


Figure 2. Elongation changes during fatigue testing - Longitudinal direction for two levels of maximum stress 16 an 17 MPa.

**Keywords:** High Density Polyethylene; Pipes; HDPE-100; cyclic loading.

## Study of the Shear Modulus Oof Wood-Based Layered Composites Under Static Load Using Finite Element Method

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This article presents research on wood laminates transferring shear stress. These laminates were used for construction of railway seats.

Reducing the weight of items and the required nature of the load transfer in the elements of the railway seat during service, requires the application of reinforcement in the form of continuous fibers. The multi layered laminate structure consists of interconnected layers of synthetic and natural fibers which provides rigidity and strength of the construction. Static shear strength tests with simultaneous registration of the in-plane deformation of the samples by means of Digital image Correlation (DIC) were aimed to the designation of critical shear stress and modulus of elasticity in shear.

This test method is most useful for determining the moduli of rigidity of orthotropic materials for which moduli of rigidity cannot be computed from elastic moduli and Poisson's ratios. The shear modulus obtained is that associated with shearing deformation in the plane of the plate. The shear test of beech veneers in bias directions (45°) of their fiber orientation show cracking along the fibers. The fractures usually happens on the entire samples surface, as it is shown in Fig.1c.

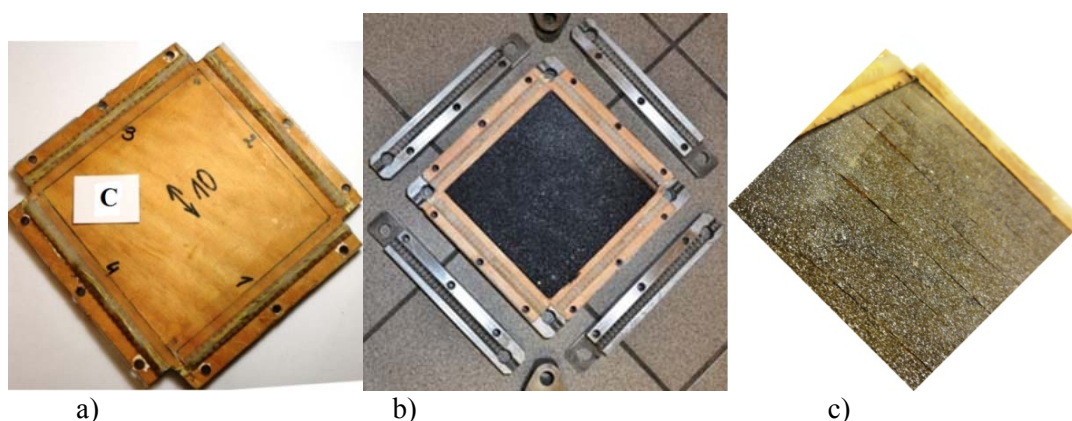


Fig. 1. Typical failure of plywood specimens; the initial state (a), closing system b), destruction c)

A geometric model simulating the samples used for mechanical properties testing was developed using the Finite Element Method (FEM). The FE models were based on the criteria of strength of single layers of orthotropic composite. Numerical results obtained by using the developed procedure for the specimen described in Fig.2. and have been compared with experimental results.

The multi layered laminate structure The FE model of a few layer wood based composite is useful for its properties optimization and for development of more efficient in large-scale simulations computational models of layered composites.

This research was co-financed by The National Center for Research and Development within the frame of Applied Research Programme (PBS1/B6/2/2012).

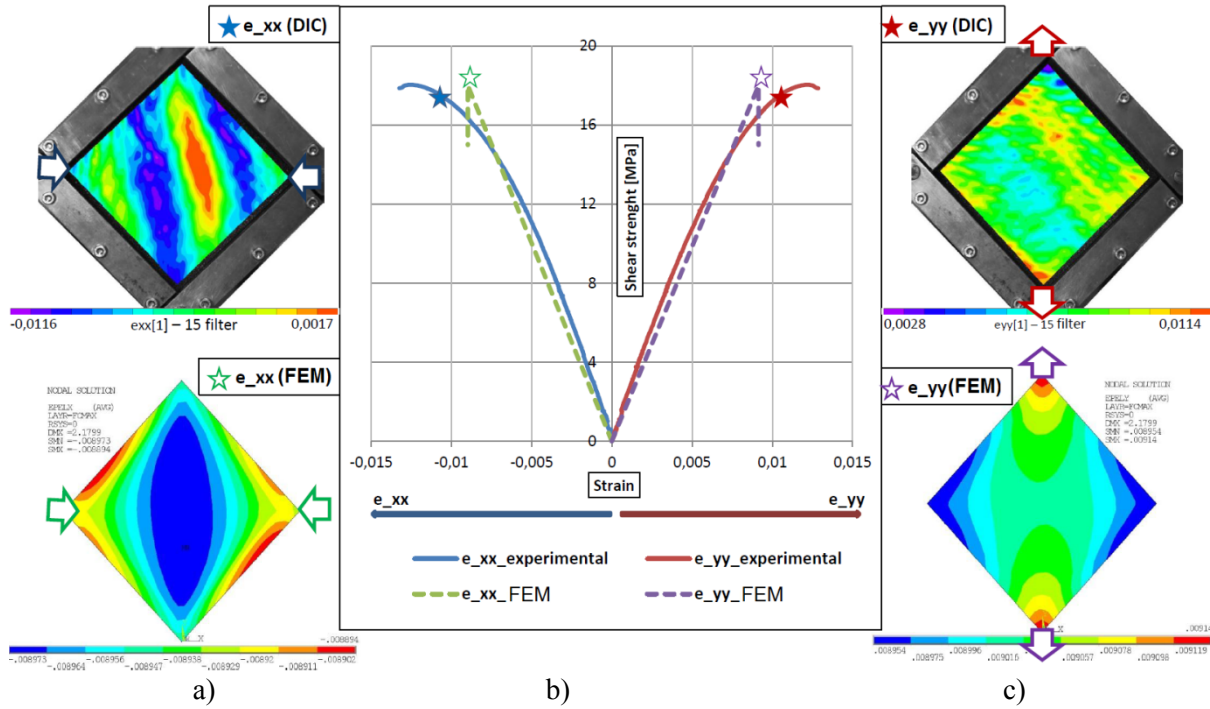


Fig. 2. The three-ply beech plywood: the summary deformation maps during compression of, obtained by DIC and FEM (a); (shear stress)–(strain) diagrams of experimental shear test finite element model (b); the summary deformation maps during tensile of, obtained by DIC and FEM (c)

**Keywords:** Wood-based composites, Strength tests, Shear modulus, Digital image correlation, Finite element method

## Standard Enthalpy of Combustion of Biodiesel From Hydroxylated Oils

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*QSPR* equations are presented to calculate the standard enthalpy of combustion developed for pure substances and mixtures of alkylesters, triglycerides, diglycerides and monoglycerides of common and hydroxylated fatty acids (i.e, castor, lesquerella oils, etc.), by using only the molecular structure of the compound and the predictability of homologous series. The molecular descriptors used in the equations are: size of the carbon chain, number of double bonds, number of hydroxyl groups and the number of carbon atoms of the alcohol in the alkylesters. For natural oils and biodiesel, which are mixtures of fatty esters, simple mixture rules and the Brönsted's Congruence Principle were applied and permitted to express the equations with the saponification, iodine and hydroxyl values. *QSPR* equations, based on stoichiometry and on Hess's law, without regression analysis, were developed with Mathcad 13.0. The values predicted by the equation were compared with data from the literature by using the MS Excel, observing the following average absolute errors: biodiesel (1.95%, n=24), natural oils (1.43%, n=69), alkylic esters (4.0%, n=62), triglycerides (1.9%, n=20) and fatty acids (6.9%, n=50). The equation obtained for the heat of combustion of natural oils represents a generalization of Bertram's equation, which is extended to hydroxylated oils, with average absolute errors of about 1.43 % in the *QSPR* equation and 1.23 % in Bertram's.

**Keywords:** Higher heating value, Biodiesel, Oxygenated biofuels, *QSPR* equations, Bertram's equation.

## **The Investigation of The Hydrocracking Process of Tar With Heavy Gas Oil of Catalytic Cracking In The Presence of High-Dispersed Halloysite**

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The main trend of development of oil refining industry is an increase of oil refining extent with involvement of heavy petroleum residues into refining with the purpose of enlargement of motor fuels production. On this purpose has been studied the -hydrocracking process of tar with heavy gas oil of catalytic cracking (tar: heavy gas oil of catalytic cracking-70:30) in the presence of suspended high-dispersed halloysite.

It should be mentioned that halloysite consists of aluminum and silica oxide layers. The thickness of the layers in hydrate mineral reduces about 10 Å, but in unhydrated mineral to 7.2 Å. These layers are covered to the pipe in the result of atmospheric condition and geothermic processes in hydrate mineral. Pure (crude) halloysite is white mineral and can be fine powdered by treating easily. Halloysite contains very small amount of other ions of metals as Fe<sup>+3</sup>, Cr<sup>+3</sup>, Ti<sup>+4</sup> and etc. besides aluminum, silica oxides and hydrated water. Ferrum oxide is a general mixture found in halloysite minerals (weight up to 3%). The generating of such a large amount of ferrum oxide can be explained in the presence of associated (combined) oxides in mineral and also izomorphic substituting of Fe<sup>+3</sup> and Al<sup>+3</sup> ions in octahedral layer of aluminum oxide.

The experiments were carried out in a rotating autoclave( of 1 l volume) at 400-460 °C temperature and 0.5-2 MPa pressure. Determined that the light oil products with weight of 50-52% are obtained by the hydrocracking process of tar in the presence of suspended high-dispersed halloysite in optimal condition. But during the hydrocracking process of tar with heavy gas oil of catalytic cracking (70:30) the yield of the light oil products makes up 59-60 % by increasing 7-9% and the coke yield reduces from 10% to 5%. It can be explained by adding naphthenes, partial hydrated polycyclic aromatic compounds, including heavy gas oil of catalytic cracking as an activator (as hydrogenous donor) to the crude in hydrocracking processes of heavy petroleum residua (fuel oil, tar) that known from the literature. However it causes the increasing of the yield of light oil products and also reducing the amount of coke during the process.

**Keywords:** Hydrocracking, Goudron, Suspended catalyst.

## Catalytic Oxidation of Dearomatized Diesel Fraction in Liquid Phase by Extraction Method

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The mixture of synthetic petroleum acids (SPA) and synthetic oxyacids (SOPA) obtained from catalytic oxidation of diesel fraction of petroleum in liquid phase are the excellent substitutes of natural petroleum acids (NPA) that largely applied in petro-chemistry industry. From this point of view the obtaining of synthetic acids mixture with high yield from the aerob oxydation of diesel fraction in liquid phase is of a great scientific and economic importance (*assumes a great scientific and economic importance*). But, it is known from the literature references that o- and p- substituted phenoles with a strong anti-oxidant properties is formed from aromatic hydrocarbons in co-oxydation process and it prevents the running of the oxydation process of naphthene-parafin hydrocarbons. In this regard it is necessary to dearomatize the diesel fraction before to oxidize. Extraction process is one of the analyze methods used in different fields of chemical industry, including oil refining industry. In order a wide range of researches on an industrial scale are recently conducted in the sphere of applying of solvents of ion-liquid content besides n-methyl pyrrolidon as a solvent extractant and the creating of ecologically clean “green” chemistry. From this point of view the use of solvents of high selectivity, being liquid in a wide temperature range, environmentally safe ion-liquid type as an extractant is actual in treatment of oil fractions and is very important in terms of industry.

By taking into consideration that the diesel fraction (DF) mentioned below boiled in 217-349 °C brought from “Azerneftiyag” ORP is purified from aromatic hydrocarbons and sulfur compounds content by extraction method and obtained positive results.

As an extractant has been used the n-methyl pyrrolidon (NMP) and its ion-liquid typed solvent containing morpholineformiate (NFM). Extraction process with NMP is realized in 3 stages. Defined that the amount of aromatic hydrocarbon in the content of fraction decreases from 16 % nearly to 1-2 % by taking NMP:df=3:1.

Additionally the diesel fraction has been extracted with help of morpholineformiate extractant. The influence of different factors as temperature, contact period, ratio of components to the process of selective treatment of diesel fraction has been studied and the optimal condition has been selected. Determined that the maximum treatment of diesel fraction from aromatic hydrocarbons and sulfur compounds is provided when morpholineformiate used as extractant. The optimal condition of extraction process of the diesel fraction with mentioned extractant: DF:NFM=1:3 (weight ratio), contact period – 3 hours, temperature – 60 °C. The amount of sulfur in fraction content has decreased from 0,09% to 0,03% during the extraction process.

The diesel fraction that partially treated from aromatic hydrocarbons and sulfur compounds by extraction method has been purified from the residua amount of sulfur content by the way of sulfurization with concentrated H<sub>2</sub>SO<sub>4</sub>. Then the diesel fraction has been oxidized in the co-catalytic presence of Cr and Mn salts of natural oil acids and has been obtained the mixture of SPA and OPA with high yield. Determined that the acid number of oxidate (oxidation products-alcohols, aldehydes, ketones, acids and oxyacids mixture) obtained by taking the ratio of salt Cr:salt Mn =3:1 (rather than weight 0,2%) is 65 mgKOH/g. The yield of SPA (for oxidate) is 5%, but the yield of OPA is 47% that removed from oxidate obtained in the presence of mixture of these catalysts (SPA + OPA =52%).

Thus, according to the obtained results we can note that the extraction method with solvents of ion-liquid type is very important in selective treatment of diesel fraction from aromatic hydrocarbons. Our researches on this field are going on.

**Keywords:** Catalytic oxidation, Extraction, Ionic liquid.

## Effect of Activation Temperature on Properties of Activated Carbon From Orange Peel by Zinc Chloride

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Activated carbons have widely used as adsorbents because of its high adsorptive capacity. Moreover, activated carbons are usually used in the separation and purification for aqueous solutions. Hence, activated carbons have played an important role in the chemical, pharmaceutical and food industries. Activated carbons can be produced by physical or chemical activation. Chemical activation is preferred to physical activation owing to the higher yield, simplicity, lower temperature, shorter activation and good development of the porous structure. Chemical activation involves reacting the raw material with chemical such as ZnCl<sub>2</sub>, KOH, HNO<sub>3</sub>, H<sub>3</sub>PO<sub>4</sub>, H<sub>2</sub>SO<sub>4</sub>, and K<sub>2</sub>CO<sub>3</sub>. Chemical activation by zinc chloride (ZnCl<sub>2</sub>) improves the pore development in the carbon structure and because of the effect of chemicals; the yields of carbon are usually high. In this study, activated carbons were prepared by chemical activation with zinc chloride (ZnCl<sub>2</sub>) of the orange peel. The influence of activation temperature on the yield, proximate and ultimate analysis results of the activated carbons was investigated. This purpose, the orange peel was activated at temperatures ranging from 500 to 900 °C, heating rate of 5 °C min<sup>-1</sup> and a ZnCl<sub>2</sub>:orange peel impregnation ratio of 3:1 under nitrogen atmosphere (150 cm<sup>3</sup> min<sup>-1</sup>). Orange peel sample contains 2.8% ash and 82.7% volatile matter. Fixed carbon content was obtained as 14.5% by finding the difference and the moisture content is 3.7%. All the values were expressed on a dry basis by weight percentage. The results showed that both yields and chemical properties of the activated carbon were significantly affected by the activation temperature.

**Keywords:** Orange peel, Zinc chloride, Activated carbon, Characterization.

## Horizontal and Vertical Optical Misura® Dilatometers

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Dilatometers will facilitate measurement of the coefficient of thermal expansion (CTE), softening point, phase and/or glass transition (T<sub>g</sub>). The measurement of the sintering curve even in materials with high percentage of glassy phase, like traditional ceramics, is possible, thanks to the complete absence of contact with the specimen. TA Instruments offers a line of optical dilatometers both in vertical and horizontal orientation. The specimens are measured by the image that the sample reflects on the CCD when it is lit by a direct beam of light. The instrument makes an image analysis of the extreme borders of the specimen. Samples such as thin films, incoherent materials, and irregular shaped samples can be measured. The available temperature is ambient to 1600°C. Examples from high temperature measurements of ceramics and glass will be presented.

**Keywords:** Dilatometer, Optical, Horizontal, Vertical, Coefficient of thermal expansion, CTE. Sintering, Phase transition, Stress relaxation.

## Scratch test of Silica and PVB Coatings Deposited on Sandblasted Glass

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In this work, we investigated the failure mechanism under scratch testing of sandblasted glass samples coated with silica and PVB coatings. To correct the surface defects generated by sand impacts on a soda lime glass. Thin layer of silica by sol-gel technique and another thicker layer of PVB were deposited on sandblasted samples. The surface damage was made by erosion tests using different sand masses (50 - 200 g). After sandblasting, the total roughness increases and reaches 11.75  $\mu\text{m}$  for a sand mass of 200 g. Meanwhile, the optical transmission decreases from 91.4% (initial value) to 13%. After deposition of silica and PVB layers, the total roughness decreases to 2  $\mu\text{m}$ , and the optical transmission increases significantly up to 88%.

The adhesion properties of the silica and PVB coatings were evaluated using a CSM Micro Scratch Instrument Scratch Tester. The scratch indenter was a diamond Rockwell with a radius of 200  $\mu\text{m}$ . The scratch length was set to be 5 mm. The applied load was progressively increased from 0.03 to 7 N at a rate of 2.5 mm/mn. Acoustic emission signals were recorded during the test. The scratch equipment enabled the measurement of the normal and tangential forces and the penetration depth. After the test a critical load  $L_c$  where a particular failure mode occurred was determined by post-mortem observation of the scratch track using an optical microscope.

The results showed that PVB layer failed by plastic deformation, the critical load of onset delamination was 0.6 N. However, the scratch track on silica layer was formed by adjacent closed rings. The critical load of delamination was 6.5 N.

**Keywords:** Erosion, Glass, Roughness, Sol-gel technique, Scratch test.

## Fundamental Equations of State for Fluorobenzene and For Mixture of Benzene with Fluorobenzene (C<sub>6</sub>H<sub>6</sub> – C<sub>6</sub>H<sub>5</sub>F)

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Based on the the most reliable experimental data, a fundamental equation of state for fluorobenzene has been developed. This equation is in the form of the reduced Helmholtz free energy and takes the reduced density and reduced temperature as variables.

$$\frac{a(\rho, T)}{RT} = \frac{a^0(\rho, T) + a^r(\rho, T)}{RT} = \alpha^0(\delta, \tau) + \alpha^r(\delta, \tau) \quad (1)$$

where  $a(\rho, T)$  is the Helmholtz free energy;  $\alpha^0(\delta, \tau)$  is the reduced Helmholtz energy in the ideal-gas state;  $\alpha^r(\delta, \tau)$  is the residual part of the reduced Helmholtz energy;  $\delta = \rho/\rho_r$  is the reduced density;  $\tau = T_r/T$  is the inverse reduced temperature; and  $\rho_r, T_r$  is reducing parameters.

The ideal-gas reduced Helmholtz energy, in dimensionless form, can be represented by

$$\alpha^0(\delta, \tau) = \frac{h_0^0 \tau}{RT_c} - \frac{s_0^0}{R} - 1 + \ln \frac{\delta \tau_0}{\delta_0 \tau} - \frac{\tau}{R} \int_{\tau_0}^{\tau} \frac{c_p^0}{\tau^2} d\tau + \frac{1}{R} \int_{\tau_0}^{\tau} \frac{c_p^0}{\tau} d\tau \quad (2)$$

where  $\delta_0 = \rho_0/\rho_c$  and  $\tau_0 = T_c/T_0$ .  $T_0$  and  $p_0$  are arbitrary constants, and  $\rho_0$  is the ideal gas density at  $T_0$  and  $p_0$  ( $\rho_0 = p_0/(T_0 R)$ ).  $h_0^0$  is the ideal-gas enthalpy at the reference state, and  $s_0^0$  is the ideal-gas entropy at the reference state.

To describe the residual part of the reduced Helmholtz energy, an optimized functional form was developed

$$\alpha^r(\delta, \tau) = \alpha_{Pol}^r + \alpha_{Exp}^r = \sum n_i \tau^{t_i} \delta^{d_i} + \sum n_i \tau^{t_i} \delta^{d_i} \exp(-\delta^{p_i}) \quad (3)$$

where  $\delta = \rho/\rho_r$ ;  $\tau = T_r/T$  are reducing parameters.

The proposed equation satisfies the critical conditions and Maxwell rule, shows correct behavior for the ideal curves and for the derivatives of the thermodynamic potentials, and allows the calculation of all thermodynamic properties including phase equilibrium of fluorobenzene over a temperature range from the triple point to 700 K with pressures up to 100 MPa.

Based on the new experimental data of system C<sub>6</sub>H<sub>6</sub> – C<sub>6</sub>H<sub>5</sub>F, a multiparameter equation of state has been developed. This equation is in the form of the reduced Helmholtz free energy and takes the reduced density and reduced temperature as variables. Pseudocritical properties that are defined based on the mixing rules were used as reducing parameters. Binary interaction coefficients, which are included in the mixing rules, were determined by the fitting of experimental data using a method of random search.

$$\alpha(\delta, \tau, x) = \alpha^0(\rho, T, x) + \alpha^r(\delta, \tau, x) \quad (4)$$

where  $\alpha(\delta, \tau, x)$  is the mixture Helmholtz energy;  $\alpha^0(\rho, T, x)$  is the reduced Helmholtz energy in the ideal-gas state;  $\alpha^r(\delta, \tau, x)$  is the residual part of the reduced Helmholtz energy;  $\delta = \rho/\rho_r(x)$ ;  $\tau = T_r(x)/T$ ;  $\rho_r(x), T_r(x)$  is the reducing parameters suggested by Kunz and Wagner

$$\frac{1}{\rho_r(x)} = \sum_{i=1}^N x_i^2 \frac{1}{\rho_{c,i}} + \sum_{i=1}^{N-1} \sum_{j=i+1}^N 2x_i x_j \beta_{v,ij} \gamma_{v,ij} \frac{x_i + x_j}{\beta_{v,ij}^2 x_i + x_j} \frac{1}{8} \left( \frac{1}{\rho_{c,i}^{1/3}} + \frac{1}{\rho_{c,j}^{1/3}} \right)^3 \quad (5)$$

$$T_r(x) = \sum_{i=1}^N x_i^2 T_{c,i} + \sum_{i=1}^{N-1} \sum_{j=i+1}^N 2x_i x_j \beta_{T,ij} \gamma_{T,ij} \frac{x_i + x_j}{\beta_{T,ij}^2 x_i + x_j} (T_{c,i} \cdot T_{c,j})^{0.5} \quad (6)$$

where  $T_{c,i}$  and  $\rho_{c,i}$  is the critical properties of component  $i$ ;  $x_i$  is the mole fraction of component  $i$ ;  $\beta_v, \gamma_v, \beta_T, \gamma_T$  is the binary interaction coefficients.

The ideal part can be defined by the following relation

$$\alpha^0(\rho, T, x) = \sum_{i=1}^N x_i [\alpha_{0i}^0(\rho, T) + \ln x_i] \quad (7)$$

where  $\alpha_{0i}^0(\rho, T)$  in the ideal part of Helmholtz energy of component  $i$ .  
The excess part can be defined by the following relation

$$\alpha^r(\delta, \tau, x) = \sum_{i=1}^N x_i \alpha_{0i}^r(\delta, \tau) + \sum_{i=1}^{N-1} \sum_{j=i+1}^N x_i x_j F_{ij} \alpha_{ij}^r(\delta, \tau) \quad (8)$$

where  $\alpha_{0i}^r(\delta, \tau)$  is the excess part of Helmholtz energy of component  $i$ ;  $\alpha_{ij}^r(\delta, \tau)$  is the excess function

$$\alpha_{ij}^r(\delta, \tau) = \sum_{k=1}^{K_{pol,ij}} n_{ij,k} \delta^{d_{ij,k}} \tau^{t_{ij,k}} + \sum_{k=K_{pol,ij}+1}^{K_{pol,ij}+K_{exp,ij}} n_{ij,k} \delta^{d_{ij,k}} \tau^{t_{ij,k}} e^{-\eta_{ij,k}(\delta-\varepsilon_{ij,k})^2 - \beta_{ij,k}(\delta-\gamma_{ij,k})} \quad (9)$$

The proposed equation of state allows the calculation of all thermodynamic properties of system  $C_6H_6 - C_6H_5F$  including phase equilibrium.

**Keywords:** Fluorobenzene, Equation of state, Helmholtz free energy, Thermodynamic properties.

## Determination of the Solid-Liquid Equilibrium of Mixtures of Sugar Alcohols for their Use as Phase Change Materials

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The use of phase change materials (PCM) based latent heat thermal energy storage (LHTES) systems can improve the energy efficiency of sustainable energies. Sugar alcohols are widespread materials that can be considered as promising candidates to be used as PCMs. However, their melting temperatures are too high to use them directly in thermal storage systems for building technologies, such as residential micro-CHP or solar thermal systems. In order to overcome this situation, eutectic mixtures of the materials were studied. The phase diagrams were calculated by the UNIFAC group contribution method. Three suitable new mixtures were identified, comprised by Erythritol and Xylitol; Erythritol and Sorbitol; and Xylitol and Sorbitol. Their melting temperatures lie within the temperature range herein sought (60-90°C). This modeling methodology showed to be suitable and can be applied to develop new PCMs. However, the mixtures identified underwent vitrification upon cooling. Therefore, research efforts should be done to develop techniques to promote the crystallization of the materials involved.

