TMS

MEMA

The TMS Middle East - Mediterranean Materials Congress on Energy and Infrastructure Systems 2015

January 11–14, 2015
Ritz-Carlton Doha • Doha, Qatar
www.tms.org/MEMA2015

PROGRAM & ABSTRACTS

Organized by: TMS

In Cooperation with: Texas A&M University; Texas A&M University at Qatar; جامعة قطر Qatar University; مؤسسة قطر Qatar Foundation; NSF; International Institute for Materials for Energy Conversion IIMEC

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