**Keywords:** Phase change materials, Sugar alcohols; Thermal energy storage, Eutectic mixture, Unifac.

## **Research of the Level of Hydration of the Low-Main Cements and Phase Composition of the Stone on Their Basis**

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Low key limes of the cements are characterized by slower progress of hydration and hardening of cements oolitovogo than that of cements from low fundamental clinkers, derived from raw materials in the region of Kizilkumskogo, along with an increased number of S2S (25-52%), also contain relatively high amounts of C3a and S4AF (6.5 to 7.0 and 14.5 15.5% ÷ is a specific theoretical and practical study of the hydration of the cement activity in the process of formation of a cement stone.

**Keywords:** Polymer composition, Chemical reactant, Physico-chemical properties of drilling fluids.

## **Manufacturing of the Additional Cements with Using Local Rocks and Wastes of Asbestos-Cement Production**

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With Kolbasova , Timasheva , Atakuzieva , MI Iskandarova works they found that cement stone of binding to particulate carbonate fillers (in particular, with limestone, shell limestone, etc.) on the strength parameters, resistance to aggressive environments and frost, not inferior without adding cements. Given that the presence of magnesium oxide MgO cement in a large amount (more than 5 %) is undesirable, dolomitic limestone and dolomite have found limited use in the cement industry as raw material component mixture to obtain a clinker.

Therefore, in this study the possibility of using local dolomite rocks as filler in it to save grinding clinker content of the cement and reducing its cost. Research hypothesis is that an cube-shaped grains of ground dolomite, its presence in the cement as a filler must provide high technological properties of cement and enhanced its adhesion to the cement particles.

**Keywords:** Cement, Clinker, Dolomit.

## **Influence of Composition on the Thermal and Mechanical Properties of Elastomeric Polyamide Blends For Industrial Applications**

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Several industrial applications require specific behavior under charge, which can be obtained by blending of polymeric components. The material answers may be achieved by the characterization of functional properties. The diversity of applications in the field of automotive materials, electrical and thermal insulators, fabrication of membranes, gaskets and sealants asks detailed study on some elastomer/polyamide 6 systems.

Starting from PA6 as basic material, this paper was accomplished on its various blends with EPDM (ethylene-propylene-diene terpolymer, ethylene 70%; Propylene 29.5% and ENB 0.5% ), EXXELOR (medium viscosity semi-crystalline ethylene copolymer functionalized with maleic anhydride), LOTARDER (random terpolymer of ethylene, ethyl acrylate and maleic anhydride) and MARFRAN (mixture polypropylene, polyethylene ethylene vinyl acetate) and SEBS additives (styrene-ethylene/butyl-styrene) bloc copolymer), whose mixing proportions cover the following PA6/elastomer ratios: 100/0, 90/10, 80/20 and 70/30.

The preparation of compounds was performed by mixing in a Brabender twin screw extruder with L/D40. Samples for analysis were then obtained by injection into a melt injection machine Dr. Boy. The specimens were subjected to tensile and bending mechanical tests and thermal tests for predicting thermal endurance.

In the case of three-point bending strength tests the increasing of elastomeric content determines lower values of mechanical resistance. The behavior of studied polymeric systems reveals different relative decreases in the resistance level of three-point bending strength:

- for PA6/EPDM blends, it decreases from 23% (PA6/10 % EPDM) to 54% (PA6/20 % EPDM) and respectively 64% (PA6/30 % EPDM) relative to pristine PA6,
- for PA6/ EXXELOR blends, the diminutions are of 45% (PA6/5 % EXXELOR), 65 % (PA6/10 % EXXELOR) and 66% ((PA6/20 % EXXELOR) relative to pristine PA6,
- for PA6/LOTARDER blends, the same property falls down by 32% (PA6/5 % LOTADER ), 48% (PA6/10 % LOTARDER) and 62% (PA6/20 % LOTARDER) relative to pristine PA6,
- for PA6/MARFRAN blends, the strength decreases by 39% (PA6/5 % MARFRAN), 40% (PA6/10 % MARFRAN) and respectively 66%(PA6/20 % MARFRAN) relative to pristine PA6.

It can be concluded that the optimal variant of composition is the formulation PA6/5 % LOTADER. The tensile strength tests revealed additionally the alteration of tensile strength as elastomeric content is enhanced. The tensile strength becomes:

- 21% for PA6/10 % EPDM, 36% for PA6/20 % EPDM and 54% for PA6/30 % EPDM relative to neat PA6,
- 36% for PA6/5 % EXXELOR, 37 % for PA6/ 10 % EXXELOR and 43% for PA6/ 20 % EXXELOR relative to pristine PA6,
- 21% for PA6/5 % LOTARDER, 31% for PA6/10 % LOTARDER and 36% for PA6/20 % LOTARDER relative to pristine PA6,
- 32% for PA6/5 % MARFRAN, 36% for PA6/10 % MARFRAN and 39% for PA6/20 % MARFRAN relative to pristine PA6.

The main conclusion regards that the optimal variant is the compound PA6/5 LOTADER.

The thermal endurance tests indicated the possibility of successful using of PA6/elastomers compounds in the same conditions as PA6 basic material, with a plus in terms of the degree of elasticity (due to additions of various elastomers), allowing identification of applications for cable insulation.

After achieving thermal endurance tests found that temperature indices are quite close to compounding studied, this being due to the majority of each mixture component.

It can be concluded that the thermally optimal variant is compounded PA/20 EPDM.

This research is the basic part of a detailed study concening the preparation of cable insulation having improved mechanical and thermal performances.

**Keywords:** Cable insulation, Mechanical resistance.

### **Rheological Characterization of the Modified Crude Oil of the Field of Tin Fouyetabankort (Illizi, Southern Algeria)**

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An optimal dimensioning of a pipe transportation network system of the crude oil requires the knowledge of the laws of behavior of the transported fluid. From the rheological point of view, the crude oils can be classified in the general field of the suspensions. Crude Oil is a mixture of various chemical components which can vary from one field to another. This study is purely experimental; its main objective is to carry out a rheological characterization of the crude coming from the field of the Northern sector of Tin Fouye Tabankort (Illizi, southern Algerian). This crude oil was modified by the addition of additive concentrations to increase its viscosity; the additive is based on oil called Geltone. The diluted solutions are prepared from a diluted mother solution. The physicochemical characteristics of the crude oil used, such as the density, the water content, and the asphalt were determined on site. The tests were carried out using a HAAKE-Viscotester-VT550, a Couette type rotation viscometer of two coaxial cylinders. The study of the rheological behavior of the modified crude oil was undertaken by using several concentrations of the Geltone additive. The rheological behavior of the crude oil changes according to the thermal and mechanical flowing conditions. The viscometer is equipped with a thermostated bath, which allowed the temperature to vary between 20 and 50 °C. A significant influence on the rheological parameters (the stress threshold of flow, the consistency,  $k$  and the flow index,  $n$ ) was recorded when the temperature increases. A correlation was established between the viscometric data and the rheological models of Ostwald De Waele, Casson, and Herschel-Bulkley without omitting that of Bingham by calculating the coefficient of correlation. While the parameters of Ostwald De Waele, Bingham and Casson lead to non satisfactory results, the model of Herschel-Bulkley makes it possible to corroborate the results satisfactorily. It can be said that the crude oil of the field of Tin Fouye Tabankort behaves like a non Newtonian fluid with a threshold of flow satisfying the rheological model of Herschel-Bulkley.

**Keywords:** Crude oil, Rheology, Polymers solutions.

### Heat Flow Meter-Fox 50

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The thermal conductivity of a specimen ( $\lambda$ ) is determined by measuring the heat flux, specimen thickness, and temperature difference across the specimen. In each component of the thermal conductivity equation the instrument provides extremely precise readings, .6mV resolution on integrating high output heat flux transducers, 0.001" precision in thickness measurement, and 0.01°C temperature control and resolution. They are designed for testing the thermal conductivity of materials in the conductivity range of 0.1W/mK to 10W/mK. The use of two heat flux transducers accelerates the tests and produces more accurate results. High-output Heat Flow Meters (HFMs, or transducers), developed are bonded to the surfaces of both plates. Samples up to 63 mm in diameter and from 0 to 25 mm thick are tested in accordance with ASTM C 518 and ISO 8301. The available temperature range is -10°C to 300°C.

**Keywords:** Heat Flow Meter, Thermal Conductivity.

### New Flame Retardant Phosphorus-Containing Polymers with Liquid Crystalline Properties. Synthesis and Characterization

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In this work we describe the successful synthesis of two new thermotropic liquid crystalline phosphorus-containing polymers. The polymers were characterized by means of FTIR, <sup>1</sup>H NMR, differential scanning calorimetry, polarized light microscopy, wide-angle X-ray diffraction and thermogravimetric analysis. Thermogravimetric analysis was performed in nitrogen atmosphere by heating the samples over a range of temperature from 25 °C to 700 °C using five different heating rates. Thermal decomposition of polymers took place in one step. Effect of the heating rate on TG and DTG curves was also presented. Activation energy and pre-exponential factor were obtained by Freeman-Carroll, ASTM E1641 and Kissinger methods. The kinetic parameters calculated by Kissinger method were the same for the whole degradation process, where as in the ASTM E1641 method, the apparent activation energy and the apparent pre-exponential factor varied with the conversion degree and revealed the complex mechanism of reaction that occur during the degradation process.

**Keywords:** Phosphorus-containing polymers, Liquid crystalline properties, Thermal stability, Kinetic study.

**Acknowledgements:** The authors acknowledge the financial support of CNCSIS–UEFISCSU, Project Number PN-II-RU-TE-0123 nr. 28/29.04.2013.

## **A New Generalized Correlation of Viscosity Coefficient of Complex Hydrocarbon Mixtures In A Wide Range of Temperatures and Pressures**

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Analysis of the most reliable and universal methods of calculation of viscosity coefficient of complex hydrocarbon mixtures has shown that most of them are applicable only in the liquid phase over a temperature range from 250 to 700 K with pressures up to 100 MPa. For gas phase and supercritical region the reliable methods of predictive calculation are not available.

This report presents two new generalized predictive correlations for the calculation of viscosity coefficient of complex hydrocarbon mixtures of different origins over a temperature range from hardening to 700 K with pressures up to 100 MPa in the liquid and gas phases and in the supercritical region. The generalization is made within the framework of the extended three-parameter corresponding states principle and takes the reduced density and reduced temperature as variables. For the density calculation, the method that built on two generalized multiparameter equations of state is used. These equations of state developed by the authors, and are applicable in a specific range of parameters.

The first equation for the calculation of the viscosity coefficient is presented in the form of a double number for temperature and density, consisting of both polynomial and exponential terms. Optimization of the numbers of terms, temperature and density exponents place simultaneously in a nonlinear form using the method of random search. The acentric factor was chosen as the determining criterion of similarity. In the second equation a special coordinate transformation is used. In the report discusses the various options for selecting reference points to determine the dimensionless variable.

The proposed method has been tested by comparison with experimental data on the viscosity coefficient of more than 200 substances of oil and gas condensates of various fields, products of their single and structural processing and so on.

Testing has shown that the new methods are characterized by significantly higher precision of calculation of viscosity coefficient and wider range of applicability.

**Keywords:** Viscosity, Equations of state, Acentric factor, Hydrocarbon.

## **A New Generalized Correlation of Thermal Conductivity Coefficient of Complex Hydrocarbon Mixtures In A Wide Range of Temperatures and Pressures**

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Analysis of the most reliable and universal methods of calculation of thermal conductivity coefficient of complex hydrocarbon mixtures has shown that most of them are applicable only in the liquid phase over a temperature range from 250 to 700 K with pressures up to 100 MPa. For gas phase and supercritical region the reliable methods of predictive calculation are not available.

This report presents new generalized predictive correlation for the calculation of thermal conductivity coefficient of complex hydrocarbon mixtures of different origins over a temperature range from hardening to 700 K with pressures up to 100 MPa in the liquid and gas phases and in the supercritical region. The generalization is made within the framework of the extended three-parameter corresponding states principle and takes the reduced density and reduced temperature as variables. For the density calculation, the method that built on two generalized multiparameter equations of state is used. These equations of state developed by the authors, and are applicable in a specific range of parameters.

Equation for the calculation of the thermal conductivity coefficient is presented in the form of a double number for temperature and density, consisting of both polynomial and exponential terms. Optimization of the numbers of terms, temperature and density exponents place simultaneously in a nonlinear form using the method of random search. The acentric factor was chosen as the determining criterion of similarity. In the report discusses the possibility of applying other criterion of similarity.

The proposed method has been tested by comparison with experimental data on the thermal conductivity coefficient of more than 300 substances of oil and gas condensates of various fields, products of their single and structural processing and so on.

Testing has shown that the new method is characterized by significantly higher precision of calculation of thermal conductivity coefficient and wider range of applicability.

**Keywords:** Thermal conductivity, Equations of state, Acentric factor, Hydrocarbon.

## Hexavalent Chromium (Cr (VI)) Adsorption Behavior Onto Poly(Pyrrole-Co-Ortho-Anisidine) Nanocomposite: Thermodynamics and Kinetics Study

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The removal of heavy metals from wastewater is an important and widely studied research area. Among these heavy metals, Cr is considered as a major pollutant. Recently, conducting polymers such as polypyrrole, polyaniline and its composites have become under attention as exciting new adsorbing materials due to their high adsorption capacity and requires a relatively short period of time to remove Cr(VI) from aqueous solution.

In the present study, poly(pyrrole-co-ortho-anisidine) copolymer was synthesized chemically by simultaneous polymerization of pyrrole and ortho-anisidine monomers in presence of FeCl<sub>3</sub>, (NH<sub>4</sub>)<sub>2</sub>S<sub>2</sub>O<sub>8</sub> as oxidants, and was used as an adsorbent to remove hexavalent chromium (Cr(VI)). A prepared poly(pyrrole-co-ortho-anisidine) powder was characterized by FT-IR, UV-Vis, XRD and SEM analysis. FT-IR and UV-Vis studies confirmed the formation of the copolymer which presents the combination between anisidine and pyrrole units. SEM and XDR confirmed also the nanostructure morphology of the copolymer.

Adsorption capacity of hexavalent chromium (Cr(VI)) onto poly(pyrrole-co-ortho-anisidine) copolymer was carried in a batch system by considering the effects of various parameters like contact time, initial concentration of Cr(VI), pH, dose of copolymer and temperature. Cr(VI) removal is pH dependent and found to be maximum at pH 3.0. Adsorption equilibrium was achieved within 20-150 min for initial Cr(VI) of 50-150 mg/L. XPS studies confirmed the presence of Cr (III) on the surface of adsorbent and suggested that ion exchange and reduction of Cr (VI) into Cr (III) on the surface of the copolymer may be possible. Adsorption kinetic was best described by the pseudo-second-order rate model and the isotherm data fitted well to the Langmuir isotherm model. Thermodynamic parameters such as standard enthalpy ( $\Delta H^\circ$ ), standard entropy ( $\Delta S^\circ$ ) and standard Gibb's free energy ( $\Delta G^\circ$ ) were evaluated. According to the thermodynamics, the adsorption process is spontaneous and endothermic in nature which means that the adsorption capacity increases with increasing temperature. Regeneration and reusability of the poly(pyrrole-co-ortho-anisidine) nanocomposite was tested for five successive adsorption-desorption cycles in which it was found that there is no loss of original capacity in the first three cycles. These results confirm that the material can be considered as an alternative adsorbent for the removal of Cr(VI) from aqueous solution.

**Keywords:** Poly(pyrrole-co-ortho-anisidine), Adsorption, Hexavalent chromium, Kinetics, Thermodynamics.

## **The Assessment of Curing Parameters and Mechanical Properties of Epoxy Resins Modified with Polyurethane based on Polycarbonate Diol**

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Due to the high reactivity of epoxy group and specific structure of segmented polyurethanes they are an excellent combination for hybrid material preparation. The objective of our work was to synthesize epoxy resin materials based on 2,2-bis(4-glycidyloxyphenyl) propane and thermoplastic polyurethanes. In the first step the segmented polyurethane elastomers (based on aliphatic hexamethylenediisocyanate, polycarbonate macrodiol and tetramethylene glycol as chain extender) were prepared by one step procedure using the. The hard segment content in elastomer samples was varied (20, 25 and 30 wt.%). In the next step the hybrid materials were prepared by reaction of melted thermoplastic polyurethane and epoxy resin in the presence of polyoxypropylenediamine as a crosslinking agent. The content of segmented polyurethanes in the reaction mixture was varied (5, 10 and 15 wt.%). The curing was followed by differential scanning calorimetry in the temperature interval from ambient to 300°C at three heating rates. Kinetic parameters of network formation reaction was determined using Friedman differential procedure and two integral procedure (Kissinger–Akahira–Sunose, Ozawa–Flynn–Wall). It was estimated that with the increase of polyurethane hard segments content the temperature maximum of the crosslinking reaction was shifted from 205 to 179°C. The significant differences was obvious for the degree of conversion higher than 60 %, where the activation energies were higher. Mechanical properties of obtained samples were evaluated from stress-strain measurements. The increase of hard segment content in polyurethane elastomer influenced the improvement of mechanical properties of prepared hybrid materials (elongation at break and tensile strength).

**Keywords:** Curing kinetic, Hybrid materials, DSC, Composites.

## Morphology and Thermal Properties of Chitosan/Bentonite Beads Prepared for Dye Removal

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Four different batches of chitosan/organically modified bentonite composite beads for dye removal were prepared. Molarity of NaOH, volume of chitosan solution and clay powder content were varied. Morphology of composite beads was studied using scanning electron microscopy (SEM). Thermal properties were investigated by thermogravimetry coupled with differential scanning calorimetry (TG-DSC) and differential scanning calorimetry (DSC). SEM results showed that beads prepared in the solution with higher NaOH concentration have more irregular spherical shape. On the basis of morphology results, it was estimated that method of chitosan/bentonite beads preparation significantly affects their morphology as well as the interaction of the boundary layer of the solid phase with water. The decomposition of the chitosane matrix starts at around 230 °C. All processes detected in TG curves are endothermic up to ~250 °C. Above mentioned temperature, the observed decomposition in air is highly exothermic for the samples prepared at lower NaOH content. The exothermic effects accompanying the decomposition are significantly lower for composites prepared at higher NaOH concentration, in accordance with their more compact structure which prevents the good contact of the beads with air. Analyzing DSC curves of all chitosan/bentonite samples, it was found that glass transition temperature of obtained beads is independent on the preparation procedure (144 °C). A significantly higher enthalpy change (393.6 J/g) for water evaporation was found for the sample with highest clay powder content, prepared at lower NaOH concentration. It was concluded that surface changes of chitosan/bentonite composite beads depend on the used preparation method. The synthesis procedure did not affect water adsorptivity of the obtained samples. It was assessed that mechanism of water evaporation strongly depends on bentonite content in the samples prepared at lower NaOH concentration.

**Keywords:** Chitosan, Dye removal, Composite beads, Thermal properties.

## Thermophysical Properties of Date Palm Fiber Reinforced Thermoset Matrix

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The development of high performance engineering products made from natural resources is increasing worldwide, due to renewable and environmental issues. Among the many different types of natural resources, date palm wood has been extensively exploited. The use of date palm fiber as reinforcing phase in thermoset matrix has been reported in this study. The thermophysical properties of the resulting composites were characterized experimentally. The effects of the fibers concentrations on the composite properties were studied. The thermal conductivity of the composite has been also investigated using 3D finite element computation. The effect of the filler size on the effective thermal conductivity of composites was considered. The present work compares theoretical and the measured thermal conductivities for various samples. It was found that the thermal conductivity of the composite decreases with fiber loading.

**Keywords:** Composites, Date palm fiber, Thermoset matrix, Thermal conductivity.

## Property Libraries and Software for Seawater, Steam, Water, Ice, Humid Air, and other Working Fluids for Calculating Desalination and Related Processes

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The program libraries for calculating the thermophysical properties for seawater, steam, water, ice, humid air, combustion-gas mixtures and other working fluids are designed for practical use by engineers who calculate desalination and related processes. The property libraries can calculate thermodynamic properties, transport properties, thermodynamic derivatives and inverse functions.

For simulating desalination processes at high temperatures, pressures, and salinities, the property library *LibSeaWa* for seawater can be used. It calculates thermodynamic and colligative properties from the IAPWS Industrial Formulation for Seawater. The range of validity in temperature and salinity of this property library is enlarged by using algorithms described by Hömig, Fichtner-Handbook [2]. So, the library *LibSeaWa* can be used at temperatures  $T$  from 261 K to 493 K, pressures  $p$  from 0.2 kPa to 100 MPa, and salinities  $S$  from 0 (pure water) to 200 g kg<sup>-1</sup>. All thermodynamic properties such as density  $\rho$ , specific volume  $v$ , specific enthalpy  $h$ , specific isobaric heat capacity  $c_p$ , and specific entropy  $s$ , transport properties such as thermal conductivity  $\lambda$  and dynamic viscosity  $\eta$ , thermodynamic derivatives, and inverse functions from given quantities  $(p, h, S)$  and  $(p, s, S)$  are computed. In addition, boiling temperature  $T_b$ , freezing temperature  $T_f$ , and properties for brine-vapor mixtures are calculable. Furthermore, the property libraries *LibIF97* for water and steam, *LibIF97\_META* for metastable steam, *LibICE* for ice including melting and sublimation, *LibHuAir* for humid air also at high temperatures and pressures, and *LibHuGas* for humid combustion-gas mixtures also at high pressures are available. In addition, property libraries for a number of other working fluids such as for ORC working fluids, refrigerants, absorption-refrigerant mixtures, gas mixtures, carbon dioxide, and hydrogen are offered. The libraries contain the most recent and accurate algorithms for calculating thermodynamic and transport properties.

The following software solutions will be presented:

Add-In *FluidEXLGraphics* for Excel<sup>®</sup>,

Add-on *FluidLAB* for MATLAB<sup>®</sup>,

Add-on *FluidMAT* for Mathcad<sup>®</sup>,

Add-on *FluidDYM* for Dymola<sup>®</sup> (Modelica) and SimulationX<sup>®</sup>,

Add-on *FluidVIEW* for LabVIEW<sup>™</sup>, and

Add-on *FluidEES* for the Engineering Equation Solver<sup>®</sup>.

The program *FluidDIA* was developed for calculating and plotting large-size and camera-ready thermodynamic charts.

Steam tables are available for iPhone, iPad and iPod touch, and for Android smart phones and tablets.

The property software on Texas Instruments<sup>®</sup>, Hewlett Packard<sup>®</sup>, and Casio<sup>®</sup> pocket calculators is particularly interesting for students.

The properties of several working fluids can be calculated at our website:

[www.thermodynamics-zittau.de](http://www.thermodynamics-zittau.de).

**Keywords:** Seawater, Thermophysical properties, Property libraries.

## Performance Evaluation of Peanut Roasting Process at Continuous Type Infrared System

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In this study, the performance of roasting process of peanut at continuous type infrared system was evaluated in terms of energy/exergy analysis, and some quality changes occurred during process. The infrared roasting was performed in triplicate by using three different processing parameters; 3 different power applications (370.62, 567.83, 847.55 W) and 3 different processing times (3, 6 and 9 min) for the application distance of 10.5 cm (distances between samples and infrared unit). The weight loss, final total moisture content, final surface temperature and color (Hue angle) properties of roasted samples and the energy-exergy efficiencies of the process were selected as responses. The initial temperature of the sample was selected as a covariate factor. The temperature measurements of peanut samples for energy and exergy performance analysis were performed non-destructively. SAS V1.5 program was used for statistical evaluation.

The maximum exergy (49.53±6.29 %) and the maximum energy (49.10±4.26 %) yields were predicted for minimum process duration (3 min) and power application of 370.62 W. The weight loss varied between 0.3502±0.0505 % (370.62 W-3 min) and 2.8812±0.7961 % (567.83 W-9 min). The power-processing time interaction was statistically significant on color (Hue angle) property of peanut sample ( $p<0.05$ ). As the power level and the processing time increased, the Hue angle value of roasted peanut increased. The non-destructive temperature measurements were practical and instant method to provide temperature distributions on the surface of peanuts during roasting process.

The obtained results are aimed to be a source for industrial scale productions.

**Keywords:** Energy, Exergy, Peanut, Quality.

## Electrochemical Detection of Uric Acid Based on Polypyrrole/Iron Hexacyanoferrate Film Modified Iron Electrode

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Hollow microparticles of polypyrrole film doped by ferrocyanide anions  $\text{Fe}(\text{CN})_6^{3-}$  are successfully synthesized by chronoamperometric mode at 750 mV/(Ag/AgCl) onto iron electrode from an aqueous solution containing pyrrole monomer, potassium hexacyanoferrate  $\text{K}_4\text{Fe}(\text{CN})_6$  and potassium tetraoxalate ( $\text{C}_4\text{H}_3\text{KO}_8$ ). The characterization of the modified electrode was realised by XRD, FEG-SEM and EDX techniques. The electrochemical behaviour of the modified electrodes towards uric acid ( $\text{C}_5\text{H}_4\text{N}_4\text{O}_3$ ) oxidation was studied by cyclic voltammetry. The results show that the incorporation of  $\text{Fe}(\text{CN})_6^{3-}$  anions into the polypyrrole matrix improve significantly the electrocatalytic activity of this film. Different experimental conditions were optimized such as imposed potential, synthesis time,  $\text{Fe}(\text{CN})_6^{3-}$  ions concentration, and solution's pH. The PPy/FCN/Fe films have a potent and persistent electrocatalytic activity towards the oxydation of uric acid with detection limit of 25  $\mu\text{M}$  and a good linear relationship between the catalytic current and urique acid concentrations.

**Keywords:** Uric acid, Polypyrrole, Ferrocyanide, Electrochemical detection, modified electrode.

## Scanning Micro and Nano-Thermal Expansion Microscopy of Polymers: Application to the Determination of Surface Glass Transition Temperature in a Wood Cell Wall

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With the increasing development of vegetal fibre reinforced biocomposites, local measurement of mechanical properties of vegetal fibres has gained a strong interest. One outcome is the control of defibrization of lignocellulosic plant fiber during processing that could be used to enhance the mechanical properties of natural fiber composites (NFC). Understanding the structural and mechanical properties of fibres at a cell wall scale is still a big challenge from a technological point of view. However, thermomechanical properties of constitutive biopolymers are closely linked to the glass phase transition in polymeric materials. At a local scale, classical thermal methods such as differential scanning calorimetry (DSC) or thermomechanical analysis (TMA) do not provide information on specific features on or within the sample at a microscopic or sub-microscopic scale and are not adequate also due to the required and destructive heating of the whole sample mass. Among the different methods capable to characterize thermo-mechanical properties at this local scale, an alternative is the local thermal analysis (LTA) based on a modified atomic force microscopy (AFM). By using both, Wollaston tip (with a resolution around 1  $\mu\text{m}^2$ ) and nano tip as thermal probes (resolution close to sub-parietal length, i.e.  $<0,3 \mu\text{m}$ ), the scanning thermal microscope  $\mu\text{TA}$  2990 has first been studied in order to identify limitations, defects and to optimize its operation for scanning localized thermal analysis. Measurements were related to local thermal expansion of the sample surface. Both types of thermal probes have been implemented through different applications on academic homopolymer samples (PET polymers, PLA, PCL) prior to test on lignocellulosic cell wall (poplar). Results have been compared with classical DSC measurements. It establishes that local measurement of  $T_g$  is feasible at a micro and sub-microscale in a scanning mode. The in-depth thickness of the investigated zone being related to the tip size, the local thermal analysis concerns the free surface which behaves like a layer that is confined on the top surface of the bulk material, particularly true with the nanotip. When compared to DSC measurements, a local temperature depression is observed. It is not only depending on scanning parameters (scanning rate and normal load) but also, on the size of the excitation and on the molecular mass of the studied sample (in agreement with the literature). Using this approach, a profile of glass transition temperature ( $T_g$ ) has been obtained across the surface of a cell wall. The data analysis has also been extended in order to map the whole distribution of  $T_g$  on the surface. The influence of the water (plasticizer) content inside the cell wall on the thermomechanical properties has also been depicted at both scales. It has been observed that the  $T_g$  of lignin and hemicellulose were not detectable in situ at low water contents. The analysis on a wet sample showed that the surface  $T_g$  is lowest when the moisture content is high. A comparison between the results obtained with the Wollaston wire and the nanotip is presented and analysed.

**Keywords:** Scanning micro and nano thermal analysis, Local thermal analysis, Thermal expansion melting point, Surface glass transition temperature polymer, Biopolymer, Wood cell wall, Poplar.

## Solid State Synthesis of Spirothia(Selena) Pyeanes Containing Condensed Pyrasole Rings

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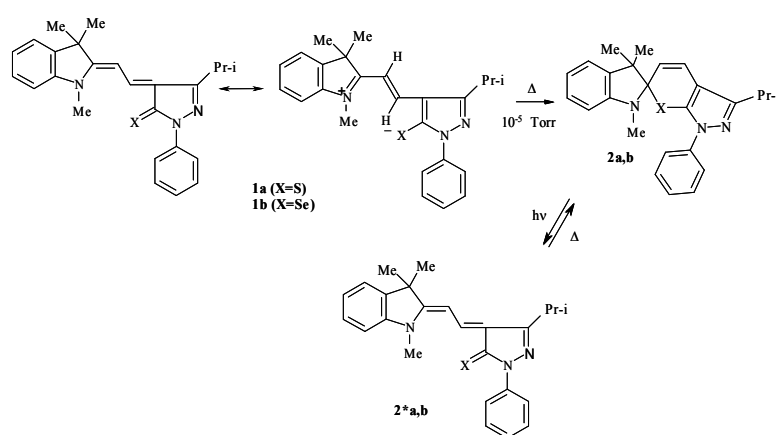
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Spiropyrans are the most promising and studied in detail type of organic photochromes. One of the most important task of their structural modifications associated with the use of spiropyrans as materials for optical information recording is the long wave shifting of the absorption spectra band of photo-colored (merocyanine) form.

We have obtained the indoline series spiropyrans containing 2H-thiapyran-and 2H-selenapyran moieties fused to heterocyclic rings during thermal vacuum deposition onto solid substrates (quartz, glass or KBr plates).



UV irradiation of the compounds **2** films activates their coloration through forming of photoinduced colored form **2\*a** (548 nm) and **2\*b** (585 nm). Irradiation with the visible light results the back reaction.

**Keywords:** Solid state synthesis, Spiropyran, Photocromism.

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## Study of Thermophysical and Mechanical Properties for New Composites Based on the Mortar and the Date Palm Wood to Use for Thermal Insulation in Buildings

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This work focuses on the experimental study of thermophysical and mechanical properties of mortar reinforced with date palm fibers (DPF) and to the evaluation of the possibility of using this material as insulating component in buildings. The thermal and mechanical investigations were carried out on different composite samples as a function of DPF loading and sizes. The biocomposites were obtained by mixing cement, sand, and water for several palm wood fibres concentrations. Drying tests were performed in the air for 48 hours in the moulds and 28 days after moulding.

The biocomposites are obtained by mixing portlandcement (CPJ-CEMII/A32.5), sand and water for several weightconcentrations of DPF (5, 10, 15, 20, 25 and 30%). The samples are performed by mixing the fibers, cement and sand in a mixer (40 turn/minutes) during 5 minutes. The dry mixing is necessary to homogenize the mixture, so water is then added gradually. Then, the mixture is versed into cubic molds (15cm × 15cm × 15cm). Drying of the samples was performed in the open air for 48 hours in the molds and 28 days after demoulding. Three types of composites were prepared:

MDP<sub>3.5mm</sub>: Mortar+ fine Fibers

MDP<sub>6.3mm</sub>: Mortar + Large Fibers.

MDP<sub>Mix</sub>: Mortar+ The mixture.

The thermal conductivity measurements were performed using a standard transient probe method based on hot wire method. The measurement is based on the analysis of temperature response of the sample to heat flow impulses.

The compressive strength was measured using a compression machine with standard NF EN196-1, type Controlab, precision of 0.001MPa, and loading speed of 0.5 MPa/S. All tested samples have undergone a surfacing.

This study shows that the thermal conductivity of mortar reinforced DPF biocomposites decreases with the increase of the fibers DPF loading. Moreover, the increase in DPF concentration leads to a decrease of mechanical properties. However, interesting mechanical strength values were obtained at low concentration wood (5%, 10%, and 15 %). For example, for fibers content of 5%, for MDP<sub>mix</sub>, the compressive strength reaches to 5 MPa.

Thus, as a conclusion, the optimum ratio of date palm fibers component is in the range of 5%-15%. For these fibers content, mechanical strength and thermal conductivity are consistent with the use of composites studied in the field of thermal insulation of buildings.

**Keywords:** Thermal properties, Mechanical properties, Date palm fibers, Thermal insulation, Composites.

## Synthesis of New Derivatives of Morpholinium with Acrylic and Metakrilovy Acids

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on the basis of synthesized 1-morpholinium-3-hloropropanol-2 interaction with acrylic acids received new reactive monomers. Physical and chemical properties of the synthesized monomers are set and their IR spectrums absorption are described.

Heterocyclic amines are reactive connections which are successfully used in synthesis of other classes of organic compounds, and also when receiving monomeric and on their basis of polymeric products. From heterocyclic amines morpholinium and its derivatives possess a broad spectrum of physiological activity. Besides they possess the increased protective properties in the conditions of acid atmospheric and biological corrosion of metals.

In particular, in operations it was proved that the component consisting of salt of morpholinium is inhibitor of acid corrosion, other authors synthesized quarternary ammoniyeve salts on the basis of morpholinium. Quarternary ammoniyeve salts are synthesized on response between tertiary amines on the basis of morpholinium and galogenproizvodny. In quality halogen of derivatives are used Benzylum chloride, butyl bromic, аллил bromic, ethylenechlorineguiderihn.

In operation results of researches by authors of perspective ionic liquids on the basis of morpholinium derivatives are considered. The ionic liquids on a basis the prizvodnykh of morpholinium with different cationic and anionic part are synthesized. All aforesaid sveditelstvoyer about relevance of synthesis and research of new organic compounds on the basis of morpholinium derivatives.

IR spectrums are removed on IK-Fourier a Perkin-Elmer firm spectrometer in liquid films or tablets from KBR. Purity of the synthesized connections controlled a method of a thin layer chromatography on Silufol plates: eluent-bensole-acetone, manifestation - vapors of iodine.

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Synthesis 1-morfolino-3-chlorine-2-propanola (1). 1 moles of morpholinium cooled, to -5 °C slowly added 1 mole of the cooled epichlorohydrin. After that a reactionary compound mixed within 12 hours in case of-5 about With and overtook in vacuum installation. The output 1-morfolino - 3-chlorine-2-propanola makes 75%.  $T_{\text{kip}}=64^{\circ}\text{C}$  (5 mm hg);  $n_D^{20}=1,4995$   $R_f=0,50$ .

Response of an eterifikation synthesized акрилатов. In the round-bottomed flask with a capacity of 250 ml supplied with the device of Dean-Starck loaded 1 mole of acrylic acid, (1% of total quantity of a reactionary compound) hydrochinone both 1 mole 1-morfolino-3-chlorine-2-propanola and the catalytic agent KU-2 slowly boiled within 3 hours. After response completion, a reactionary compound overtook in vacuum installation. Product yield (85%),  $T_{\text{kip}}=72^{\circ}\text{C}$  (6 мм.рт.ст);  $n_D^{20}=1,5208$ .  $R_f=0,48$

**Keywords:** Morpholinium, Acrylic acid, Metakrilovy acid, Hydrochinone, Monomer.

## **Models and Numerical Study of Thermal Conductivity For Conductive Particle Filled Polymer Composite**

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Physical properties of composites materials have won more importance in new system designs. The reasons of raising interest for polymer composites are electrical and thermal properties of polymer composites are close to metallic filler materials and the other physical properties are maintained for plastics. For many applications of materials, thermal properties of composites are needed. Determining the thermal conductivity of composite materials is very important for many industrial applications to simulate the heat transfer ability of composite materials. The thermal conductivity of materials is needed to define the optimum conditions along materials process and heat transfer of materials during applications. Some relationships are offered to determine composite materials' effective thermal conductivity. Many empirical, semiempirical, theoretical and numerical models were improved to predict the effective conductivity value depend on the dispersion, the each component characteristics and shape of the fillers.

In this study, thermal conductivity of polymer composite are investigated numerically, the obtained results are compared with the results calculated from the theoretical model. Numerical analyses are made in the finite-element program package ANSYS-Workbench in 3D for various filler materials. Graphene and aluminum were selected as filler material, high density polyethylene was selected as matrix material. For 3-D model, shape of the matrix material has been chosen as cube, whereas shapes of the filler material (particle) have been chosen as cube and sphere. The dimensions of the cube matrix material are fixed and have been taken as unity.

15 different theoretical thermal conductivity models, Series, Parallel, Geometric Mean, Maxwell, Cheng & Vachon's, Springer & Tsai's Model, Russell, Rayleigh's, Woodside & Messmer's Theoretical Model, Lewis & Nielsen's Semi-Theoretical Model, Hamilton & Crosser's, Bashirrow & Selenew, Zehner & Schlünder's, Meredith & Tobias Model and Hashin & Shtrikman have been investigated in this study.

It is found that type of filler material hasn't significant effect on thermal conductivity in low concentrations. Increasing concentration of filler material in matrix material, increasing difference between thermal conductivity values of graphene and aluminum high density polyethylene composites. The thermal conductive of aluminum-high density polyethylene is bigger than other. This result was foreseeable, because thermal conductivity of aluminum is higher than that of graphene.

The effective conductivities estimated by numerical analyses are compared with the results calculated from theoretical models. It may be seen that one of the closest models to numerical models are Hamilton and Crosser's and Hashin and Shtrikman's Theoretical Model. at low filler concentrations, there is good agreement between the numerical and theoretical estimations, the reason for this being that the fillers are evenly distributed in the matrix without any interactions between them.

**Keywords:** Thermal conductivity, polymer composite, models, ANSYS

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## Thermophysical Properties of Ionic Liquids with [NTf<sub>2</sub>]<sup>-</sup> Anions

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Typical ILs have a stable liquid range of over 300 K and have a very low vapor pressure at room temperature. As well known the ILs have been suggested as potentially “green” replacements for conventional organic solvents since they are nonvolatile (negligible vapor pressure), nonflammable, thermal stable, and recyclable. While scientific and technological interest in the properties of room-temperature ILs and their mixture with other fluids are rapidly increasing.

One of the most important advantages of ionic liquids is their physical-chemical properties and the phase behavior of the systems based on the ILs can be tuned/controlled by tailoring their structures. To do this, however, it is crucial to assume that ILs are the solvents of which the local structural (i.e., electronic and steric) features may be correlated with their physical-chemical properties and then deal with the effect of their cation and anion structures in altering the abovementioned properties and phase behavior.

A homological series of the 1-alkyl-3-methylimidazolium bis(trifluoromethanesulfonyl)imides or [C<sub>n</sub>mim][NTf<sub>2</sub>] where *n* = 2, 4, 6, 8 is the *even* chain length of the alkyl-imidazolium cation has been the most frequently investigated class of aprotic ionic liquids. In contrast, thermodynamic data on the representatives of this family with the odd alkyl chain-length, where *n* = 3, 5, 7, are practically absent in the literature, probably because the precursors for synthesis of these ionic liquids are hardly commercially available.

In this case, we have tried to find the community between even and odd alkenes number ionic liquids 1-C<sub>N</sub>mim-3-methylimidazolium (*N* = 2, 3, 4, 5, 6, 7, 8) with [NTf<sub>2</sub>]<sup>-</sup> anion using the molecular weight of ionic liquid. For this purpose, the (*p, ρ, T*) data of even alcohol number ionic liquids with bis(trifluoromethylsulfonyl)imide [NTf<sub>2</sub>]<sup>-</sup> anions ([EMIM][NTf<sub>2</sub>], [BMIM][NTf<sub>2</sub>], [HMIM][NTf<sub>2</sub>] and [OMIM][NTf<sub>2</sub>] at *T* = (273.15 to 413.15) K and pressures up to *p* = 140 MPa are reported with an estimated experimental relative combined standard uncertainty of  $\Delta\rho/\rho = \pm(0.01 \text{ to } 0.08) \%$  in density. The measurements were carried out with a newly constructed Anton-Paar DMA HPM vibration-tube densimeter, which based on the dependence of the period of oscillation of a unilaterally fixed U - tube (Hastelloy C - 276) on its mass. This mass consists of the U - tube material and the mass of the fluid filled into the U - tube.

The temperature in the measuring cell where the U – tube is located is controlled using a thermostat (F32 - ME Julabo, Germany) with an error of  $\pm 10$  mK and is measured using the (ITS-90) Pt100 thermometer (Type 2141) with an experimental error of  $\pm 15$  mK. Pressure is measured by pressure transmitters P-10 and HP-1 (WIKA Alexander Wiegand GmbH & Co., Germany) with a relative uncertainty of (0.1 and 0.5) % respectively, of the measured value.

An empiric equation of state for fitting of the (*p, ρ, T*) data of ionic liquids has been developed as a function of pressure, temperature and molecular weight of ionic liquids. The fitting using the group contributions will be discussed. This equation is used for the calculation of the thermophysical properties of IL, such as isothermal compressibility, isobaric thermal expansibility, thermal pressure coefficient, internal pressure, isobaric and isochoric heat capacities, speed of sound and isentropic expansibility.

The literature (*p, ρ, T*) values of [C<sub>3</sub>MIM][NTf<sub>2</sub>] were compared with our calculated values and good agreement was obtained.

**Keywords:** Density, vibration tube densimeter, equation of state, thermal properties.

## Simulation of Convection Heat Transport in Open-Cell Metal Foam

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In this paper a large domain made up of numerous idealized geometrical cells in the flow direction is used to simulate heat transfer due to air flow in open-cell metal foam. The large number of cells avoided periodicity issues and ensured minimal or no size and entrance effects. The flow and heat transfer equations are solved directly at the pore scale; and the temperature fields are obtained for various approach velocities using a commercial package. The details of the geometrical modeling and simulation are given. The commercial foam simulated has 20 pores per inch and porosity of 91.5%. The simulation shows a clear thermal-development region. To validate the simulation results and the modeling approach, direct comparisons to analytical local fluid temperatures from the solution of volume-average two-equation model in the thermally fully-developed region from the literature are presented. Good agreement between the simulation and analytical results are displayed.

**Keywords:** Unit cell, Simulation; Metal foam, Convection.

## The Density-Salinity Relation of Standard Seawater

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The ocean is essential for understanding climate. A main aspect is its ability to store and transport great amounts of thermal energy by means of currents. Their quantification requires the knowledge of thermophysical properties that are depending on salinity, temperature and pressure. The salinity represents the amount of dissolved salts in seawater.

Salinity is commonly determined from measurements of the electrolytic conductivity. The conductivity measuring devices are calibrated with so called standard seawater that is prepared from natural seawater and, therefore, may change its properties during long periods. For this reason, another approach to determine salinity is reasonable. One way is to define salinity by density – a quantity directly traceable to the International System of Units (SI) and is also a key variable for the description of deep-sea currents as density gradients are the driving forces for ocean currents.

This is one main issue of the European Metrology Research Project “Ocean Metrology” that includes the experimental determination of the relationship between salinity and density with highest precision. The measurements cover wide ranges of salinities, temperatures and pressures common in the ocean. These are in detail 2 g/kg to 42 g/kg, 5 °C to 35 °C, and 0.1 MPa to 70 MPa.

The density measurements were performed using a vibrating tube densimeter. A substitution method was used to minimise uncertainty. A relative expanded uncertainty for density of  $2 \cdot 10^{-6}$  at atmospheric pressure has been achieved using this method. at high pressure this uncertainty is larger, first estimations yield a value of  $40 \cdot 10^{-6}$ .

The relation between salinity and density was approximated by a polynomial equation. Associated measurement uncertainties of the polynomial coefficients were determined to allow the calculation of the total uncertainty of the relation between density and salinity. Measurement uncertainty calculations were done according to JCGM 100-2008: *Evaluation of Measurement Data - Guide to the Expression of Uncertainty in Measurement* (GUM).

**Keywords:** Seawater, Salinity, Density, SI traceability.

## Characterization of Oscillating Water Transport in Metal Foam

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Oscillating flow in porous media is a phenomenon that occurs in many engineered systems, e.g., heat pipes, regenerators, Stirling engines, cooling designs of nuclear power plants and reciprocating internal combustion engines. Due to superior heat removal rates, there has been interest in using oscillatory flow in porous media for cooling high-power-density high-speed electronic components. Such flow provides enhanced heat removal rates and uniform substrate temperature.

Oscillating flow of water in traditional porous media (e.g. packed spheres) has been studied before. Metal (aluminum, copper, etc.) foams are relatively new class of porous materials. They have extremely large surface area density, up to 10,000 m<sup>2</sup>/m<sup>3</sup>, and have very high porosity, over 90%. The cells of open-cell metal foams are connected tetrakaidecahedra. Oscillating flow of water in metal foam has never been investigated. All the available studies are for oscillating air flow in metal foam. Flow characteristics of oscillating flow of water in metal foam are critical for convection heat transfer designs. Water is a much better medium for removing heat compared to air. Also, liquid flow is known to have strong dispersion (an added mechanism of heat transfer), which is very weak for gas flow in porous media.

This paper shows experimentally obtained flow characteristics of oscillating water flow in commercial aluminum metal foam. In particular, data and correlations for the pressure drop, friction factor, permeability and inertial coefficient using the kinetic Reynolds number are given.

The information provide insights as to how the pumping power can be reduced/optimized, which means energy savings. The results of this study are the groundwork for studying convection heat transfer due to oscillating water flow in metal foam.

**Keywords:** Metal foam, Porous media, Oscillating flow, Kinetic Reynolds number, Water.

## Thermophysical Characterization of a Urea Based Eutectic Mixture for Thermal Energy Storage

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Eutectic mixtures of urea with other materials could be suitable materials for latent thermal storage. The mixtures could show a melting point in the domestic hot water (DHW) systems. The main advantage would be the low cost of the urea although many authors have dismissed it mainly due to its poor thermal stability.

The present article deals with the thermo analytical evaluation of the eutectic mixture based on urea and sodium nitrate in the temperature range 60-90°C. The potential application of this material is focused on thermal storage systems for cogeneration and solar ACS facilities. The material degrades with increasing temperature. However, if its degradation takes place slowly enough below 90°C, this material could be integrated in the system. That would prove the suitability of the mixture to be applied in latent heat thermal energy storage, in the specific temperature range. Therefore, the objective of this work is to determine the stability of the urea and urea based eutectic mixtures in the temperature range 60-90 °C. In the case that the stability is good enough in this temperature range, the urea mixtures could be used as PCM with a lower cost than the currently commercialized materials.

**Keywords:** Phase change materials, PCM, Thermal storage, Thermal decomposition, Urea mixtures.

## Modeling of the Bubble Growth Dynamics in PS/CO<sub>2</sub> Foaming System

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Polymeric foams have a cellular structure composed of two phases; a polymeric solid and a gaseous phase. They are produced using many methods which are basically consisting of incorporating a blowing agent into polymeric matrix through a mixing process. In foaming process, cell structure is developed by expansion of a blowing agent in polymer melt. In the case of physical blowing agent, upon reducing the system pressure, bubble nucleation starts and is followed by bubble growth due to gas diffusion into the bubbles. The growth of the bubble plays an important role in the polymeric foaming dynamics and has dramatic impact on the final product properties. Generally speaking, the bubble growth process is very complicated since it consists of simultaneous mass, momentum and heat transfer between an expanding bubble and the surrounding polymeric media associated with changes in the rheological properties. In the most studies on the bubble growth field, the single bubble growth model is considered. The single bubble growth model describes the growth of a surrounded single bubble by a finite or infinite fluid. The focus of the present study is on the bubble growth process as the second stage of the foaming process. In this work, the bubble growth processes with limited and unlimited dissolved gas available were modeled using finite difference and integral methods. The predicted results also were compared to experimental results and the integral model was modified to limit the growth of bubble. To study the growth of a gas bubble in a finite pool of liquid, a gas bubble concentrically surrounded by a shell of viscoelastic melt of constant mass is considered. The gas inside the bubble is assumed to behave as an ideal gas and its pressure is always greater than the ambient pressure. Fluid around the spherical bubble is considered to be incompressible and flow assumes to be a creeping flow. Since in the foaming process, the bubble is growing, its boundary is changing. So trial and error method was used to calculate the radius of the growing bubble. First the bubble radius is estimated, then bubble pressure is calculated from overall force balance on the melt and compared with calculated pressure from mass balance between the gas bubble and polymer-gas shell. To calculate bubble pressure from overall force balance on the melt, it is needed to have normal stress around the bubble, so the upper convected Maxwell model is used to describe the polymer viscoelastic behavior. In order to calculate the bubble pressure from mass balance, concentration gradient of blowing agent in bubble-shell interface should be known, so gas diffusion equation in shell was used to calculate the concentration distribution in shell around the bubble.

In order to solve the mass transfer equations, the integral method can be used. In this method, a polynomial concentration profile is used to describe the gas concentration profile in a thin layer. The mass balance equation is obtained by integrating the assumed polynomial profile. In the present study, two mass transfer equations of the integral method at the gas-polymer interface of a bubble are considered. In order to solve the ordinary and partial differential equations, 4th order Rung-Kata (RK4) and implicit finite difference methods were used, respectively. The necessary experimental parameters for modeling were extracted from literature for PS/CO<sub>2</sub> foaming system to verify the predicted results from modeling. The results showed if the bubble pressure is calculated using quadratic concentration profile (QCP), the theoretical prediction will be approached to the experimental results compared to the cubic concentration profile (CCP). But these models did not predict the plateau behavior in the equilibrium size whereas the experimental results show that the bubble grows up to an equilibrium size. This contradiction arises from the fact that in the integral models (QCP and CCP) take an infinite source of gas available for bubble to grow.

The QCP and CCP models should be modified to limit the growth of bubble. Therefore, in the present study, the gas concentration profile in the shell was obtained from the numerical solution (finite difference method) of the mass transfer equations and then the value of the gas concentration at the outer boundary shell was updated and used in QCP and CCP integral models. It is observed that the modified integral method can predict the steady-state stage of the bubble growth. Comparing the modified method results to experimental ones reveal that there is a remarkable difference between them. The reason of this difference can be explained that in the modified integral method, the total thickness of

the shell was considered as the concentration boundary thickness. Since the concentration gradient at the interface of the bubble and shell is needed to calculate the bubble pressure. So using of finite difference method and the gas concentration gradient at the interface has led the results more consistent with the experiments.

**Keywords:** Polymeric foam; Bubble growth dynamics; Viscoelastic fluid; Mass diffusion; Polystyrene; Carbon dioxide.

## The IAPWS Industrial Formulation for the Thermodynamic Properties of Seawater

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The development and operation of desalination plants or cooling of power plants using seawater require the knowledge of accurate thermodynamic properties of seawater and their fast calculation.

In 2013, the International Association for the Properties of Water and Steam (IAPWS) adopted the "Advisory Note No. 5: Industrial Calculation of the Thermodynamic Properties of Seawater" (IAPWS 2013) [1] as an international standard for the calculation of the thermodynamic properties of seawater for industrial use. This standard contains an equation of state for the Gibbs free energy for seawater consisting of Gibbs free energy equations for pure liquid water and for saline. The water part is computed from the "IAPWS Industrial Formulation 1997 for the Thermodynamic Properties of Water and Steam" (IAPWS-IF97) and the saline part from the "IAPWS Formulation 2008 for the Thermodynamic Properties of Seawater" (IAPWS-08) [2]. For seawater in contact with ice, the "Revised IAPWS Release on an Equation of State 2006 for H<sub>2</sub>O Ice Ih" is used.

The industrial formulation is valid for seawater with sea salt of the reference composition at temperatures  $T$  from 261 K to 353 K, pressures  $p$  from 0.3 kPa to 100 MPa, and salinities  $S$  from 0 (pure water) to 120 g kg<sup>-1</sup>, with some restrictions in certain regions as described in and.

All thermodynamic properties such as density  $\rho$ , specific volume  $v$ , specific enthalpy  $h$ , specific isobaric heat capacity  $c_p$ , and specific entropy  $s$ , thermodynamic derivatives, and inverse functions from given quantities ( $p, h, S$ ) and ( $p, s, S$ ) can be computed. In addition, boiling temperature  $T_b$ , freezing temperature  $T_f$ , osmotic pressure  $p_{\text{osm}}$ , and properties for brine-vapor mixtures and brine-ice mixtures are calculable.

When using the industrial formulation IAPWS 2013, the uncertainties of the calculated seawater properties are slightly greater than those of the scientific formulation IAPWS-08. The differences between both formulations result from the use of IAPWS-IF97 for the pure-water part in the industrial formulation and the use of IAPWS-95 in the scientific formulation. They will be discussed in this paper.

The computing speed of the industrial formulation IAPWS 2013 for seawater is increased in the order of 100 to 200 depending on the property function in comparison with the use of the scientific formulation IAPWS-08. Details will be shown in this paper.

The industrial formulation IAPWS 2013 for seawater can be applied in calculations for analyzing, designing, simulating, operating, and optimizing desalination and cooling processes.

**Keywords:** Seawater, Thermodynamic properties, Industrial standard.

## Enhancement of Compression Performances of Foam Core Sandwich Composites

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Sandwich composites are composed of the core, which is lighter but thicker and has lower strength, and the facesheet, which is rigid and stronger. Sandwich composites have been preferred to be popularly used in marine applications, wind turbines, space and aircraft vehicles due to their high bending rigidities in addition to lower weight necessitates. However one of the disadvantages of using sandwich composite is their lower strength against out-of-plane compression loadings, because there is no loading resistance material in this direction. To overcome this disadvantage the core should be reinforced in that direction.

In this study it is aimed to improve the compression performance of sandwich composites manufactured using foam as the core and woven glass fabrics as the sheet material by vacuum infusion method. With this purpose two different applications are performed and compared. As the first application; the cores are perforated and then the sandwich composites are manufactured using woven glass fabrics. As the second application; the core is perforated, glass rovings (fibres) are placed in the holes with hand stitching and then the sandwich composite is manufactured by using woven glass fabrics as the sheet material. For this set of specimens, rovings of different counts (having different fineness/diameter) are also considered to investigate the effect of fiber (roving) diameter on the composite performance. In addition, for comparison purposes, sandwich composites of the same material but without perforating the core are also manufactured; this is the classical method popularly used. Flat-wise compression tests are performed according to ASTM C365 standard for all types of specimens and the results are compared.

It is seen that both of the application methods increase the compression strength of the investigated sandwich composites in comparison to the classically manufactured sandwich composites. Especially the sandwich composites with glass rovings (fibers) in the perforated core have the highest compression strength however the increase in the strength of the composites is not observed to be proportional with the increase in the fiber diameter of the glass rovings used in hand stitching.

**Keywords:** Sandwich composite, Compression, Glass, Foam.

## Molecular Simulation of Nano-Dispersed Fluid Phases

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Dispersed phases are ubiquitous both in nature and in technological applications. Their character poses a particular challenge to thermodynamic approaches which attempt to reduce the complexity of a system to a few macroscopic degrees of freedom. For a dispersed phase, a bulk-like region does not exist. Thus, thermodynamic properties in the centre of a nanoscopic bubble or droplet may deviate substantially from the bulk phase under similar conditions, i.e. at the same chemical potential and temperature. Interfacial properties may dominate the behaviour of the whole system, and the heterogeneity of the dispersion further complicates its thermodynamic description. It is therefore attractive to apply molecular simulation to these problems, supplementing experimental results where they are available, and replacing them where suitable experiments have not yet been devised.

Fluid phase equilibria involving nano-dispersed phases, where at least one of the coexisting phases is confined to a small volume, are investigated by molecular dynamics simulation of the truncated-shifted Lennard-Jones fluid. Simulation volumes containing a nanoscopic gas bubble surrounded by a subsaturated liquid under tension (i.e. at negative pressure), a nanoscopic droplet, or a thin liquid slab surrounded by vapour, are conducted in the canonical ensemble. The boundary conditions are chosen such that the phase equilibrium is thermodynamically stable. The curvature dependence of the surface tension is considered, employing an approach based directly on the average radial density profiles to obtain the excess equimolar radius, which is found to be small and positive, corresponding to a small and negative Tolman length.

Regarding nanoscopic bubbles, two distinct size-dependent effects are found, which are of opposite sign: Curvature induces a subsaturation of the system, leading to a smaller liquid density. For the gas in the centre of the bubble, the small diameter has an additional obverse effect, increasing its density. Furthermore, curvature-independent finite size effects are examined by varying the thickness of planar liquid slabs. It is found that the density in the centre of the liquid region as well as the surface tension decreases significantly as the slabs become thinner. The influence of the slab thickness  $S$  on the liquid density and the surface tension is found to scale with  $1/S^3$ , and a linear correlation between both effects is obtained. With respect to the surface tension of liquid nanodroplets, the results corroborate the analysis of Maličevský and Jackson.

**Keywords:** Molecular Dynamics, Surface tension, Dispersed phases, Curved interfaces.

## Mechanical Properties, Microstructure and Density of Rigid Crosslinked PVC/Organoclay Nanocomposite Foams

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Rigid polymer foams represent a group of lightweight materials currently used in a wide variety of industries, such as packaging, building and insulation owing to their attractive properties including lightweight, excellent strength/weight ratio, superior insulating capability and energy absorption. Foam density and its cell size are the most important structural parameters which greatly affect the mechanical performance of the foam. It is well documented that the microcellular foams have superior mechanical properties over conventional foams. Due to large surface area as well as extremely fine dimensions, the addition of nanoparticles into the matrix usually decreases density and cell size of the foam. The main objective of this work was to investigate the effects of incorporating organoclay (Cloisite 30B) as a nanofiller, foaming temperature and the immersion time on the cell morphology, foam density and compressive mechanical properties of rigid PVC foams. Gel content test, optical microscopy, scanning electron microscopy (SEM), x-ray diffraction (XRD) analyses were employed to characterize the cell morphology of prepared foams and dispersion state of organoclay in the polymer matrix, respectively. Attempt was made to establish a correlation between microstructural parameters and compressive properties of the resulting foams. The following materials were used for PVC foam preparation. Suspension PVC with a K value of 70 was supplied by LG, Korea, di-octyl phthalate (DOP) was used as plasticizer, Ca/Zn stearate as heat stabilizer, maleic anhydride, styrene monomer, toluene di-isocyanate (TDI) and Cloisite 30B organoclay were used for production of nanocomposite foams. An established method for manufacturing such cross-linked PVC rigid foams is based on a discontinuous process which takes place in at least three stages. In order to production of neat PVC foam samples, at first PVC plastisol was prepared in a mechanical stirrer and all components were mixed together until obtaining a homogeneous mixture. The formulation used contained 100 phr PVC, 40 phr DOP, 2 phr Ca/Zn stearate heat stabilizer, Maleic anhydride, Vinyl monomer, polymerization catalyst and TDI. For producing of nanocomposite foams, the modified nanoclay (Cloisite 30B) was mixed with Toluene diisocyanate (TDI) and di-octyl phthalate (DOP) ultrasonically and then added to PVC and other components. In the second stage of the process the blend is poured into a mold heated under pressure to gel PVC. During this molding (gelling) the polymerization catalyst which is a free radical yielding agent, such as azo-bis-iso-butyronitril (AIBN), induces the copolymerization of maleic anhydride with the vinyl monomer. Polymerization catalyst can also easily extract hydrogen atoms, so the combination of the maleic anhydride-styrene copolymer with PVC backbone takes place. at the third stage of the process the molded samples are immersed in hot water or steam to cross-link rigid PVC foam. All of the specimens were immersed at four different temperatures, 80, 90, boiling water, and 120 °C ( $\pm 1$  °C) and were cross-linked for different periods of time (2–12 h). The material is quite hydrophilic, because of the presence of diisocyanate and maleic anhydride in the grafted chains. Water or steam will diffuse rather quickly into the samples. Water can react as well with maleic anhydride to crosslink the samples as well as with diisocyanate to produce carbon dioxide to expand the molded samples. SEM micrographs show that there is a reasonably good uniformity and homogeneity in the overall cell morphology of nanocomposite foams. Neat foams tend to have thicker cell struts and walls, but similar cell size distribution. Nanocomposite foams, on the other hand, have a narrower cell size distribution. The density of the nanocomposite samples decreased as the organoclay added. The decrease in foam density in the case of Cloisite 30B is mainly due to the increase in cell nucleation sites caused by the dispersed nanoclay in the PVC matrix, as well as the increase of generated CO<sub>2</sub> gas levels in the melt due to the moisture trapped in the nanoclay. The immersion temperature has a significant effect on the foam density. The density of the samples decreases as the temperature increases. With increasing temperature the viscosity and the cell strength of the foam cores reduces that probably controls the bubble growth, so the cell size distribution improves. The heterogeneous nucleation in nanocomposite foams in the case of Cloisite 30B improves the diffusion of water and due to the direct relationship between the crosslinking and the diffusion process, the rate and degree of crosslinking

increases. Compressive results of the PVC foams illustrate the influence of nanoclay incorporation and foam density on the mechanical properties. The compressive strength increases significantly with the incorporating of nanoclay because of the strengthening of the cell struts in the foam. Density is found to improve by incorporating organoclay in the polymer matrix and increasing the immersion time and temperature. Cellular microstructure of the neat samples shows that the presence of Cloisite 30B nanoclay increases foam cell density and decreases cell sizes. While with immersion temperature and time increasing, both neat and nanocomposite foams show a drop in mechanical behavior due to the higher water uptake which lead to decrement in density.

**Keywords:** Rigid PVC foam, Cell microstructure, Mechanical properties, Nanocomposite, Organoclay.

## Experimental and Theoretical Analysis of Heat Transfer in Micro-Models of Porous Media

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Micro-models of porous media have been recently constructed and employed in the proposition and analysis of conceptual models for contaminated soils remediation and enhanced oil recovery from mature reservoirs. Different micro-fabrication techniques have been utilized in constructing such pore scale two- and three-dimensional physical models of the porous medium to be studied, also known as ROC (rock-on-a-chip), followed by the metrological and hydraulic characterization of the micro-model. The present work employs a combination of integral transforms and Bayesian inference in the proposition of a direct-inverse problem analysis for the characterization of two-dimensional micro-models of porous media, based on the availability of non-intrusive measurements of the external surface wall temperatures. The physical dimensions and properties are taken from an actually constructed micro-model, manufactured through micro-milling on a PMMA substrate, according to tomography images of an actual rock sample, and sealed with a thermal pressing machine. An infrared camera is assumed to be employed to capture the temperature distributions on the external surface of the micro-fluidic chip, while flowing hot water through the micro-model. A conjugated heat transfer model is proposed for the conduction-convection analysis which provides the direct problem solution for the theoretical external surface temperatures, which is then combined to the inverse analysis through the MCMC approach with the Metropolis-Hastings algorithm, so as to identify the hydraulic and thermal parameters of the tested micro-model. The direct-inverse problem with the non-intrusive temperature measurements is then analyzed for different porous media configurations of known geometries and thus different dimensionless parameters, so as to demonstrate the consistency of the proposed approach in the parameters identification and characterization of the micro-porous model.

**Keywords:** Porous Media, Micro-Models, Experimental Analysis, Theoretical Analysis.

## **Solubility and Diffusivity of Normal Pentane and Supercritical CO<sub>2</sub> In St-MMA Copolymer With Different Compositions**

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In this study, styrene- methylmethacrylate (St-MMA) copolymer particles were synthesized in a batch reactor by suspension polymerization process at different copolymer compositions. Also for further comparisons, the neat polystyrene (PS) and polymethyl methacrylate (PMMA) were synthesized by the same method. Supercritical carbon dioxide (scCO<sub>2</sub>) and normal pentane (n-pentane) were used as blowing agents. The solubility and diffusivity of scCO<sub>2</sub> and n-pentane into the synthesized copolymers at different temperatures and pressures were measured by a magnetic suspension balance (MSB) and our designed solubility measuring system, respectively. The MSB makes it possible to weigh samples under the high pressure and temperature environments without holding the balance in the environments. at the first, CO<sub>2</sub> was pressurized and introduced into the MSB measuring chamber using a plunger pump (Isco 260D/USA), for purging the atmosphere. In the chamber, the pressure could be built up to maximum 25 MPa pressure and temperature could be increased to 523K. The resolution and the accuracy of the balance were 10<sup>-5</sup> g ±0.002%, respectively. A disk-shaped polymer sample about 0.001 kg in weight was set in a stainless basket and the basket was attached on a hook of the magnetic suspension balance. The chamber was heated to keep the sample in molten state and under vacuum for 1800 seconds at the specified temperature. Then, CO<sub>2</sub> was introduced into the chamber. The data of the electronic microbalance readouts, temperature and pressure were acquired on-line by a computer. The measurements were performed by changing CO<sub>2</sub> pressure stepwise in the pressure range from 5.0 to 12.0 MPa and temperature of 393 and 423K. To perform accurate measurements we have one equation which consists of the weight of dissolved CO<sub>2</sub> measured by MSB readout should be corrected by considering of the buoyancy effect and then the true amount of dissolved CO<sub>2</sub> was calculated. The solubility of n-pentane in samples was conducted as well in our designed solubility measuring system, which consisted of the self-sealing observation cell equipped to the pressure and temperature controller. For measuring the amount of solubility n-pentane in samples, the synthesized copolymer particle was weighted (m1) and impregnated by pentane and finally solubility measurement was done by decreasing the temperature while the pressure of the chamber is still high. When the temperature reached below the boiling temperature of n-pentane, the sample was taken out from the chamber and weighted (m2). The solubility of n-pentane in sample is defined as (m2-m1)/m1. In this experiment a very small amount of the evaporated n-pentane from particles was neglected in calculations and the solubility of n-pentane in different St/MMA copolymers and corresponding homopolymers were compared at the same conditions. The volume of polymer/gas mixture is a function of temperature, pressure and weight of blowing agent and could be estimated by employing the Sanchez-Lacombe (SL) equation of state. The characteristic parameters of samples were determined by fitting SL equation to PVT experimental data of samples, individually. The PVT data of all polymeric samples were obtained by a high-pressure GNOMIX PVT apparatus (GNOMIX, Inc., USA) with an isothermal cooling procedure for the range of temperature from 313 to 503 K and pressure from 0.1 to 100 MPa. We weighted and put our samples in powder form to its cylinder shape sampler in which worked with air compressor and then using the software from the connected computer, in different selected pressure, the specific volumes versus temperature were obtained and recorded. When the polymer/gas mixture reaches at an equilibrium state at temperature, T, and pressure, P, the chemical potentials of blowing agent should be the same at the interface between the gas phase and the polymer/gas mixture. The last equation required for solubility calculation is the equation of phase equilibrium, which equates the chemical potentials of blowing agent in the two phases. Mutual diffusion coefficients of n-Pentane (with our apparatus) and CO<sub>2</sub> (with MSB) gas in molten polymer were measured in the different temperatures and pressure ranges and determined by measuring the time evolution of the weight of molten polymer in the course of reaching a new steady state from an old one. Fick's second diffusion law was given for estimating the diffusion coefficient from the weight data. The dissolved blowing agents in-

duce swelling of the polymer and change the specific volume of the polymer. Therefore, since the swelling occurs during the diffusivity measurement, Fick's second law cannot describe the diffusion process when the swelling effect is large. Thus, by making the stepwise change in pressure for diffusivity measurements small enough to make the swelling small, the mutual diffusion coefficient could be treated as a constant parameter during the measurement. We calculated the diffusion coefficient by fitting the solution of Fick's second diffusion equation to the taken data of the weight of molten polymer versus the time evolution in every pressure step. There are interactions in CO<sub>2</sub> and copolymers with higher amount of MMA, in which with MMA content increment, the carbonyl groups were increased and consequently their interactions with CO<sub>2</sub> also increased. Therefore in the case of CO<sub>2</sub>, due to the higher affinity of CO<sub>2</sub> to MMA units than St units, its solubility in samples increased with increasing of pressure and methyl methacrylate (MMA) units in copolymer and decreased with temperature increment. Meanwhile the results revealed that the diffusion coefficients of CO<sub>2</sub> in samples increased with pressure as well as with temperature increment. In the case of n-pentane, due to non polarity of n-pentane and St groups, n-pentane was dissolved in St units of copolymer more than its MMA units and the solubility of n-pentane in samples was improved with increasing of pressure and declined with rising of temperature and methyl methacrylate (MMA) units in copolymer. In the case of St/MMA: 53/47 copolymer composition, it was concluded that two different pressure ranges could be observed in dissolved gas content isotherms, one is lower than 3 bar and the second is higher than 3 bar, in which the contradictory behavior was observed with temperature increment. In low pressures the solubility was reduced with temperature rising, but in the high pressure range the trend for St/MMA: 53/47 was different from other samples. Furthermore the diffusivity results revealed that the diffusion coefficients of n-pentane in samples increased with pressure, St content as well as with temperature increment. The probable reason for contrary behavior of n-pentane solubility in higher and lower pressures than 3 bar could be found as follows. In the case of St/MMA 53/47 copolymer, we had three dominant parameters: the sorption pressure, the sorption temperature and the copolymer composition. While the sorption pressure was lower than 3 bar, the driving force for pentane dissolved content was not high enough and the less amount of pentane could dissolve in St units of copolymer. In this condition with temperature increment, the dissolved pentane molecules go out of copolymer and the solubility of n-pentane was decreased. As the sorption pressure was higher than 3 bar, the driving force for pentane dissolved content was high enough and the higher amount of pentane was dissolved in St units of copolymer and in this condition with temperature increment, the solubility of n-pentane in copolymer matrix was increased.

**Keywords:** St/MMA copolymer, Solubility, Diffusivity, CO<sub>2</sub>, n-pentane.

## **Simulation Under Uncertainty of Heat Conduction in Heterogeneous Media Combining Integral Transformation and Polynomial Chaos**

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Deterministic solution techniques for partial differential equations that govern diffusion-convection phenomena are already a well-defined research field, with the Integral Transformation technique highlighting in this context as a powerful tool for this class of problems, allowing analytical and hybrid numerical-analytical solutions for many applications. On the other hand, a key factor that has been less considered in the analysis of classical problems is the understanding and quantification of the impact of uncertainties in the input data, for instance from the experimental determination of thermophysical properties. Uncertainty quantification, as has been called this area of research, seeks to provide more reliable predictions to practical problems, having received increasing attention. This work is based on the analytical treatment of uncertainty in the spatially variable coefficients of the governing equations of heat conduction problems in heterogeneous media. The available methods are reviewed, focusing on the promising approach using Polynomial Chaos. The traditional application of this method is analyzed both in its Galerkin approach, as in the stochastic collocation approach. Then a fusion of this method with the integral transformation technique is proposed, in order to reduce the stochastic problem to a simpler problem, while allowing to obtain an entirely analytical solution. Efficiency and convergence of the results are compared with exact solutions as well as solutions obtained by Monte Carlo simulations.

**Keywords:** Integral transforms, Stochastic partial differential equations, Heterogeneous media, Polynomial chaos, Simulation under uncertainty.

## **Thermal Degradation and Burning Behavior of a Commercial Epoxy Resin Blended With an Organophosphonate**

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Herein, a detailed characterization of the thermal properties and fire behavior of a bifunctional bisphenol-A based epoxy resin (DGEBA) cured with an aromatic aminic hardener (DDM) as a function of the weight fraction of the phosphorus flame retardant (PFR) was conducted. The experimental results regarding the burning behavior and thermal decomposition mechanism were compared to the reference system based on the cured epoxy resin (DGEBA/DDM) without the organophosphorus additive. It was shown that with a very low content of phosphorus element, the fireproof epoxy resins (PFR-DGEBA/DDM) exhibited significantly improved flame retardancy. A concentration of 1 wt% was enough to increase the value of the limiting oxygen index (LOI) with about 30%. In addition, the peak of total heat release rate (p-HRR) of the fireproof PFR-DGEBA/DDM composites was reduced up to 45% of that of the DGEBA/DDM system, depending on the content of the flame retardant additive introduced into the epoxy matrix. The thermogravimetric analysis (TGA) showed that the incorporation of PFR significantly increased the char yield and the thermal stability of the gradually forming phosphorus-rich carbonaceous layer at elevated temperatures. These results suggested that the main flame retardancy mechanism of the fireproof cured epoxy resins was the condensed phase mechanism.

**Keywords:** Epoxy resin, Thermal degradation, Flame retardancy.

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## **Effect of Stamp Forming Pressure and Temperature on Polyvinylchloride Sheets**

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Materials that have been used in this work were formed in stamp forming. A stamp forming mould which has a shape that has rectangular geometry was designed and manufactured to use this mould in this operation. Unreinforced polymer sheets were heated with an external heater to temperature which is close to melting limit but under melting point for each different material and formed by the mould which has been employed at room temperature to shape any parts from unreinforced PVC. Some useful parameters for stamp forming of the polymer sheets such as heating time of polymer sheets, mould velocity, stamping pressure etc. were determined before the experimental operation started. These materials were formed in different temperature and pressure conditions. Some specimens were cut and taken from these sheets by machining. Tensile characteristics of these materials were investigated. According to tensile test results obtained from experimental stamp forming operations, after changing the stamp forming parameters as stamping pressure and stamping temperature PVC materials showed different characteristics in (%)elongation at break and ultimate tensile strength.

**Keywords:** Compression, Temperature, Sheet, Polyvinylchloride (PVC), Strength.

## Calibration of Moisture Sensor for the Monitoring of Temperature-Moisture Regime in Volcanic Tuffs (Natural Rock Dwellings) in Brhlovce Village (Slovakia)

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The underlying research is based on in-situ monitoring of the temperature-moisture regime of natural rock mass /volcanic tuffs/. Temperature-moisture regime is the control parameter that influences deterioration process of rock massive. Depending on thermodynamic conditions, the moisture sensor utilizes changes of thermal conductivity of porous structure when pores are filled by air/vapor, water or ice. The relationship between thermophysical properties and water content in certain pore material needs to be known. Therefore it's necessary to calibrate the moisture sensor and determine change of thermal conductivity of tuff pore material in dry and water saturated states in the temperature range that is typical for the climate of Brhlovce locality. The calibration is carried out in a temperature range of different degrees of moisture content.

The construction of moisture probe is based on hot ball sensor in combination with rock cylinder made of tuff and assembled in a proper way. The probe can be used for the measurement in quasi steady-state regime or in transient regime. The new probes were calibrated in transient regime that is more sensitive for the properties change and the results improved accuracy of measurement. The difference in thermal conductivity of dry and moisture saturated states is about 50% that gives big sensitivity for relative changes of moisture content. The four probes were constructed and calibrated for the in-situ monitoring of temperature and moisture at the four distances from the surface within the range of depths from 10 cm up to 190 cm. The results are discussed.

**Keywords:** Moisture sensor, Monitoring, Preservation of historical monuments.

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## Dilatometry- Theory, Instrumentation and Applications

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The goal of this article is to provide an understanding of TA Instruments line of dilatometers. In the last three years TA Instruments has acquired Baehr and ESS with the intention of getting into high temperature measurements of metals, ceramics and glass. Dilatometry will facilitate measurement of coefficient of thermal expansion, softening point, determination of phase and glass transitions by measuring sample temperature, furnace temperature and change in length. All the available models of TA Instruments dilatometers will be discussed with respect to the measurement transducer, operational range, resolution and applications. In the first part of this article, the theory of thermal expansion will be discussed. The selection of materials is very important for practical applications for them to have the thermal compatibility and the ability for it to work in harsh environments and temperature extremes. In second part will be on the TA Instruments line of optical, horizontal and vertical dilatometers and their properties will be presented such as furnace options, measuring systems, and calibration materials. Examples from potential applications will be presented including glass transition (T<sub>g</sub>) determination and softening point detection. This paper will provide the reader with an overview of TA Instruments products

**Keywords:** Dilatometer, Optical, Horizontal, Vertical, Coefficient of thermal expansion.

## Optimum Design of the Vehicle Energy Absorber

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Accidents concluded with injuries and deaths which are related with the increase in the number of vehicles are force engineers to design and manufacture much safer vehicles. Nowadays, a lot of research works have been conducted in the field of crashworthiness in order to define crash performance of vehicles and crash boxes. The purpose of these works is to realize the optimum design that provides maximum structural absorption of the energy which emerges on the instant of an accident in order to preserve passengers' safety as much as possible. As a result of this, structural components that are used in vehicles should be designed to absorb the kinetic energy which emerges during the crashes.

Crash boxes are structures which can partially or completely convert kinetic energy to another form of energy. It is aimed to absorb a great deal of crash energy inside of box irreversibly, during the design of a deformable crash box. Thus injury of passengers and equipment damages could be reduced. Transformation of kinetic energy to plastic forming energy depends on the parameters such as applied force intensity, method, mode of deformation or replacement and material properties.

The structures that are mainly used in vehicle passive safety systems are deformable crash boxes and there are many studies about energy absorbers can be found in literature. Crash boxes that examined in these studies can be classified as straight and tapered. Straight ones are the crash boxes where structural walls are extended parallel to the axis of the impact, whereas the tapered ones, a certain angle is located between absorber's walls and axis of the impact. The most important design parameter of the crash boxes is cross-sectional geometry which is generally used as spherical, squared, rectangular and hexagonal.

In this paper, crash boxes is tested in both numerical and experimental for front impact of vehicles. Numerical studies include determination of energy absorption characteristics of different geometries of crash boxes. In addition, these studies include making changes in existing profiles with wall thickness of crash boxes, changing the positions of some of the profiles and adding new profiles. Optimum geometries of crash boxes which obtained by numerical studies are tested and improvement of energy absorption characteristics are defined.

**Keywords:** Frontal impact, Crash box, Optimum product design.

## **Adaptive Nanomechanical Response and Elastic Property Analysis of Polymer Brushes by AFM Nanoscale Probing**

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Stimuli-responsive polymer brushes made of surface tethered macromolecules have been widely applied to prepare sensors, to regulate cell culture, to control wetting and adhesion, and in many other areas. Small changes in the external environment (e.g., temperature, pH, or solvent quality) can generally trigger a sharp and large response in the structure and properties of these grafted polymer chains. Various polymer brushes have been synthesized via the surface-initiated atom transfer polymerization (SI-ATRP) approach from different substrates using surface-attached initiators. This method allows one to accurately control the structure and properties of the polymer grafts. In this work, a high-density, ultrathin (~ 50 nm) polymer brush of (2-hydroxyethyl methacrylate) (PHEMA) was precisely prepared as a model responsive polymer brush on the surface of a flexible poly(dimethylsiloxane) (PDMS) substrate via SI-ATRP. The elastic properties and dynamic response of PHEMA brush within a two-dimensional polymer thin film structure are investigated using *in situ* atomic force microscopy (AFM) nanoindentation analysis under external stimuli. To date, only a few studies have addressed the question of the resultant mechanical properties of such a smart brush under complex environmental triggers. The reversible conformational changes of PHEMA brush between extended (hydrated state) and collapsed (dehydrated state) chain upon immersing in selective and non-selective solvents dictated elastic modulus, derived from force-indentation curves, which are almost estimated to be two and one order of magnitude smaller than the modulus of dry PHEMA brush, respectively. There is a quite uniform spatial distribution in the elastic modulus, with a narrower elastic modulus obtained for selective solvent and a little broader one for non-selective solvent. Such uniformity and the extremely low friction of the tethered polymer film contribute to precise controlled and well-defined structure of PHEMA brush for water-based lubrication under boundary condition.

**Keywords:** Nanomechanical property, Ultrathin polymer brush, Responsive surface, AFM nanoindentation.

## Low Velocity Impact Response of Sandwich Composites with Different Core Thicknesses

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Due to their excellent mechanical properties over metallic materials, structural sandwich composites are commonly used in various engineering applications like aerospace, automotive and wind turbine blades and so on. Sandwich composites used in these applications are often subjected to transverse impact loads resulting in different damage modes. Since these damage modes can cause significant decrease in the composite stiffness, the impact properties of sandwich composites have been investigated by many researchers.

In the present work, sandwich composite plates were manufactured by using vacuum assisted resin infusion molding (VARIM). E-glass fabrics 0/90 having density of 300g/m<sup>2</sup> as a reinforcing material and Epoxy ARALDITE LY 1564 SP resin and ARADUR 3487B hardener as a matrix material were used. The stacking sequence of sandwich composites was considered as [0/90/0/core/0/90/0] and AIREX PVC foam core in three different core thicknesses (5, 10 and 15mm) was selected as a core material.

Low velocity impact tests were performed CEAST 9350 with High-Energy System (Fractovis Plus) impact testing machine. A number of impact energy levels ranging from 10J to 50J were performed. Contact force-deflection, absorbed energy-impact energy, contact force-impact energy curves were depicted. Also, the photos of cross sectional area of the impacted zone were given to evaluate the damage modes.

It is seen from the contact force-deflection curves that there are two peaks at higher impact energy levels which demonstrate the failure of upper and bottom face sheets, respectively. Also, the contact force values decrease by increasing the core thickness while maximum deformation values increase by increasing the core thickness. According to photos of cross section area, the fiber cracks, matrix cracks and delamination between face sheets and core material were observed.

**Keywords:** PVC foam, Core thickness, Sandwich composite, Low velocity impact.

## **Nature and Surface of Steel Effects on Coatings Obtained by Galvanization at Various Immersion Times**

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In the last few years, the use of galvanization coating as material treatment to improve notably the chemical properties of steel parts has shown a large and extensive development. Zinc and some of its alloys have a number of characteristics that make it well suited for use as a protective coating against the corrosion of steel substrates under severe atmospheric conditions. The metal zinc, which represents the main galvanization element offers then a cathodic protection to the ferrous materials.

Because of these excellent characteristics, galvanization coatings are expected to be used for different protective applications fields. The aim of this research work is to study the effect of nature and surface of steel substrates on intermetallic compounds of galvanization coatings obtained at different immersion time. Steels substrates to be coated in this case are used in agriculture field as tubes and irrigation elements in pivot.

After a best preparation of here surfaces by different roughness process, various steel of substrates were galvanized by immersion in a molten zinc bath maintained at 450°C During the galvanization process, the chemical reactions that take place between the steel and the liquid zinc give rise to the formation of different intermetallic. Thus, three phases of  $\Gamma$  (Gamma),  $\sigma$  (Delta) and  $\xi$  (Zeta) are produced on the steel substrate. Theses metallic compounds have been coated then by a solid solution of iron in zinc  $\eta$  (Eta).

These intermetallic compounds are hard and fragile and the product that is obtained is not suitable for working, since this would inevitably lead to cracking and detachment of the coating. The morphology and thickness of phases formed the coatings at different parameters took place with scanning optical microscope. Finally the hardness of coatings was measured with a Vickers hardness tester with different loads.

**Keywords:** Steel, Zinc, Galvanization, Iron.

## Investigation of The Ribs Effects on Dynamic Response of Grid Composite Structures Under Impact Loading

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Grid cylindrical composite structures are being increasingly used in aerospace, aircraft and defense industries due to their attractive properties in strength and stiffness to weight ratios. The material examined in this research is manufactured by the filament winding process with  $[\pm 65]_{12}$  stacking sequence lay-up.

All the ribs are made of continuous and unidirectional fibers so they are intrinsically stiff and strong. The specimens were characterized by an external diameter of 140 mm and an overall length of 360 mm, Average mass of stiffened samples is 530gr and the thickness of outer shell is about 2.4 mm. 3 clockwise and 3 counter-clockwise helical ribs with square cross section ( $6 \times 6 \text{ mm}^2$ ) were used in each specimen. Table 1 shows geometrical dimensions of samples.

Table1: Geometrical characterize

| Cylindrical shell |                         |                   |
|-------------------|-------------------------|-------------------|
| Length            | thickness               | External Diameter |
| 360 mm            | 2.4 mm                  | 140 mm            |
| Ribs              |                         |                   |
| length            | Cross section           |                   |
| 360 mm            | $6 \times 6 \text{ mm}$ |                   |

The ballistic test was performed by a gas gun in the impact velocity of 107m/s and 139m/s. In the present research, the dynamic response and the damage of grid cylindrical composite structures subjected to high velocity lateral impact loading are experimentally investigated. Moreover, the effects of the ribs on residual velocity of projectile and overall damage area are investigated. General results show that presence of ribs reduces the overall damage area. In fact, discrete ribs prevent spreading cracks from one cell to its adjacent cells, as it can be seen in figure 1.



Figure 1. Damaged area

Due to reduce fracture area, overall and local deformations after impact in velocity which is higher than ballistic limit, projectile has been come out from grid samples with higher velocity than simple composite shells.

At first the center of each cell was chosen as position of collision, in this situation 107 m/s was recorded as residual velocity for mentioned structure subjected to impact by a projectile with an initial velocity of 139 m/s. This velocity was exactly the same unstiffened tested composite shell so in this situation ribs had no effects on output velocity of projectile.

In second step, for analyzing the ribs effects on output velocity, we changed the position of projectile collision. For impacting near intersection ribs (5.5 cm), 119 m/s was recorded as residual velocity of projectile with 140 m/s initial velocity.

In this paper, delamination in outer composite shell and ribs, debonding between shell and ribs, residual velocity of projectile, fracture area of the grid specimens and the effects of curvature in two different velocities were reported and commented upon as results.

**Keywords:** Grid composites, Damage, Delamination, Failure, Impact, Cellular shape.

## **The Modelling of Solar Air Collector with Thermal Efficiency Analysis and Artificial Neural Networks**

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Solar air collectors are widely used from space heating to dry agricultural products in many engineering applications. Despite solar air collectors have simple design and have a long life, thermal efficiencies are low. Many studies in the literature are performed to increase the thermal efficiency.

In this study, thermal performance of trapezoidal absorber plate of solar air collectors have been experimentally investigated. The collector is manufactured from steel sheet having a thickness of 0.8 mm and 1000x2000x200 mm in size. The aluminum absorber plate having 0.2 mm thick trapeze shaped is used in the collector. The absorber plate is painted with selective paint. 3.2 mm thick glass with low iron ratio was used on the collector as a transparent cover.

Experimental measurements are carried out under normal weather conditions. Global radiation value is measured with a pyranometer mounted on the collector. Temperatures of three points on the absorber plate and collector input-output air temperatures are recorded at regular intervals. on collector output, air flow rate is measured by using hotwire type anemometer. As a result of all these measurements, its efficiency is determined experimentally.

According to the data obtained in the experiments, a model of neural network of collector is created considering five inputs and two outputs data. As the collector inlet air temperature, global radiation and temperatures of the absorber are evaluated input parameters, however the collector outlet air temperature and the thermal efficiency values of the collector are evaluated as output parameters. By training an artificial neural network with some of the experimental data, the output parameters are estimated corresponding to different inputs data.

**Keywords:** Solar air collector, Thermal efficiency analysis, Artificial neural network.

## **A New Fatigue Damage Model for Mechanic Parts Subjected To High-Cycle Fatigue Loadings**

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Damage in metals is mainly the process of the initiation and growth of micro-cracks and cavities. A reliable lifetime prediction is particularly important in the design, safety assessments, and optimization of engineering materials and structures. With the accumulation of fatigue damage, some accidents will occur. Manufacturing companies always search the means to find the defects of their machines and to determine the maintenance date in order to replace the damaged parts before their failure. Indeed, it is important to formulate a method to evaluate the fatigue damage accumulation in order to predict the fatigue life. Various theories and models have been proposed to predict damage accumulation in materials.

The purpose of this work is to develop a numerical tool, based on the finite element method, in order to determine the cumulative damage evolution and the remaining lifetime for mechanic parts under high-cycle fatigue (HCF) loadings. A nonlinear cumulative fatigue damage model, extended to multi-axial loading, taking into account the effects of the amplitude and sequence of variable-amplitude fatigue loadings is proposed. Various load histories were applied and the resulting cumulative damage was evaluated using a numerical simulation. In order to demonstrate the features of the model, the results were compared to those obtained according to the Palmgren-Miner's rule.

Our approach belongs to the category of the nonlinear damage cumulative models. An effort was made to get a better life prediction capability and applicability of the proposed model. It was done by considering the influence of both static and cyclic loadings on damage and the effects of load sequence. An example is provided to demonstrate the applicability of the method. In order to determine the cumulative damage, it is necessary to replace the real sequence of cycles by an irregular loading with an assumed sequence of groups of uniform cycles. The block-loading data was transformed into an equivalent constant amplitude data using the concept of maximum equivalent stress defined by Crossland's criterion. To estimate the fatigue life, the damage model requires the whole S-N curve. For this end, we have model the low-cycle fatigue (LCF) region through a mathematical expression. The proposed nonlinear damage theory, which includes the effects of the magnitude cyclic load, the static load and the sequence of applied fatigue loadings, allows more realistic fatigue analysis of concrete structures.

The main aim of the present study was to determine the damage evolution and the lifetime of mechanical parts under high-cycle fatigue (HCF) loadings. We have developed a numerical tool, based on the finite element method, in order to determine the damage evolution and the remaining lifetime. The model was tested on a carbon steel type S 45 C. The present damage model, with use of a numerical technique, was applied to a rectangular plate with low thickness under various load sequences. Three different types of load histories were investigated: High-Low (H-L), Low-High (L-H) and random block-loading sequences. The predicted curves of cumulative damage evolve nonlinearly with the number of cycles. The loading sequential effects are clearly noticeable. Compared with the expectations of the Palmgren-Miner's rule, the model predicts shorter fatigue life under H-L sequence and longer fatigue life under L-H one. The cumulative damage was found to be higher than unity when the sequence is in the L-H order and lower than unity when it is in the H-L order.

The results obtained by the proposed model confirm the findings of many researchers. In particular, it was established that the sum of the fractions of life is greater than unity under the L-H loading sequences; on the contrary, it is less than unity under the H-L loading sequences. It can be summarized that for a mechanical part subjected to high-cycle fatigue (HCF) loadings, the fatigue damage strongly depends on the mechanical behavior of its material, the nature of the loading with its both parts (static and cyclic), the geometry and the shape of the structure, the number of cycles of each load-block and the type of load sequences. The encouraging results indicate that the present damage assessment meth-

odology will be a very useful tool for the lifetime prediction in the field of maintenance. In fact, the current model is capable of predicting fatigue life of structures subject to cyclic loadings. In addition, the present model could be extended to very-high-cycle fatigue (VHCF) regime through the known of this region of S-N curve.

**Keywords:** Fatigue, High-cycle fatigue, Cumulative damage, Finite element method.

## **Preparation of Dense and Interconnected Porous Cordierite Ceramics**

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This study presents our investigations on the synthesis of cordierite from a Algerian kaolin, and the development of dense ceramics, and porous ceramics over a wide range of pore volume that reaches more than 90% of the total volume of the ceramic.

The preparation of cordierite ceramics is carried out from a mixture of kaolin, precipitated magnesium hydroxide, and silica fume in accordance with the stoichiometric composition of cordierite ( $2\text{MgO} \cdot 2\text{Al}_2\text{O}_3 \cdot 5\text{SiO}_2$ ). Kaolin is washed and sieved below 25 microns, and magnesium hydroxide is precipitated by reacting magnesium chloride with ammonia hydroxide. The synthesis of the cordierite phase is investigated with the TG-DTA thermal analysis, and dilatometer. Pellets of diameter 40 mm and thickness 5 mm are pressed and sintered at 1300 °C to prepare dense cordierite ceramics, and for develop porous ceramics, glucose is added to the starting mixture to create an interconnected porosity during sintering (1300 °C) pressed powder pellets.

The DTA analysis shows two exothermic peaks; the first peak which happens at 950 °C is attributed to the  $\alpha$ -cordierite, and the second peak at 1200 °C shows the crystallisation of  $\alpha$ -cordierite (Indialite) starting from m-cordierite. The identification of the formed phases performed on the starting mixture sintered at 1300 °C by XRD analysis, shows the predominance of the cordierite phase.

The maximum densification of sintered pellets at 1300 °C reaches 96 %. With the addition of glucose two structures porosities are obtained. For a pore volume less than 60 %, the pore size is about 10 to 100 microns, and for more than 60 %, the pores are approximately 100 to 1000 micrometers having a cellular structure. The thermal coefficient of expansion between 50 and 1000 °C is  $< 3.0 \times 10^{-6} \text{ }^\circ\text{C}^{-1}$ .

The cordierite ceramic was prepared from kaolin and magnesium hydroxide precipitate, with a densification which varies of 5% to 95% successfully. Glucose is used to develop two structures porosities. For a pore volume less than 60 %, the pore size is about 10 to 100 microns, and for more than 60 %, the pores are approximately 100 to 1000 micrometers having a cellular structure. The thermal coefficient of expansion between 50 and 1000 °C is  $< 3.0 \times 10^{-6} \text{ }^\circ\text{C}^{-1}$ .

**Keywords:** Cordierite, Synthesis, Porous ceramics, Kaolin.

## **Determining of Thermal Properties of LiCl and LiBr used As Anode Materials in Thermal Batteries**

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The batteries are a device that they used to store chemical energy and convert it to electrical energy. Thermal batteries are more powerful and more durable than regular batteries. So, they are preferred for defense and military purposes mostly. The Thermal Battery (TB) is composed of a series of cells each cells having an anode, an electrolyte, a cathode and a heating mass. In order to make any numerical model for thermal batteries, it is required to determine their some thermophysical properties such as enthalpy, melting point, ionic conduction and thermal conductivity. DSC analyzes shows that thermophysical properties such as materials purities, enthalpy values were obtained for different temperatures. For this aim, the Differential Scanning Calorimeter (DSC) analyzes was performed to determine heating features of Lithium chloride (LiCl) and Lithium bromide (LiBr), which are used as anode materials in thermal batteries in this work.

Energy storage for both electrical and thermal energies is a rapidly emerging field of interest toward the development of more sustainable energy systems. The Thermal Batteries are (TB) the complex chemical systems which are composed of a series of cells each one having an anode, electrolyte, cathode and a heating mass. In order to understand these systems, it is necessary to decide their thermal, chemical and physical properties.

Thermal energy can be stored as latent heat or sensible heat. Some kinds of rocks such as granite, basalt, sand, limestone can be used to store sensible heat. However, liquid-vapour or solid-liquid phase change is used mostly in latent heat storage. As to thermal batteries, they work on the principle of latent heat storage. at the moment of activation, the pyrotechnic material (heat source) releases energy into the cells. Thus, temperature increases, the electrolyte melts, ion exchange occurs and the power in the cell is liberated. In this study, the Differential Scanning Calorimeter (DSC) analyzes of LiCl and LiBr chemical materials were performed.

According to the DSC curve of LiCl shown in the Fig. 1, a peak is seen at a lower temperature than a melting temperature. This peak is thought to result by breakage of the bonds in the chemical. The melting point of LiCl is 600 °C. As the reservoir of the DSC device is made of aluminium and the working temperature is up to 600 °C. According to the formed peak, for temperature range between 61.6 °C and 108.2 °C, the enthalpy value is 40.8 mJ / mg.

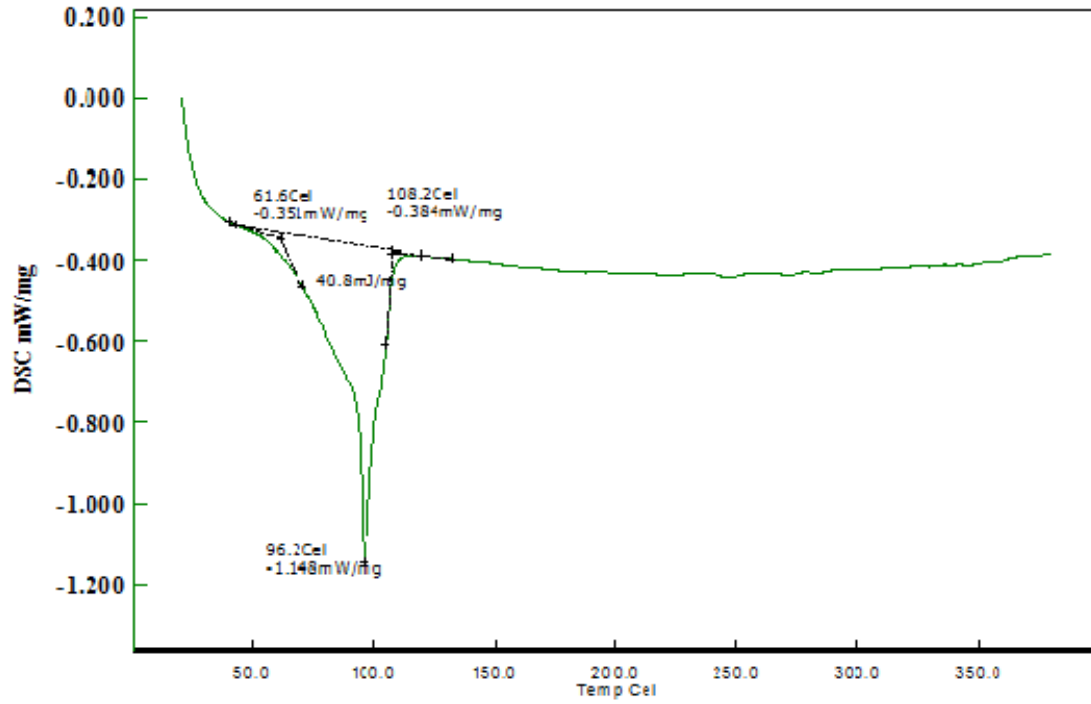


Figure.1. DSC curve of LiCl.

**Keywords:** Thermal Battery, DSC, Anode Materials, Thermal Properties.

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## Density of Bosphorus Seawater

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The Bosphorus is a strait that forms part of the boundary between Europe and Asia. The world's narrowest strait used for international navigation, the Bosphorus connects the Black Sea with the Sea of Marmara, after this connection Mediterranean Sea. These area located in the high ship navigation. The Bosphorus, as connection between these water basins, play important role for international ship transport. of course, such intensive transportation play also negative role to ecology and atmosphere of this region. The one of biggest city of the world, Istanbul, located directly in the both side of strait. The daily life of 12 million people of this city also connected with Bosphorus. The correct regulation of sanitary sewer system in Istanbul play important role for the water quality of Bosphorus. Istanbul's wastewater consisted many pumping systems, pre-treatment and biological wastewater treatment plants. Most part of treated wastewaters is discharged into the Bosphorus and small part to flow to Black Sea.

At the result of these discussions, it is to be seen, that the study of water quality of the Bosphorus is very important. We studied three water sample taken from south, middle and north parts of Bosphorus. The main interest was to study the changing of water quality from distances. at the first, the chemical analysis of Bosphorus water was studied. After this, the density, viscosity, speed of sound, vapour pressure etc. thermophysical properties analysing. In this work, the chemical analysis and density measurements are presented.

The chemical analysis of these samples (cations and anions) were analysed using the IRIS Intrepid II Optical Emission Spectrometer and DX 100 ion chromatography.

The density measurements were carried out using the Anton-Paar DMA HPM vibration-tube densimeter, which based on the dependence of the period of oscillation of a unilaterally fixed U - tube (Hastelloy C - 276) on its mass. The temperature in the measuring cell where the U – tube is located is controlled using a thermostat (F32 - ME Julabo, Germany) with an error of  $\pm 10$  mK and is measured using the (ITS-90) Pt100 thermometer (Type 2141) with an experimental error of  $\pm 15$  mK. Pressure is measured by pressure transmitters P-10 with a relative uncertainty of 0.1 % respectively, of the measured value.

An empiric equation of state for fitting of the  $(p, \rho, T)$  data of water samples of Bosphorus has been developed as a function of pressure, temperature and salinity of water. This equation is used for the calculation of the thermophysical properties of samples, such as isothermal compressibility, isobaric thermal expansibility, thermal pressure coefficient, internal pressure etc.

**Keywords:** Seawater, Bosphorus, Density.

## **SAC305 vs. SnPb Solder Joint Electrical and Mechanical Properties Measurements as Function of Working Temperature and Soldering Thermal Profile**

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The paper presents a comparative study between the electrical and mechanical properties of solder joints in case of lead-containing and lead-free alloys as function of the working temperature and the soldering thermal profile. The soldering method employed is Vapour Phase with two thermal profiles having different cooling rates: a slow one of 0.5K/s and a fast one of 4.0 K/s. For the measurement of the electrical properties, i.e. resistance of the solder joint, a new method has been developed and used in order to eliminate the errors caused by the thermo-electric effect. For the measurement of the mechanical properties, experiments have been designed to determine the shear force of the solder joints. Both measurements have been made while keeping the surface of the test boards at different working temperatures: 25°C, 75 °C and 125 °C.

Since the introduction of the RoHS European Directive, lead-containing alloys have stopped being used in the electronic industry with few exceptions like military equipment, medical equipment, aerospace and automotive fields. The more recent RoHS 2 European Directive forbids the use of lead-containing alloys even in the fields mentioned above. The designers, users and producers of such equipment are trying now to find solutions to replace the lead-containing alloys with lead-free alloys in order to comply with the latest European Directive. They have to do this keeping in mind the requirements for reliability and safety of such types of equipment.

The paper is answering this issue with two sets of measurements, electrical and mechanical, for two types of solder pastes, lead-containing SnPb and lead-free SAC305. Both the electrical resistance and the shear strength of solder joints have been measured by special designed tests as function of the working temperature and the soldering thermal profile. A test vehicle has been developed for these tests. The soldering method employed is Vapour Phase with two thermal profiles having different cooling rates: a slow one of 0.5K/s and a fast one of 4.0 K/s.

So far, measurements have shown that the electrical resistance of SAC305 solder joints is smaller than the electrical resistance of SnPb solder joints at room temperature (25 °C). Another observation is that the shear strength of SAC305 solder joints is greater than the shear strength of SnPb solder joints, especially when the fast cooling rate is used.

**Keywords:** Lead-containing, Lead-free, Solder joints, Electrical properties, Mechanical properties.

## **Residual Stresses in the Precipitation Layer of Gas Nitrided Alloy Steels**

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In this contribution, the residual stresses in the precipitation layer of selected alloy steels after gaseous nitriding process was investigated. Gaseous nitriding was performed at different temperatures and times, which resulted in different diffusion depth for atomic nitrogen. As a result of diffusion of atomic nitrogen, the crystal lattice of steel deforms, and as a consequence residual stresses in tension and compression appear. These residual stresses affect the strength increase and improvement of other surface properties of steels. Investigation of composition, cross-sectional morphology, hardness and residual stress of nitrided alloy steels (16MnCr5 and 31CrMoV9) was carried out using Electron Probe Micro Analysis (EPMA), Light Optical Microscopy (LOM), micro-hardness according to Vickers and X-ray Diffraction (XRD) techniques. The results show that intensity of stresses and hardness increase depend on the nitrogen diffusion depth, that is on nitriding process parameters.

**Keywords:** Gaseous nitriding, Residual stress, Precipitation layer, XRD.

## **The Influence of Silica Nanoparticles on Thermal Properties of Poly(lactide) Based Hybrid Materials**

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Poly(lactide) is biodegradable and biocompatible material derived from renewable resources and it is one of the most interesting subject for academic and industry researches today. In order to broadening the application of poly(lactide) (PLA) based materials, there is need for improving their mechanical and thermal properties. The incorporation of small amount of nanoparticles into a polymer matrix can markedly improved many properties of PLA based nanocomposites. In this paper, thermal properties of composites based on poly(lactide) and silicon(IV) oxide were investigated using the Differential Scanning Calorimetry. Two types of PLA were used (film grade type 4032D and bottle grade type 7032D designed for injection stretch blow molded applications). Nanocomposites were prepared with different level (2, 5, and 10 wt%) of silica nanoparticles with average size of primary particles 12 nm. Samples were prepared using a Haake Rheomix by melt mixing PLA and appropriate amounts of nanofiller at a temperature of 180 °C. Significant influence of the nanoparticles addition on the glass transition temperatures of obtained samples was not observed. The addition of 10 wt% of silica decreased T<sub>g</sub> value of pure PLA from 61.56 °C to 57.9 °C. The addition of silica nanoparticles influenced the significant change of the melting and crystallization temperatures for prepared composite materials.

**Keywords:** Thermal Properties, Poly(lactide), Nanocomposites, DSC.

## Thermodynamic and Thermo-Physical Properties of Liquid Li-Zn Alloys. Molecular Dynamics and CFM Study vs. Experiment

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The aim of this work is to obtain a complete description of thermo-physical properties of liquid Li-Zn alloys by analysing the mixing behaviour in terms of energetics and structure, through the study of thermodynamic, surface and transport properties.

Firstly, the measured thermo-physical properties in the liquid phase of  $\text{Li}_x\text{Zn}_{1-x}$  alloys, where  $x$  is changing from 0.09 to 0.4, are presented. The volume, transport and surface properties of the liquid Li-Zn alloys have been measured using draining crucible method (DC).

Secondly, the compound formation model (CFM) with an assumption of existence of the most favoured  $\text{LiZn}_2$  cluster, was applied to calculate the thermodynamic, thermo-physical and surface properties of the liquid Li-Zn alloys. Clustering effects have also been examined using two microscopic functions, i.e. the concentration fluctuation function in the long-wavelength limit and the Warren-Cowley short-range parameter obtained from molecular dynamics simulations.

The missing values of surface tension and viscosity have been modelled. The experimental data related to surface tension were compared to the relevant data obtained by modelling, using Butler model and CFM formalism. For viscosity calculations, the Kucharsky model was also applied. Experiments show a decrease of density, surface tension and viscosity with increasing Li content in liquid Li-Zn alloys. The surface tension data are in fair agreement with computed data using the Butler model and CFM formalism. Also, satisfactory matching in viscosity modelling is achieved. The examined diffusivity and macroscopic functions signify that the  $\text{LiZn}_2$  clusters can exist like transient structural units in the melt.

**Keywords:** Liquid Li-Zn alloys, Density, Viscosity, Surface Tension.

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## A New Class of Maraging Steel with Increase Heat Working Stability

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The aim of the paper is to increase the field work of Maraging steel up to 750°C and keep-up the mechanical properties as the classic M300 one. The new class of Maraging steel perform the following marks: the Ni content is fall down to 12 wt%, with the goal to increase the  $m \rightarrow \gamma$  transformation temperature; contains refractory alloying elements, such as Si, Nb, Ti, Mo, Zr. Increasing of the precipitation stability area and the martensitic phase by reducing the Ni content from 18% to 12%. The new steel belong to Schaeffer-martensitic zone in the DeLong diagrams, with ferrite factor  $F = Cr_{\text{equiv}}/Ni_{\text{equiv}}$  between  $0.5 \div 1$ .

The experimental researches presented in the paper were conducted in the structural kinetic transformations and in optimize the heat treatments parameters. It was evaluated the kinetic reactions by examine the typical expansion and diffusivity plots, in order to get the answer of the following two main questions:

- 1) Which is the increasing rate of  $\gamma \rightarrow \alpha$  temperature transformation, with the %Ni decreasing?
- 2) The precipitate and respectively solution temperatures are associated with the  $\gamma \rightarrow \alpha$  or  $\alpha \rightarrow \gamma$  structural temperature transformations?

The decreasing of Ni content increase the martensitic transformation temperature and in the same time the stability of intermetallic compounds (IMC) precipitates, up to 750 °C. At cooling, the shrinking of martensitic transformation hysteresis is also observed, as the effect of increasing the  $\gamma \rightarrow m$  temperature transformation, from about 200 °C, to about 400 °C. The heat working stability was perform by identify the recalescence points from expansion graphs, both at heating and cooling.

The heat treatment experiments managed to the optimum heat treated parameters are: solution at 950°C for 1h air cooling and aging at 550 °C for 3h air cooling.

After that the maximum tensile load indicate the uncommon value of 2090 N/mm<sup>2</sup> and for the proportionality limit the value was about 1930 N/mm<sup>2</sup>.

Our determinations have identified three types of precipitated phases: *orthorhombic phase*  $\gamma - Ni_3Mo$ ; *hexagonal phase*  $\eta - Ni_3Ti$ ; *tetragonal phase*  $\sigma - FeTi$ .

The presence of spherical IMC (2-9 nm in size), obliges dislocations in motion to form looping or shearing, with effect in increasing mechanical resistance, maintaining in the same time endurance characteristics at high level.

The presence of Si, Zr and Nb enhance structure stability at high temperature (for example the ultimate tensile strength at 550°C is about 1440N/mm<sup>2</sup>).

**Keywords:** Maraging steel, Expansion, Heat working stability (HWS).

### Dielectric Properties of *PZT-PBC-ZTIS* Piezoelectric Ceramics

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The main objective of this work is based on the synthesis and dielectric characterization of a new material in ceramic PZT with a perovskite structure  $ABO_3$ . We are interested in the study of the Quaternary system (doping in site A and site B) of general formula:

$Pb_{0.96}Ba_{0.02}Ca_{0.02}[(Zr_{0.52}Ti_{0.48})_{0.94}(Zn_{1/3},Ta_{2/3})_{0.03}(In_{1/3},Sb_{2/3})_{0.03}]O_3$  short *PZT-PBC-ZTIS*.

The sample selected for this study has been prepared by the method of synthesis with solid way. Heat treatment has been applied to these compositions at different temperatures: 1100, 1150, 1180 and 1200 °C successively to optimize the sintering temperature optimal where the density of the sample is maximum (near theoretical density) and therefore the product is better physical quality.

The study of dielectric properties of all samples showed a high permittivity dielectric  $\epsilon_r = 18018$ , low dielectric loss:  $\tan\delta = 7.62\%$ , for the composition sintered to 1180 °C included in the phase morphotropic zone (FMP).

**Keywords:** Ceramics PZT, Dielectric properties, Dielectric constant, Loss constant.

### Simulation of the Process of an Electro-Thermal Interaction in the Diode Laser System

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The physical-thermal characteristics of the modern thermal conducting materials, for example diamond of different types, in wide temperature range were investigated. It is shown the necessity to consider the interaction inharmoniousness of high orders of the atoms in crystals to satisfy a good agreement between calculated data with the experimental ones in definition of thermal conductivity of the materials and evaluation of the corresponding nonlinear coefficients. Spatial distribution of the thermal fields in the model with some discrete sources (elements) in the condition of electrical current flow was numerically and analytically simulated for the active region – heat transfer substrate (contact layer) system. The proposed calculation method for thermal fields allows optimizing the structure of the devices in order to increase their thermal stability.

**Keywords:** Power diode lasers, Thermal conductivity, Inharmoniousness of atoms interaction, Electro-thermal interaction, Diamond heatsinks.

### **Cooling Condition Effects on Phase Transformation, Crystal Structure and Microstructure of Cu-Al-Co Shape Memory Alloy**

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The purpose of this study is to investigate the cooling conditions of the Cu-%at.21Al-%at.1Co shape memory alloy on its crystal structure, transformation temperature and microstructure. For this purpose, samples were first subjected to a heat treatment at 850 °C for 1 hour and then cooling was applied at four different conditions. After cooling process, XRD, DSC, optical microscopy and micro-hardness measurements were conducted. The experimental studies showed that crystal structure, microstructure and transformation temperature of Cu-Al-Co alloy were affected from the cooling conditions, i.e., from decreasing cooling rate.

**Keywords:** Shape memory materials, Indentation and hardness, Phase transformation.

### **Status and Perspective of Production of Cement with Use Non-traditional Raw materials - Volcanic rocks of Uzbekistan**

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For the solution of this actual problem retrieval operations whenever possible uses of volcanic rocks as ferriferous a mineralizer and the conditional aliyumosilikatny component of a raw compound are carried out by production of clinker instead of traditional components, and their huge inventories are available in the territory of Uzbekistan in close proximity to each operating cement works.

**Keywords:** Glass of the phase, Aluminates, Alumferrite.

## Formation and Physical Properties of $\text{Sb}_2\text{O}_3$ - $\text{PbO}$ - $\text{MnO}$ Glasses

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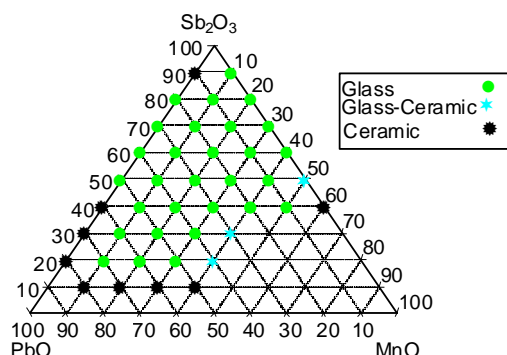
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The glass forming ability of antimony oxide  $\text{Sb}_2\text{O}_3$  was predicted by Zachariasen, and confirmed by various authors, either in oxide systems or in combination with halides or sulfides. Antimony has been incorporated in oxide glasses and some antimony phosphate glasses have been reported. Many glass samples from these systems contain micro crystals and show local variations in chemical composition, which increases light scattering. This study is about the ternary glasses based on antimony oxide in association with  $\text{PbO}$ ,  $\text{MnO}$ . We determine the glass forming ranges, glass stabilities and some physical properties.

| Composition<br>(80-x) $\text{Sb}_2\text{O}_3$ -20 $\text{PbO}$ -x $\text{MnO}$ | T <sub>g</sub> (°C) | T <sub>x</sub> (°C) | T <sub>p</sub><br>(°C) | T <sub>x</sub> -T <sub>g</sub> | Density<br>(g/cm <sup>3</sup> ) | Vickers micro-<br>hardness(Kg/mm <sup>2</sup> ) |
|--|---------------------|---------------------|------------------------|--------------------------------|---------------------------------|---|
| 05   | 280                 | 402                 | 432                    | 122                            | 5.308                           | 261.02  |
| 10   | 291                 | 444                 | 484                    | 153                            | 5.313                           | 296.61  |
| 15   | 298                 | 458                 | 498                    | 160                            | 5.384                           | 318.41  |
| 20   | 310                 | 496                 | >500                   | 186                            | 5.542                           | 336.84  |
| 25   | 312                 | 467                 | /                      | 155                            | 5.557                           | 362.63  |
| 30   | 317                 | 467                 | >500                   | 150                            | 5.564                           | 383.82  |
| 35   | 332                 | 441                 | /                      | 109                            | 5.565                           | 394.63  |

*Summary of data on various physical parameters of  $\text{Sb}_2\text{O}_3$ -  $\text{PbO}$ - $\text{MnO}$  glasses*



*Compositional limits for glass formation in the  $\text{Sb}_2\text{O}_3$ -  $\text{PbO}$ - $\text{MnO}$  system.*

**Keywords:** Density, Antimony oxide, Glass.

## **Influence of the Magnetic Field on the Morphology of the Wear of the Cutting Tool**

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This paper reports the study of the influence of a magnetic field on the morphology of the wear of the cutting tool as a function of the cutting speed during the cutting operation, and observed the weight losses (wear) and their morphologies. The wear of the cutting tool was quantified by weight loss during cutting. While carrying out experiments, we have noticed the existence of a critical value of the magnetic field intensity  $H = 16.5 \text{ kA.m}^{-1}$ , for which the depth of the crater wear of cutting is minimal and the cutting edge of the cutting tool is preserved. The presence of the magnetic field in the manufacturing contact modifies completely the morphology of cutting, shape of chips of manufacturing, and quality of the surface state of the cutting edge. Moreover, the increasing of the magnetic field was found to change the cutting temperature. In the present manuscript we presented the different behaviours of manufacturing observed with and without magnetic field.

**Keywords:** Cutting tool, Magnetic field, Surface quality, Wear.

## **Investigation of the Temperature Stability of Perovskite Phase Formation and the Electromechanical Properties of $\text{Pb}(\text{Zr}_{1-x}\text{Ti}_x)\text{O}_3$ Ceramics Modified with Certain Additives**

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The  $\text{Pb}(\text{Zr}_{1-x}\text{Ti}_x)\text{O}_3$  ceramics with perovskite structure is used in various fields in particular in electronics because of its interesting dielectric and electromechanical properties. However for specific application (ex. Transducers), It is necessary to develop reproducible ceramic with characteristics according to the temperature. In this objective, the study focused on the development and characterization of powders precursors and based PZT pure and doped. But also to link their electromechanical properties on their composition in particular on the nature of substitutions in A site and B site as well as in their chemical homogeneity and their microstructure. Several compositions  $\text{Pb}_{1-x}\text{M}_x[(\text{Zr}_{0.52}\text{Ti}_{0.48})_{0.98}(\text{Mg}_{1/3}\text{Sb}_{2/3})_{0.01}(\text{Ni}_{1/3}\text{Nb}_{2/3})_{0.01}]\text{O}_3$  (M: Gd; Eu; Ca; Sr,  $x = 2\%$ ) was synthesized by conventional ceramic method and characterized by the point of structural, microstructure and electric view. The results of these studies have been discussed.

**Keywords:**  $(\text{Zr}_{1-x}\text{Ti}_x)\text{O}_3$  ceramics, Perovskite structure, PZT pure and doped, Conventional ceramic method.

## Study of Glass Formation in the $\text{Sb}_2\text{O}_3\text{-Li}_2\text{O- MoO}_3$ Ternary System

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Antimony oxide based glasses are ones of the Heavy Metal Oxide glasses. They are subject of many researches in the recent years for their low phonon energy, high refractive index and large optical transmission spectrum [1,3]. In this work, new Vitreous system based on antimony oxide  $\text{Sb}_2\text{O}_3$  have been investigated. The  $(80-x) \text{Sb}_2\text{O}_3\text{-}20\text{Li}_2\text{O-xMoO}_3$  glasses with the value of  $x$  (ranging from 0 to 40 mol%) were prepared. A number of studies, viz. differential scanning calorimetry, elastic modulus, thermal expansion, microhardness, infrared and UV transmission spectra on these glasses were carried out as a function of molybdenum ion concentration ( $\text{MoO}_3/\text{Sb}_2\text{O}_3$ ).

Density decreases linearly from  $4.96 \text{ g}\cdot\text{cm}^{-3}$  to  $4.48 \text{ g}\cdot\text{cm}^{-3}$  as  $\text{MoO}_3$  replaces  $\text{Sb}_2\text{O}_3$ . However the evolution of glass transition temperature, thermal expansion and microhardness is not monotonous.

**Keywords:** Antimony glasses; Physical properties; Mechanical properties; Optical properties.

## Fatigue Damage Modelling of Polymeric Matierials: Case of HDPE

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In this Paper, the cumulative fatigue damage behavior for HDPE-100 was experimentally investigated. The S–N curve was, first obtained to establish the fatigue life of The HDPE-100 subjected to constant stress levels. The Cumulative Fatigue Damage versus Number of Cycles (D–N) curve was deduced from stiffness degradation versus Number of Cycles (E–N) to characterize the three-stage cumulative fatigue damage.

Based on this three stage damage trend, the remaining fatigue life of the second stage was numerically predicted by considering a double term power damage accumulation model originally proposed for composite materials since the Linear Cumulative Damage rule, i.e., the Palmgren–Miner rule, did not show good agreement. Further, the specimen stiffness during the preliminary constant-amplitude fatigue tests was utilized to describe the fatigue damage and the corresponding damage curves were developed to predict the cumulative fatigue life.

By comparing the prediction results with the experimental data, it shows that the Miner's rule fails to evaluate the cumulative fatigue life, while the non-linear damage theories based on the variation of the stiffness provide good estimated results of the cycle ratio of the second stage.

The proposed model is found to be more accurate than existing models, both in modeling the rapid damage growth early in life and near the end of fatigue life. The parameters for the proposed model are obtained with experimental data and numerical results illustrate that the proposed model is able to accurately fit several different sets of experimental data.

**Keywords:** HDPE-100, Fatigue damage, Semi-crystalline, Damage accumulation, Stiffness degradation, Two-bloc loading.

## **Study of Thermal Conductivity and Morphology of Bio-Polymer Based Nanocomposites with Expanded Graphite and Montmorillonite**

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The polymer based composites have been used for several years in many industrial fields. It allows an improvement of the pure polymer properties or the access to some almost non-existent properties of the neat materials such as gas permeability, fire resistance, electrical and thermal conductivity. In recent years, the accumulation of toxic waste and the degradation of the ozone layer, among others, led to a gradual replacement of petrochemicals materials by biodegradable polymers coming from renewable resources. Aliphatic polyesters represent an important family of biodegradable polymers. Our study focuses on two polymers of this family which are the poly (lactic acid) (PLA) and the poly (butylene succinate) (PBS). It aims, on one hand, to improve their barrier properties to some gases and water vapor, and on the other hand, to make these materials heat conductors.

Among different minerals used to reinforce polymers, two of them were studied. The first one, organically modified montmorillonites (OMMT) were particularly interesting since a small amount (almost 5 wt %) is required to achieve a significant improvement in the mechanical and barrier properties of the polymer. The second one, expanded graphite (EG) proved its capacity to increase the heat transfer properties of polymers. In this study, we present the effects of silane functionalisation (f) and the particles size distribution on the thermal properties and the morphology of prepared nanocomposites. To facilitate the implementation, the PLA was made more ductile by adding plasticizer: 15 wt % of Triethyl Citrate (PLA15). OMMT nanocomposite samples were prepared by melt intercalation in a mini twin screw extruder and by casting in chloroform and EG nanocomposites were prepared in a melt mixer.

Different series of samples were studied: i) PLA15/PBS + 4.5 and 6 wt % OMMTf/OMMT, and ii) PLA15/PBS + EGf/EG of 50 / 200  $\mu\text{m}$  (particle sizes) at two amounts 7 and 15 wt %. The nanocomposite properties characterization was performed by different techniques: mechanical and thermal properties were obtained by tensile test and differential scanning calorimetry (DSC); X-ray diffraction (XRD) and rheological analysis showed the morphology of nanocomposites; the thermal diffusivity measurements were performed by flash method and the silane grafting were evaluated by Fourier transform spectroscopy (FTIR).

**Keywords:** Nanocomposites, PLA, PBS, Montmorillonites, Expanded graphite, Barrier properties, Thermal properties.

## Structural and Optical Properties of Tin Oxide Thin Films Prepared by Spray Ultrasonic Technique

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Transparent conducting SnO<sub>2</sub> films were fabricated by employing an inexpensive, simplified spray ultrasonic technique using an ultrasonic generator at different substrate's temperatures (300, 350, 400, 450 °C). The structural studies reveal that the SnO<sub>2</sub> films are polycrystalline (at 350, 400, and 450 °C) with preferential orientation along the (200) and (101) plane, and amorphous at 300 °C. The crystallite size of the films was found to be in the range of 20-50 nm. The optical transmittance in the visible range and the optical band gap are 75% and 3.9 eV respectively. The films thicknesses were varied between 466 nm and 1840 nm. This simplified Ultrasonic spray technique may be considered as a promising alternative to conventional spray for the massive production of economic SnO<sub>2</sub> films for solar cells, sensors and opto-electronic applications.

**Keywords:** Tin oxide, Thin films, Spray ultrasonic, Structural properties, Optical properties.

## Fatigue Life Calculation By Cycle Counting Method and Spectra Methods Under Random Loading

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The vast majority of structural failures are due to some sort of fatigue in the component material caused by stress. Fatigue damage increases with applied load cycles in a cumulative manner. Fatigue damage model plays a key role in life prediction of components and structures under random loading. These cyclic or repeated loads often lead eventually to structural failure caused by fatigue.

Damage is calculated in the time domain using stress cycle counting methods such as the Rainflow counting algorithm which is used here as a control method.

The aim of this paper is the evaluate methods of predicting fatigue damage. examination of the performance of the “ Damaged Stress Model (DSM)”, proposed and validated, against other models in fatigue under random loading before and after reconstruction of the load histories.

To achieve this object, some linear and non-linear models proposed for fatigue life estimation and a batch of specimens made of 6082T6 aluminum alloy is subjected under random loading.

Damage was cumulated by Miner's rule, (DSM), Henry model and Unified Theory (UT) and cycles were counted with the rain-flow method with various number of classes.

A computing Matlab-based algorithm of the fatigue life prediction methodology was developed where studied models are connected cycle by cycle to the Wöhler curve before and after signal reconstruction.

Experimental data on high-cycle fatigue by complex loading histories with different mean and amplitude stress values are analyzed for life calculations and models predictions are compared.

**Keywords:** Damaged stress model, Rainflow, Performance, Random loading, Number of class.

## **Influence of Fatigue on Mechanical Properties of Kevlar Fibers Epoxy Composite and Characterized Damage by Acoustic Emission Technique (AE)**

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This paper presents the results of experimental investigations of the effects of fatigue of composite materials. The plates of Kevlar fiber and SR 1500 epoxy resin with SD 2505 composite were realized by vacuum molding. This operation is done under a 0.3 bar vacuum for 6 hours, with the help of vacuum pump, followed by 8 hours polymerization in 80°C electric heater. Afterwards specimens are cut in the recommended dimensions (200x20x1 mm).

Experimental tests were carried out on a standard hydraulic machine INSTRON 8516. The capacity of machine is  $\pm 100$  kN, which can be used for static and fatigue tests. The machine is interfaced with a dedicated computer for controlling and data acquisition.

In static tests, the specimens were loaded at a constant rate of 1 mm/min. The fatigue tests were performed using sinusoidal type of waveform at a displacement control with frequency of 10 Hz.

The protocol of the tensile tests of studied composite materials is done in 3 stages:

- the 1st stage of loading is done at a constant speed of 1mm/mn under the displacement controlled up to 50% of displacement to the rapture in statics tests ;

- the 2nd stage is a phase of fatigue with a form of sinusoidal wave of 10 Hz frequency with the amplitude of 10% of displacement to the rapture. Three numbers of fatigue cycles were chosen and they are 500, 5000 and 50000 cycles;

- the 3rd stage is a phase of unloading of the specimens after being subjected to fatigue with the imposed number of cycles.

At the end of the 3rd stage the specimens are broken directly by 1mm/min speed of traction.

The local damage in composite materials was identified and characterized by acoustic emission technique (AE).

In this paper, it is investigated how these three stages of stiffness degradation. The first stage of deterioration by fatigue is observable by the formation of damage zones, such as fiber/matrix interface failure and pull-out of fibers from the matrix. Hence damage starts very early, and a sharp initial decline of the composite's stiffness is observed. This early damage is followed by a second stage of very gradual deterioration of the material, characterized by a gradual reduction of the stiffness. More serious types of damage appear in the third stage, such as fiber fracture and instable delamination growth, leading to an accelerated decline.

Degradation of mechanical properties was observed. In fact, elastic modulus and stress were decreased.

**Keywords:** Kevlar, Epoxy, Fatigue, Acoustic.

## **Molarity Effect on The Optical and Structural Properties of Sprayed Indium Oxide Thin Films**

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Transparent conductive Indium oxide ( $\text{In}_2\text{O}_3$ ) thin films were deposited on glass substrates by ultrasonic spray technique. The study was in one series by varying the molarity from 0,05 to 0,3 mol/l at substrate temperature 400°C. To investigate the influence of precursor molarity on structural, optical and electrical properties of indium oxide thin films, several characterizations were carried out such as: XRD to determine the grains size and the stress, SEM for microstructural study and to determine films thickness, EDS to assure chemical composition of the films and UV-Vis-Nir Spectroscopy for optical studies like the absorption coefficient, the optical gap, the disorder and the refraction index. The results of both characterizations are presented in this report.

**Keywords:** Indium oxide, TCO, Ultrasonic Spray, optical and structural properties.

## **Simulation of carbon ion implantation in mono-crystalline silicon substrates**

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Silicon carbide is a very promising material for electronic industry. Among the various methods which may be used to elaborate this material, carbon ion implantation (into silicon wafers) is one of the interesting tools. In this work, several phenomena related to carbon ion implantation into Si(100) targets were simulated. The investigation was performed using Crystal- TRIM code under different conditions. Two particular cases were taken into account: (i) implantation of 80 keV  $\text{C}^+$  with a dose of  $2.7 \times 10^{17}$  ion/cm<sup>2</sup> at room temperature; (ii) implantation of 40 keV  $\text{C}^+$  with a dose of  $6.5 \times 10^{17}$  ion/cm<sup>2</sup> at substrate temperature of 400°C. To avoid the study of channelling phenomena, we used a tilt angle of 7°.

Several results were obtained and compared with RBS and ERDA measurements provided in literature. The simulated carbon profiles were in agreement with experimental, in particular for ERDA case. Besides, the radiation damage was predicted for interstitials and vacancies defects. The projected range of these defects ( $R_d$ ) was inferior to the projected range of carbon ( $R_p$ ) atoms which is expected by literature.

**Keywords:** Carbon, Silicon, Ion implantation, Crystal-trim code.

## Perovskite Formation and Dielectric Responses in PZN Modified PMF-PZT Ceramics

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PMF-PZN-PZT ( $0.01\text{Pb}(\text{Mo}_{1/3}\text{Fe}_{2/3})\text{O}_3-x\text{Pb}(\text{Zn}_{1/3}\text{Nb}_{2/3})\text{O}_3-(0.99-x)\text{P}(\text{Zr}_{0.53}\text{Ti}_{0.47})\text{O}_3$  piezoelectric ceramics), where  $x = 0.00, 0.01, 0.03, 0.05$  and  $0.07$  were prepared by a conventional mixed-oxide method. The results show that the pure perovskite phase forms in these ceramics. X-ray diffraction analysis indicated that the phase of the material is a MPB (morphotropic phase boundary) structure. The effects of PZN content on the crystal structure and electrical properties were investigated. optimal dielectric properties were achieved at composition  $x = 0.07$  ceramics by calcination at  $800^\circ\text{C}$  and sintering at  $1180^\circ\text{C}$ , with a curie temperature of approximately  $430^\circ\text{C}$ . These results clearly show the significance of PZN in controlling the electrical responses of the PMF-PZN-PZT system.

**Keywords:** Perovskite, Dielectric properties, MPB, Curie temperature.

## Thermophysical Properties of Nitrous Oxide ( $\text{N}_2\text{O}$ ) from a New Highly Precise *ab initio* Pair Potential

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Nitrous oxide is an important industrial fluid. Its application ranges from the use as an anaesthetic in medicine, the use as a propellant in food industry, to the use as a performance increasing oxidant in rockets and jet engines. High-precision thermophysical fluid properties of nitrous oxide are therefore of great importance for the efficient design of the respective applications.

Computational methods allow for the theoretical calculation of thermophysical properties. The pair interaction energies for nitrous oxide have been calculated using highly precise quantum-chemical *ab initio* methods, and an analytical pair potential function has been fitted to the computed interaction energies. The potential function has been used to calculate the second virial coefficient, shear viscosity and thermal conductivity of dilute nitrous oxide gas. The results have been compared with experimental data.

**Keywords:** Nitrous oxide, *ab initio*, Pair potential, Thermophysical properties.

## The Investigation of Usability of Wasted Cross-Linked Polyethylene in Production of Insulation Materials

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Cross-linked polyethylene, commonly abbreviated XPE, is a form of polyethylene with cross-links. It is used predominantly in insulation for heat transfer pipes, and high tension electrical cables. The amount of plastic waste is on the rise day after day. It is related with green house gas emissions and hazardous potential if left untreated at the landfill. This work explores the recycling of cross-linked polyethylene waste-plastic that is generated at a considerable amount from the insulation industry. It also undertakes the usability of the cross-linked polyethylene waste by mixing ready plaster prescription at different waste weight ratio, i. e. 0%, 5%, 10%, 15%, 20%, 25%, 30%, and 35%. The heat transmission coefficient of every sample was measured by Shoterm QTM-D2 equipment. The changes of heat transmission coefficient is found depend on weight ratio waste XPE.

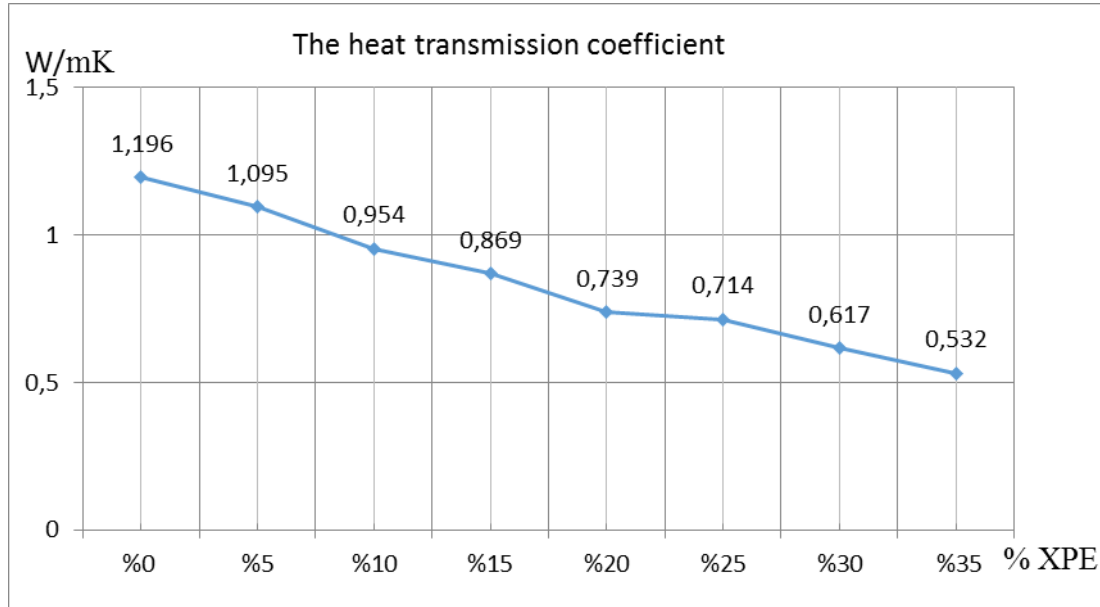


Fig. 1: The changes of the heat transmission coefficient in ready plaster prescription at different waste weight ratio

The heat transmission coefficient of ready plaster prescription without any wasted XPE is measured 1,196 W/mK. The heat transmission coefficient is decreasing from 1,196 W/mK to 0,532 W/mK with improving XPE waste in ready plaster prescription.

**Keywords:** XPE, Cross-linked, Insulation.

## Mechanical and Thermodynamic Properties of $Zr_2Al$ Under High Temperature and Pressure From First-Principles Calculations

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Lattice constants, Mechanical and thermodynamic properties of hcp structure  $Zr_2Al$  are studied using first-principles calculations based on the plane wave pseudopotential density functional theory method within the generalized gradient approximation (GGA) for exchange and correlation. It is demonstrated that the ratio  $c/a$  of about 1.206 is the most stable structure for the hcp  $Zr_2Al$ , which is consistent with the experimental data. Through the quasi-harmonic Debye model, in which the phononic effects are considered, the dependences of relative volume  $V/V_0$  on pressure  $P$ , cell volume  $V$  on temperature  $T$  are successfully obtained. The variations of the Debye temperature  $\Theta$ , the thermal expansion  $\alpha$ , the Grüneisen parameter and the heat capacity  $C_v$  with pressure  $P$  and temperature  $T$  are investigated systematically in the ranges of 0–120 GPa and 0–2000 K.

**Keywords:** Mechanical properties, thermodynamic properties, Debye temperature, DFT.

## Proposal to Reduce GUM's Recommendations to Practice in Thermophysics

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Since the first formulation of the principles of flash techniques, given by Parker et al. in the 60-ies of the last century, lots of models were developed to examine diffusivity from the thermal response of a sample. Current models mainly consider both, the interaction of a sample with its environment and the finite pulse length of the thermal impact. They do not consider any thermal effect coming from the sample itself. Till today the basic idea in flash techniques traces back to the thermal balance of a thermally inert sample without any consumption or release of heat during the measurement process. This basic assumption more and more is not fulfilled for complex materials or processing materials. Thus, current models often do not describe the thermal response of a sample in a sufficient way. This causes non negligible contributions to the uncertainty of the measurement result – mainly the so called Model Specific Uncertainty MSU. Currently only rough estimations can be done, because models operate numerically and are like a black box for the user. Therefore this contribution cannot give a final method how to formulate the MSU sufficiently. But it tries to propose a concept to formulate the uncertainty of diffusivity results using three fundamental sources of uncertainty: the Model Specific Uncertainty MSU, the Sample Specific Uncertainty SSU and the Equipment Specific Uncertainty ESU. This construction principle is applied to dilatometry and DSC methods too. Results are shown and discussed

**Keywords:** Dilatometry, DSC, Flash Techniques, Uncertainty Model.

## Production Technology of Clinker and Cement Raw Mix Bicomponent Using Gabbro from Akchinsk Field

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Open Joint Stock Company "Angrentsement" to the 90s of the last century specialized in the production of white and colored cements. For the production of white Portland cement clinker raw materials were limestone, kaolin clay slurry on the basis of which had a high humidity (45 %). Due to the fact that the firing of white Portland cement clinker was carried out at 1500-1550°C and demanded high costs of liquid fuels - oil, which at that time lacked, at the beginning of 1990 the enterprise ceased its activities. Currently, the company carries out a number of activities on modernization, technical and technological re-equipment of production. In this regard, of particular importance issues related to economical use of energy resources in the production of clinker, which is necessary to establish the possibility of using solid fuel instead of liquid, to explore the possibilities of formation of highly reactive compounds raw mixes for clinker production on local raw materials and man-made waste on firing which complete digestion of calcium oxide and the formation of clinker minerals of basic can occur at relatively lower temperatures than conventional firing temperature of raw mixtures. In this regard, the volcanic rocks, as previously noted, are of particular interest as a conventional aluminosilicate materials with low melting point. Given the geographical proximity to the LLC "Angrentsement" and to develop recommendations for possible use in raw mixtures as a conditional aluminosilicate component selected gabbro Akchinskogo Oilfield. As part of the carbonate used limestone deposit "Podzemgaz".

Calculation of two-component raw mixtures was conducted at a constant value of 0.90 kN and the changing values of silicate  $n$  (1.94; 1.95; 2.10) and alumina  $p$  (1.44; 1.46; 1.64) modules. Given the possibility of use as a solid fuel coal mine "Angren" when performing the calculations take into account the composition of the raw mixes additive ash at the highest 20% ash content. Gabbro is vysokoaluminatnoy matrix containing on average 19.65%  $Al_2O_3$ , ie almost as much as in the alumina kaolin clay (19.99%), so the resulting clinker with its use is also characterized by a high content of  $C_3A$  (from 8.89 to 9.82 %) and  $S_4AF$  (11.25 to 12.74 %), which could have a negative effect on the corrosion resistance of cements. In this regard, a composition of the raw material mixture was calculated at a relatively high value of  $n = 2.25$  and low  $p = 1.25$  (Table 1). To increase the silica modulus in the feed mixture introduced an additional component - the sand, which is formed during the enrichment of fluorite ores. The amount in the mixture was 11.87 %.

Taking into account the chemical composition of the clinker was determined theoretical amount of heat during the firing of new clinker raw mixes. It was found that the theoretical heat of clinker, depending on the values of  $n$  and  $p$ , ranging from 1690.79 to 1712.14 kJ / kg, which is 160-178 kJ / kg less than the heat of clinker traditional limestone and kaolin raw mixture (Table 2). Increasing values of silica alumina and reduced module module does not have a material impact on the theoretical heat of clinker new raw mixes. Determination of the mineralogical composition of clinker showed that the content of  $S_3S$ ,

Table 1. Raw material composition of the mixtures based on gabbro Akchinskogo field Number values of the raw mix composition, %

KH  $n$   $p$  \* Coal Limestone Gabbro (ash) Sand (departure)

|   |      |      |      |       |       |            |
|---|------|------|------|-------|-------|------------|
| 1 | 0.90 | 1.94 | 1.46 | 73.97 | 20.03 | 30 (6.0) - |
| 2 | 0.90 | 1.95 | 1.44 | 73.97 | 24.03 | 10 (2.0) - |
| 3 | 0.90 | 1.95 | 1.46 | 73.97 | 22.03 | 20 (4.0) - |
| 4 | 0.90 | 2.10 | 1.64 | 79.26 | 18.74 | 10 (2.0) - |
| 5 | 0.90 | 2.10 | 1.64 | 79.30 | 17.70 | 15 (3.0) - |
| 6 | 0.90 | 2.10 | 1.64 | 79.50 | 16.50 | 20 (4.0) - |
| 7 | 0.90 | 2.25 | 1.25 | 76.34 | 11.79 | - 11.87    |

• average ash content of coal Angren deposit accepted 20%.

S2S and the amount of C3A + S4AF they comply with the requirements of GOST 22266 for clinker manufacturing Portland cement and sulphate- pozzolan cement for general construction purposes. Based on the experience of establishing the reactivity of raw mixtures with volcanic rocks, firing them in the form of tablets silit realized in the laboratory oven at a temperature range of 900 – 135 °C at intervals of 50 – 100 °C and one hour at each temperature exposure.

Table 2 Chemical composition of clinkers( Values Contents oxides %)

| KH n p | SiO <sub>2</sub> | Fe <sub>2</sub> O <sub>3</sub> | CaO  | MgO   | Al <sub>2</sub> O <sub>3</sub> | pr   | qteor |                   |
|--------|------------------|--------------------------------|------|-------|--------------------------------|------|-------|-------------------|
| 1      | 0.90             | 1.94                           | 1.46 | 19.98 | 6.10                           | 4.19 | 61.70 | 2.02 6.01 from    |
| 2      | 0.90             | 1.95                           | 1.46 | 19.92 | 6.07                           | 4.16 | 61.71 | 2.11 6.02 1694.42 |
| 3      | 0.90             | 1.95                           | 1.44 | 19.88 | 6.03                           | 4.18 | 61.74 | 2.17 6.00 1694.65 |
| 4      | 0.90             | 2.10                           | 1.64 | 20.53 | 6.06                           | 3.70 | 62.80 | 1.74 5.17 1707.17 |
| 5      | 0.90             | 2.10                           | 1.64 | 20.53 | 6.08                           | 3.71 | 62.82 | 1.71 5.15 1705.56 |
| 6      | 0.90             | 2.10                           | 1.64 | 20.45 | 6.06                           | 3.70 | 63.01 | 1.65 5.13 1710.62 |
| 7      | 0.90             | 2.25                           | 1.25 | 20.93 | 5.16                           | 4.13 | 62.70 | 2.94 - 1712.14    |
| 8'     | 0.87             | 21.82                          | 6.12 | 1.03  | 68.6                           | 0.54 | 1.73  | 1872.11           |

8'- technological parameters, Chem. composition and heat klinkerobrazovaniya Lime kaolin raw mixture LLC " Angrentsement ."

Determination of free calcium oxide in clinkers showed that absorption of lime and clinker completion by firing raw mixes containing gabbro Akchinskogo Oilfield occurs practically at 1350C , which is 100 to 150 °C below the temperature of calcination of limestone , kaolin raw batches . Synthesized at 1300 °C is characterized by the structural heterogeneity of clinkers : in some parts of the cleavage clearly marked accumulation of crystallized grains belita oval, between which the hexagonal prisms and alite and brownmillerite rhombic crystals that are on the stage of growth and dissolution of clinker weight. Marked some areas where around alite grains arranged cubic crystals of tricalcium aluminate . Fired at 135°C promotes reception clinker with loose packing major minerals in the intergranular pore space observed that determines the relatively high grindability synthesized clinkers . Cements based on them are characterized by rapid set strength at initial stages of hardening, uniform and steady rise in its time with the achievement of 28 days to 48,6-52,4 MPa.

A high efficiency gabrro Akchinskogo field for the production of low-temperature clinker. With this kind of volcanic rocks is reached about 12-18 % savings coolant and increase productivity rotary kilns by 10-15%.

**Keywords:** Raw materials, Clinker, Minerals.

## Heat Treatment of Wood

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The wood has the major disadvantage of being susceptible to biodegradation agents and untreated, it can quickly deteriorate. To give the wood a better durability against agents and insects, and prolonged use of chemical treatments are carried out before its implementation. However, these treatments often use chemical products harmful to the environment.

In the context of environmental protection, the heat treatment may be an interesting alternative to the agents of decay.

In the present paper, three-dimensional equations for coupled heat and mass conservation equations for wood are solved to study the transient heat and mass transfer during high thermal treatment of wood. The model is based on Luikov's approach, including pressure. The model equations are solved numerically for the temperature and moisture content histories under different treatment conditions. The simulation of the proposed conjugate problem allows the assessment of the effect of the heat and mass transfer within wood. A parametric study was also carried out to determine the effects of several parameters such as initial moisture content and the sample thickness on the temperature, pressure and moisture content distributions within the samples during heat treatment.

**Keywords:** Heat and Mass Transfer, High Temperature Wood Treatment, Mathematical Modeling

## Synthesis and Characterization of Ni Containing LaAlO<sub>3</sub> Perovskite

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Our contribution has focused on the synthesis and characterization of Nickel containing LaAlO<sub>3</sub> perovskite, La (Al, Ni) O<sub>3-δ</sub> by a co-precipitation method. Nano-powders were successfully synthesized using nitrate salts of lanthanum, aluminum and nickel as cations precursors and mixture of sodium hydroxide such as base precipitant by this method and calcined at low temperatures. They were characterized by several techniques: Fourier transform infrared spectroscopy (FT-IR), thermogravimetric and differential thermal analysis (TGA/DTA), X-ray diffraction (XRD), scanning electron microscopy (SEM), and laser diffusion. All the results for physico-chemicals characterizations show that the crystallization temperature of the La (Al, Ni) O<sub>3-δ</sub> precursor gels precipitated are estimated as 780 °C by TG/DTA. The XRD pattern of the La (Al, Ni) O<sub>3-δ</sub> precursor gels calcined at 700 °C for 6 h have a perovskite structure and the presence of crystalline impurities is not found. The microstructure and morphology of the compounds show that the particles are nearly spherical in shape and are partially agglomerated.

**Keywords:** Perovskite, Coprecipitation, Thermal Analysis.

## Mössbauer Study of Feco-8nb-30b Nanocomposite Prepared by Mechanical Alloying

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Nanostructured Fe<sub>31</sub>Co<sub>31</sub>Nb<sub>8</sub>B<sub>30</sub> alloy samples were prepared by the mechanical alloying process using planetary high-energy ball mill. The alloy formation and different physical properties were investigated as a function of milling time, t, (in the 0–125 h range) by means of the X-ray diffraction (XRD) technique, scanning electron microscopy (SEM), and Mössbauer spectroscopy. The Mössbauer spectra were computer fitted using Mosfit program. The crystallite size reduction down to about 9 nm is accompanied by the introduction of internal strains up to 1.4 % (root-mean square strain, rms). Nb(B) and Fe(Co) solid solution are formed after 1 and 25 h of milling, respectively. Above 10 h of milling, the paramagnetic behavior of the amorphous phase, as evidenced by Mössbauer spectrometry, is due to the presence of non magnetic elements (Nb and B). After 125 h of milling, an amorphous matrix (~95%), where FeCo and Fe<sub>2</sub>B nanograins are dispersed, is obtained. The reduction of the magnetic moment leads to the decrease of the average hyperfine magnetic field,  $\langle H_{hyp} \rangle$ . Curie temperatures which are close to the ambient temperature reflect the compositional non-homogeneity of the paramagnetic amorphous matrix.

**Keywords:** Mechanical alloying; Nanocomposites; Mössbauer spectrometry.

## Numerical Study of Two Phase Laminar Convection Nanofluid In Microchannel

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A numerical study has been performed by using two phase method on the convective heat transfer of Al<sub>2</sub>O<sub>3</sub>/water nanofluid flowing through a microchannel under the laminar flow conditions (nanofluids are liquid suspensions of nano-sized particles).

The effects of nanoparticles concentrations, Reynolds number and diameter-size of particle are investigated on the flow and the convective heat transfer behavior.

The results obtained by the FLUENT software show that the presence of nanoparticles in the base fluid results in a considerable increase of heat transfer.

Heat transfer coefficient increases by increasing the concentration of nanoparticles in nanofluid and Reynolds number but it decreases as the particle's diameter increases.

**Keywords:** nanofluid/ two phase/ heat transfer/ FLUENT.

## Development and Characterization of Triaxial Porcelain System

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Triaxial porcelain is one of the most widely studied ceramic systems. In this study, The porcelain is obtained by the mechanical alloying of kaolinitic clay (50 wt. %), quartz (25 wt. %) and feldspar (25 wt. % powders. The pressed samples were heated at different temperatures (1100–1300 °C). The structural and mechanical changes during firing temperatures were followed by X-ray diffraction, measuring the bulk density, porosity and flexural strength. The results show that the samples achieved higher densities (max. 2.52 g cm<sup>3</sup>) in the entire temperature range (1100–1300 °C). The final porosity of porcelain tiles results from the incomplete densification of the material during the stages of processing. at 1200°C, XRD studies revealed that the crystalline phases are mullite and quartz

**Keywords:** Microstructure; Porcelain; Mechanical properties.

## Buoyancy Effect on Laminar Mixed Convection In A Horizontal Tube

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Laminar mixed convection heat and mass transfer in fluid flows constitute a subject which continues to cause much interest. This continuous interest is due to the occurrence of these transfers in nature and in many industrial applications. For example, the design of heat exchangers, solar energy collectors, thermo-protection, chemical distillatory processes and others. In all these situations, the flows are characterized by the presence of temperature and / or concentration gradients which generate thermal and / or solutale buoyancy forces. For this reason, a great number study numerical and experimental relate to the heat and mass transfer in mixed convection in various geometrical configurations.

The numerical majority studies which deal with this subject are based on the resolution of the transport differential equations (mass, momentum, energy and concentration) in their parabolic form. Because of the phenomenon importance, we are interested, in this study, with the solution of these same equations in their elliptic form by considering a three-dimensional fluid flow in mixed convection heat and mass transfer in vertical tube with aiding and opposing buoyancy forces. This tube is divided into three parts various lengths ( $L_1$ ,  $L_2$ ,  $L_3$ ), the walls of the first and third parts are considered adiabatic and impermeable whereas that located in the central part is subjected to uniform heat and mass fluxes at the walls. The elliptic differential equations governing the phenomenon are discretized by the finite volume method. The effects of buoyancy ratio  $N$  on the velocity, temperature and concentration profiles and the Nusselt number and Sherwood number have been presented. The results show that the buoyancy effects have a significant influence on the characteristics of fluid flow, heat and mass transfer.

**Keywords:** Heat transfer; Mass transfer; Horizontal Tube (3D); Elliptic Equations; Buoyancy Ratio.

## Deposition of ZnO Thin Films on Glass, ITO and ZnO:Al Coated Glass Substrates

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Zinc Oxide (ZnO) is one of the most important group II–VI semiconductor materials. It is a piezoelectric, dielectric and transparent. It has direct band gap of 3.37 eV at room temperature and a large excitation binding energy (60 meV). These characteristics have made ZnO thin films used for several applications such as transparent conductors, thin film solar cells, gas sensors and light-emitting diode (LEDs).

In the present study, ZnO thin films were deposited on glass, ITO (In<sub>2</sub>O<sub>3</sub>; Sn) and on ZnO: Al coated glass by spray pyrolysis. The substrates were heated at 350°C. Structural characterization by X-ray diffraction (XRD) measurements shows that films crystallize a hexagonal structure with a preferential orientation along (002) direction.

XRD peak –shift analysis revealed that films deposited on glass substrate (-0.173) were compressive, however, films deposited onto ITO (0.691) and on ZnO:Al (0.345) were tensile. Scanning electron microscopies (SEM) show that the morphologies of surface are porous in the form of nanopillars. The transmittance spectra indicated that the films of ZnO/ITO/glass and ZnO/ZnO:Al/glass exhibit a transmittance around 80% in the visible region.

**Keywords:** ZnO Thin Films, Spray Pyrolysis, Stress, Refractive Index Substrate.

## Optical properties and Raman investigations of CuInSe<sub>2</sub> thin film prepared from CuInSe<sub>2</sub> powder

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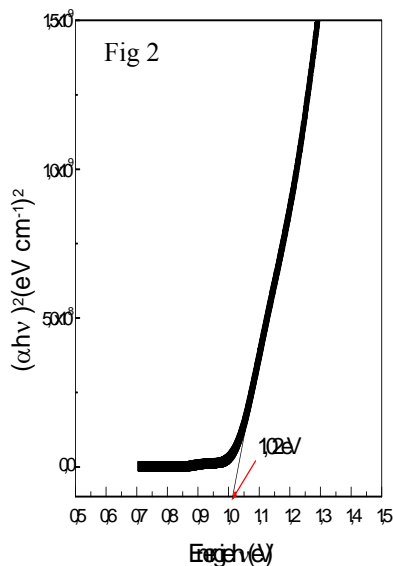
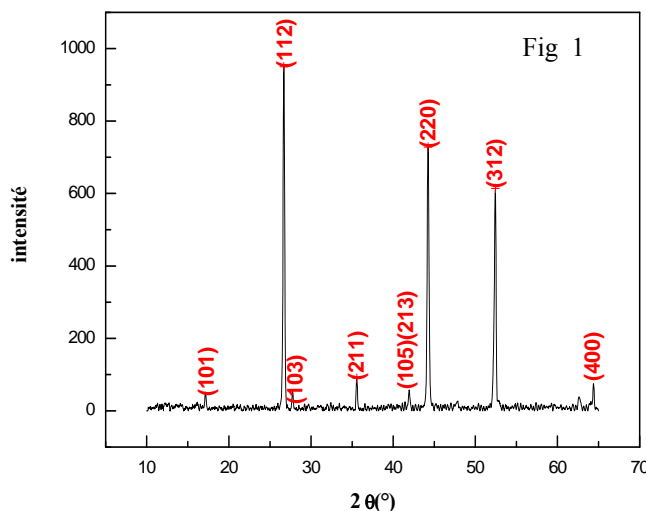
CuInSe<sub>2</sub> is a semiconducting I–III–VI<sub>2</sub> compound with chalcopyrite structure. It is a promising material for the fabrication of thin film solar cells due to its high absorption coefficient ( $\alpha \approx 10^5 \text{ cm}^{-1}$ ), direct band-gap energy ( $E_g = 1.05 \text{ eV}$ ) and excellent thermal stability in air. Currently, efficiencies above 19 % have been achieved.

Thermally evaporated thin film was deposited from CuInSe<sub>2</sub> powder obtained via mechanical alloying of Cu, In and Se elements. The ball milled powder is achieved with a rotational disc speed of 300 rpm and a milling time of 30 min. The investigated materials were analysed by X-ray diffraction. They exhibited a chalcopyrite-like structure (Fig. 1). The Raman spectra of CuInSe<sub>2</sub> powder and CuInSe<sub>2</sub> thin film show a dominant A<sub>1</sub> mode at 171 cm<sup>-1</sup> and 179 cm<sup>-1</sup> respectively.

The optical absorption is calculated using the equation:

$$\alpha h\nu = A (h\nu - E_g)^n \quad (1)$$

Transmittance measurements performed on thin film indicated that the material has a band gap of 1.02 eV (fig 2).



In summary, the ternary I-III-IV<sub>2</sub> semiconductor of CuInSe<sub>2</sub> thin film has been successfully Prepared via mechanical alloying. All the investigated samples were chalcopyrite in nature. The compositions of the powder and film have been determined from EDX. Performing Raman studies, we confirmed the formation of a single chalcopyrite phase in the film. In addition, the optical band gap has been evaluated using the transmittance spectra and is found to be direct allowed and the band gap value is about 1.02 eV.

**Keywords:** CuInSe<sub>2</sub>, Chalcopyrite, Thin Film

### **Structural, Optical and Magnetic Characterisations of Mndoped MgO Nanoparticles**

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Structural, optical and room temperature magnetic properties of Mn-doped MgO nanoparticles with Mn fractions (5-50 at.%), were investigated. The as-prepared pure MgO, with grain size of about 15 nm, exhibits two magnetization components, one is diamagnetic and another is superparamagnetic. After removing the diamagnetic contribution, the magnetization curve exhibits superparamagnetic behavior which may be attributed to vacancy defects. As the Mn content increases, the lattice parameter decreases, the ferromagnetism appears and the emission bands were considerably blue shifted. First principle electronic structure calculations reveal the decrease of both the gap and the Curie temperature with increasing Mn concentration. The obtained results suggest that both Mn doping and oxygen vacancies play an important role in the development of room temperature ferromagnetism.

**Keywords:** Nanostructures; Chemical synthesis; Ab initio calculations; Magnetic properties.

## Surface Properties of Activated Carbon From Different Raw Materials

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In this study is described the development of new adsorbents from lignocellulosic wastes of vegetable origin. Agricultural wastes such as coffee grounds (CG), melon seeds (MS) and orange peels (OP) were used for this purpose. The activated carbons obtained were characterised using infrared spectroscopy (FTIR), thermogravimetric analysis (TGA), X-ray diffraction (XRD), scanning electron microscopy (SEM) and the Boehm titration method. The adsorption efficiency of these new materials was tested with two model organic pollutants: o-nitrophenol and p-nitrotoluene. The elimination ratio obtained with new adsorbents was in the range from 70% to 90%. The kinetics of adsorption of these compounds were measured and described using a pseudo-second order model. The time necessary to attain the adsorption equilibrium was between 75 and 135 min. It was demonstrated that the adsorption kinetics as well as the maximum uptake of the pollutants were dependent mainly on the chemical properties of the adsorbates.

**Keywords:** Adsorption; Activated Carbon, Lignocellulosic Wastes, Industrial Wastewater, Organic Micropollutants.

## How To Optimize Data Quality of Thermophysical Properties of Nickel Based Superalloys

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Nickel based superalloys are representatives of a huge class of materials showing significant chemical reactions with air constituents – specially oxygen. Worse: oxygen acts as a catalyst in reactions with usual lining materials in technological processes and measurement crucibles. Thus the measurement of thermo-physical properties of materials like these is definitely challenging and the mentioned chemical interactions become reason for faulty measurements so far they are ignored during the measuring process.

This contribution focusses on the measurement of the basic set of thermo-physical properties: thermal expansion, specific heat and thermal diffusivity. Thermal conductivity is presented as the product of these quantities. For measurements a push rod dilatometer, a dynamic scanning calorimeter and a laser flash device were used. From technical measurement reasons the application of OTS components (OTS = Oxygen Trapping System) in measurement devices is recommended to minimize distorting effects as parasitic reaction enthalpies or corrosion of crucibles. An elementary physical theoretical background is given and methods how to optimize measurement procedures are explained. Last but not least a concept to formulate the uncertainty of the measured data is proposed, which allows to separate equipment related effects and limitations caused from the chosen mathematical examinations from sample related effects. The thermo-physical properties of a typical representative of a Nickel based superalloy are given in a temperature range from ambient temperatures up to 1600 °C.

**Keywords:** Thermophysical properties, Uncertainty, Sample-crucible interaction, Oxygen trapping

## Investigation of Polyethylene/Graphite Composites and their Electrical, Thermal and Mechanical properties

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Electrical conductivity, thermal conductivity and ultimate mechanical properties, namely elongation at break and stress at break of low and high density polyethylene/graphite composites were investigated in this paper. Percolation concentration at about 11 vol.% of the filler was found. The degree of crystallinity of polyethylene matrix did not have a significant influence neither the percolation concentration nor electrical conductivity of composites. DSC measurement indicated that filler has no significant influence on the change of degree of crystallinity of polyethylene matrices. The thermal conductivity of filled high-density polyethylene is higher than thermal conductivity of filled low-density in the whole concentration range due to higher degree of crystallinity of high density polyethylene. The nonlinear behavior was observed for the dependency stress at break versus filler content. After initial decrease in stress at break, a reinforcing effect was observed. The reinforcing effect was more pronounced for high-density polyethylene matrix.

**Keywords:** Polymer composite, Electrical properties, Thermal properties, Mechanical properties.

## Thermal Conductivity of Epoxy Resin Cross-linking

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The cross-linking process of epoxy resin has been studied. In the presence of selected cross-linking agent depending on the temperature epoxy resins are capable of polymerizing creating a three-dimensional net. During epoxy cross-linking different physical processes can be detected, mainly formation of polymer chains and 3D net formation. Thermodynamic and transport characteristics of epoxy change significantly. A new thermal conductivity sensor was used for monitoring of the cross-linking process. The sensor is based on the hot-ball method for measuring the thermal conductivity and recognizes the processes operating during polymerization. This paper deals with investigation of the cross-linking process of diglycidylether of bisphenol A (DGBA) epoxy resin modified with aromatic reactive diluent, where the curing rate was controlled by the temperature and boron trifluoride as cross-linking agent. A short description of the measurement method has been given.

**Keywords:** Polymer, Thermal conductivity, Cross-linking Process.

## **Thermal Analysis of Bipolar Microelectronic Devices**

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The Deep Trench Isolation (DTI) wells have crucial importance in bipolar microelectronic devices since they serve as heat insulator to reduce the parasitic capacitance and crosstalk. However, under self-heating effect of bipolar devices, DTI wells may cause temperature increase near the heat source region which results in a decrease in performance of bipolar devices. In this study, the effect of the DTI on temperature distribution near heat source region is investigated numerically for trench isolated devices. The investigation is performed for different power of heat source and different lengths of DTI wells to obtain the variation of temperature gradients near the heat source.

**Keywords:** Deep Trench Isolation, bipolar device, self-heating effect.

## INDEX

### A

A Amrouche, 109  
A. Attaf, 120  
A. Amara, 137  
A. Benaldjia, 137  
A. Benyoussef, 138  
A. Boudenne, 36  
A. Bouguerra, 127  
A. Bousseksou, 137  
A. Boutarfaia, 118  
A. Drici, 137  
A. El Kenz, 138  
A. R. Caramitu, 72  
A. Boucekkine, 135  
A. Pasturel, 116  
Abdallah Attaf, 125  
Abdallah. Attaf, 127  
Abdelaziz Drici, 136  
Abdelaziz Lachemet, 133  
Abdelaziz Lallam, 139  
Abdelhak Kareche, 84  
Abdelkader Gherabli, 79, 84  
Abdelkrim Aid, 45, 61  
Abderrahim Boudenne, 79, 84  
Abdessamed Azzez Rahmani, 42  
Abzar Mirzaliyev, 113  
Adrian Bibiș, 117  
Ahmad Ali Amadeh, 57  
Ahmed Boutaous, 50  
Ahmed Boutarfaia, 128  
Ahmed S. Suleiman, 88  
Ahmet Koca, 111  
Ahmet Yönetken, 44  
Aicha Bouhezza, 135  
Aicha Chennoufi, 127  
Aid Abdelkrim, 122, 125  
Aidel Kadum Jassim Al-Shamary, 105  
Akhan Tleoubaev, 74  
Akmal Buriev, 131  
Akramov E.M., 119  
Akramov E.M.<sup>1</sup>, 119  
Albert Van Reenen, 41  
Aleksandra Miletić, 115  
Alelaziz Amara, 136  
Ali Bouchoucha, 121  
Ali Boumedien, 56  
Ali Modarressi, 139  
Ali Rostami, 51  
Ali S. Turabi, 25, 119  
Ali Yildiz, 103  
Allel Mokaddem, 50  
Alpaslan Turgut, II, VI, VII, 16, 18  
Alvaro Campos-Celador, 90  
Ana García-Romero, 70, 90  
Anar Ahmadov, 55  
Anatoly A. Gerasimov, 75, 76  
Anatov A. Gerasimov, 69  
Anil Gündüz, 129  
Anton Popelka, 140

Asma Adelhafidhi, 46  
Assarar Mustapha, 126  
Astan Shahverdiyev, II, V, VII, 52, 54, 55, 87, 113  
Atabek Begjanov, 71  
Ayhan Erol, 44  
Ayse Aroguz, 79  
Ayşe Aydoğdu, 119  
Azadeh Karimpour, 95  
Azzedine Ayadi, 35

### B

B. Boudjema, 135  
B. Garnier, 36  
Bachir Boucekima, 139  
Bachir Gahmani, 41  
Bahia Ghernouti, 35, 110  
Bahruz Ahmadov, 54  
Barreto Orlande, 23  
Bartłomiej Toroń, 34  
Bayram Şahin, 24, 40  
Benarioua Younes, 106  
Bendouba Mostefa, 61, 122  
Bensaid Boulekbache, 41  
Bernard Lamien, 23  
Bezazi Abderrezak, 59  
Bich, E., 128  
Boris A. Grigor'ev, 75, 76  
Boris A. Grogor'ev, 69  
Bouakba Mustapha, 59  
Boudjemâ Agoudjil, 84  
Boudjema Boudjema, 33  
Boudjemaa Agoudjil, 79  
Branka Pilić, 115  
Bruno Abreu Alexandra, 26  
Bruno Lamas, 26  
Bulent Murat İçten, 93  
Bunyatova Elvira M., 59  
Burak Atakan, 9  
Burak Basaran, 25

### C

Carlos Calvo Anibarro, 140  
Carolina Palma Naveira-Cotta, 23, 96  
Cemal Meran, 129  
Cevdet Kaynak, 53  
Chahrazed Djilani, 139  
Chaouki Benabbas, 60  
Corneliu Hamciuc, 37, 74, 100  
Crusius, J.-P., 128

### Ç

Çağatay Kaptan, 30

### D

D. Oukil, 81  
Daeyong Kim, 31

Danica Fidiriková, 39, 102  
Daniel Lager, 139  
Daniel Teichmann, 10  
Daryush Ila, 14  
Diana Serbezeanu, 37, 74, 100  
Dilek Angin, 67  
Dimitri Tzetzis, 37  
Djebli Abdelkader, 45, 61, 122  
Djilani Necib, 121  
Dominika Trefon-Radziejewska, 34  
Dominique Baillis, 8  
Domingue Baillis, 8  
Donatella Giuranno, 27  
Dong-Yoon Seok, 31  
Doroshenko A.O., 83

## E

Egon Hassel, II, IV, VII, 52, 54, 55, 87, 88, 113  
El Mahi Abderrahim, 126  
Elarbi O. Khalil, 43  
Elif Begüm Elçioğlu, 20  
Elif Büyük Öğüt, 30  
Enes Kurtuluş, 103  
Enrica Ricci, 27  
Ercan Ercan, 111  
Erkin Akramov, 131  
Ersel Obuz, 81  
Ertugrul Selçuk Erdogan, 31, 100  
Eyüphan Manay, 24, 40

## F

Fabrizio Valenza, 27  
Fadi Chaat, 41  
Faezeh Majidi, 49, 51  
Fahrettin Yakuphanoglu, 111  
Farhang Abbasi, 104  
Farrukh Atabaev, 71  
Fayçal Djazi, 139  
Fethi Dağdelen, 119  
Filiz İçier, 81  
Fisnik Aliaj, 115  
Fonseca Nelson Martins, 26

## G

Gabriel Mansour, 37  
Gabriela Lisa, 74  
Gamze Gediz Ilis, 22  
Gamze Kor, 81  
Gamzepelin Aksoy, 111  
Gaudențiu Vărzaru, 114  
Georgios Tsotridis, 19  
Gerhard Schreiber, 115  
Gholam Hossein Liaghat, 107  
Gholam Hossein Rahimi, 107  
Gonzalo Diarce, 70, 90  
Gökhan Ömeroğlu, 24  
Gulbeniz S. Mukhtarova, 65  
Gulrukh Begjanova, 71  
Gülden Demir, 67

## H

H Guechichi, 109  
H.Nadjette, 125  
Hakan F. Öztö, 111  
Haluk E. Karaca, 24, 25  
Hamid Reza Azimi, 49, 97  
Hamza Bendjedidi, 125, 127  
Hanane.Saidi, 127  
Hannane Saidi, 125  
Hannes Schmidt, 88  
Hans Hasse, 94  
Hans-Joachim Kretschmar, 80, 92  
Hasan Karabay, 142  
Hasanov Vagif H., 59  
Hassel, E., 128  
Hayet Benzarouk, 136  
Hazal Arıkan, 129  
Heinrich Oettel, 115  
Helcio Rangel, 23  
Hellmann, R., 128  
Heng Ban, 1  
Henning Wolf, 88  
Hesam Abdollahi-Sevini, 58  
Hikmet I.Ibrahimov, 65  
Hind Laouamri, 68  
Hirobumi Tobe, 24  
Huseyin Erdem Yalkin, 93

## I

I. Hakkı Tavman, 16, 86, 140  
I.M. Mahbubul, 15, 17  
I.M. Shahrul, 17  
Igor Krupa, 140  
Igor Novák, 140  
Igor S. Alexandrov, 69, 75, 76  
Imane Meriam Babaghayou, 46  
Inaki Gandarias, 70  
Ines Stoecker, 80  
Ionela-Daniela Carja, 37, 74, 100  
Ionuț Cristea, 117  
Irfan Kaya, 24  
Iskandarova M. I., 119  
Ismail Hakkı Tavman, IV  
Ismail Yildiz, 44  
Ivan Chodák, 140  
Ivan Ristić, 115

## İ

İsmail Özdemir, 16

## J

J. J. Suñol, 134  
J. Judith Vijaya, 138  
J. M. Greneche, 134  
Ján Vlčko, 102  
Jaroslava Budinski-Simendić, 78, 115  
Javid Safarov, II, V, VII, 52, 54, 55, 87, 113  
Jean Stéphane Antoniow, 82  
Jean-Eudes Maigret, 82

Jelena Pavličević, 78, 79  
Jerzy Bodzenta, 32, 33, 34  
Ji Hoon Kim, 31  
Joaquín Ariel Morón-Villarreyes, 64  
Johnny Beaugrand, 82  
Jose Maria Sala, 70, 90  
Justyna Juszczak, 32, 33

## K

K. Almi, 130  
Kabache Malika, 60  
Kadir Geliş, 24, 40  
Karima Boukerma, 134  
Karima Bounab, 128  
Karol Strzałkowski, 34  
Katalin Mészáros-Szécsényi, 79  
Khadice T.Eyyubova, 65  
Khadra Bendjillali, 41  
Khaled Boumchedda, 35, 110  
Khelil Foudhil, 61  
Khira Ben Nacer, 125  
Kiyumars Jalili, 104  
Konstantinos Tsongas, 37  
Kutlay Sever, 16  
Kwansoo Chung, 31

## L

L. Avădanei, 72  
L. Makhloufi, 81  
L. Saad Hamideche, 137  
L.Hennet, 116  
Laid Makhloufi, 77  
Lala Azizova, 55  
Lala M. Afandiyeva, 66  
Lan Tighzert, 124  
Lenka Kralovičová, 102  
Letif H. Nuriyev, 66  
Linda Saad Hamideche, 136  
Ljiljana Tanasić, 78, 79  
Ludmilla Kakurina, 71  
Ludovít Kubičár, 140  
Łukasz Drewniak, 34  
Łukasz Gołębiowski, 62  
Lukyanov B.S., 83  
Lukyanova M.B., 83  
Lynda Djoudi, 133

## M

M Benkhettab, 109  
M. Nouadji, 120  
M. Poulain, 120  
M. Abba, 118  
M. Aslam Siddiqi, 9  
M. Bahattin Akgül, 108  
M. Bououdina, 138  
M. Brzozowski, 29  
M. El-Hilo, 138  
M. Ibrir, 130  
M. Oktay Alniak, 6, 7  
M.A. Amalina, 15, 17

M.Sayeh Goual, 41  
M.Trybula, 116  
Mabrouka Boubeche, 127  
Maciej Kowalski, 62  
Magdalena Bosomoiu, 19  
Magdalena Jurczyk Kowalska, 62  
Mahammadjon Tursunov, 85  
Mahdi Salami Hosseini, 91  
Mahfoud Kadja, 134  
Mahi R. Singh, 13, 29  
Mahmoud Omari, 133  
Malika Nouadji, 127  
Manel Haddadi, 79  
Marcelo J. Colaço, 99  
Marek Rogalski, 139  
Mariana Nicke, 80  
Mariano Paganelli, 67  
MarianValentin, 140  
Martin Horsch, 94  
Masahide Terazima, 11, 12  
Mastura Iskandarova, 71  
Mataoui Amina, 60  
Matthias Kunick, 80  
Maycon Magalhães, 23  
Mediha Kok, 25, 119  
Mehmet Cem Menteş, 111  
Mehmet Sarikanat, 16  
Menail Younès, 126  
Merzoug Boucheur, 60  
Mesut Abuşka, 108  
Mete Egemen, 67, 74, 102  
Metelitsa A.V., 83  
Mihaela Pantazică, 114  
Mihai Brânzei, 117  
Mihai Chirtoc, 3, 32, 124  
Milena França, 23  
Milena Špírkova, 78  
Miloš Brzić, 115  
Minevver C.Ibrahimova, 66  
Minkin V.I., 83  
Mirjana Jovičić, 78, 79  
Misirkhan Talibov, 55  
Mohamed Alami, 50  
Mohamed Chemrouk, 41  
Mohammad Hedayatian, 107  
Mohammad Hossein Pol, 107  
Mohammed Chemrouk, 42  
Mohammed Nabil Ouissi, 40  
Mohsen Adabi, 57  
Mónica Oliveria, 26  
Mostafa Kolli, 68  
Mostafa Rezaei, 49, 91, 95, 97  
Mostafa Salehi, 91, 97  
Mouas Amar, 73  
Mounia Benyamina, 60  
Mounira Mekhnache, 136  
Mourad Mordjaoui, 33  
Muhittin Bilgili, 19  
Mustafa Aydemir, 142  
Mustafa Özdemir, 89  
Müslüm Arıcı, 30, 142

## N

N. Abdessalem, 118  
N. Benslim, 137  
N. Mamouni, 138  
N.Jakse, 116  
Nadia Benmansour, 84  
Nadia Madoui, 133  
Nadir Beldjoudi, 50  
Naim Sylva, 115  
Nassima Bouguerra, 77  
Nassima Tarfa, 33  
Natalija Budinski, 78  
Negmatov Sayibjan, 71  
Nevena Vukić, 115  
Nicolas Horny, 3, 124  
Nihad Dukhan, 88, 89  
Noureddine Bentaieb, 133  
Noureddine Bouaouadja, 68

## O

Okan Özdemir, 105  
Olçay Eksi, 31, 100  
Olivier Fudym, 2  
Omar Kholai, 135  
Omar Sultan, 41  
Oskar Bera, 79  
Oytura Maksumova, 85

## Ö

Özer Bağcı, 89

## P

Paul Svasta, 114  
Peizhen Li, 25  
Peter Dieška, 39, 140  
Peter Hess, 4, 5  
Petr P. Bezverkhly, 47  
Piotr Marek, 62

## R

R. Aitout, 81  
R. El Abdi, 120  
R. Labbani, 127  
R. Saidur, 15, 17  
Rachida Zaghdoudi, 139  
Rada Novakovic, 27  
Radmila Radičević, 78  
Rafika Souag, 110  
Rainer Feistel, 92  
Ramazan Karakuzu, 105  
Ramdane Yousfi, 56  
Razika Aitout, 77  
Rena Hamidova, 52  
Renato M. Cotta, 99  
Reza Izadpanah, 95  
Reza Zamani, 107  
Rukhasare I. Huseynova, 65

## S

S Benkabouche, 109  
S. Alleg, 134  
S. Azzaza, 134, 138  
S. Mitrea, 72  
S. Narayanan, 138  
S.Balakrishnan, 29  
S.Lakel, 130  
S.S. Khaleduzzaman, 17  
Sabina A.Ahmadova, 66  
Saeid Reza Allahkaram, 58  
Safri Abdelhamid, 73  
Said Debbakh, 110  
Salah Belaadi, 133  
Salah Yahiaoui, 125  
Saleh Mirzayev, 54  
Sandra Gómez-Cavia, 70, 90  
Sang-Woo Kim, 31  
Scarpa Fabrizio, 59  
Sebastian Herrmann, 80, 92  
Sefer Avdiaj, 115  
Sergel V. Stankus, 47  
Sergey V. Lishchuk, 94  
Serkan Doğanay, 18  
Sevara Atabaeva, 131  
Sevinc Babayeva, 55  
Shahverdiyev Astan N, 59  
Sidi Mohammed Hamza-Cherif, 40  
Sławomir Krauze, 62  
Soheil Mahdavi, 58  
Soner Haldenbilen, 129  
Souhila Kadem, 133  
Souhir Semari, 127  
Souhir Semmari, 125  
Stefano Amore, 27  
Stephan Werth, 94  
Süha Sergin, 129

## Ş

Şeref Doğuşcan Akbaş, 21

## T

T. Zaharescu, 72  
T.Gancar, 116  
Tachita Vlad-Bubulac, 37, 74, 100  
Tahar Aouroun, 35  
Tamara Erceg, 115  
Tatiana Durmeková, 102  
Thiago M. Campos, 99  
Tomasz Brynk, 62  
Tuba Alpyildiz, 93  
Tuba Evgin, 86  
Tuba Okutucu-Özyurt, 20

## U

Ulugbek Urinov, 85

## V

V. Levchenko, 36  
V. Tsakiris, 72  
Vagif A. Nagiyev, 66  
Vagif M. Abbasov, 66  
Vagif M. Abbasov, 65  
Valentin V. Parashchuk, 118  
Vesna Teofilović, 78, 79  
Viktor G. Martynets, 47  
Viktor Mazur, 28  
Viktoriia Karnauh, 28  
Viliam Vretenár, 39, 102, 140  
Vinicius Zacharias, 96  
Vittorio Mercurio, 67  
Vlastimil Boháč, 39, 102  
Volkan Altıntaş, 108

## W

W.Gasior, 116  
Wolfgang Arlt, 10

Wolfgang Hohenauer, 130, 139  
Wolfgang Wagner, 92  
Wonjae Kim, 31

## Y

Y. Mamunya, 36  
Yasin Varol, 111  
Yelda Meyva, 53  
Yempab Kanake, 124  
Yıldırım Aydoğdu, 119  
Yildirim Aydogdu, 25  
Yoldaş Seki, 16  
Youcef Bennouar, 56  
Young-Seon Lee, 31

## Z

Z. Haktan Karadeniz, 18  
Z. Necira, 118  
Zengah Sahnoun, 125  
Zilong Hua, 1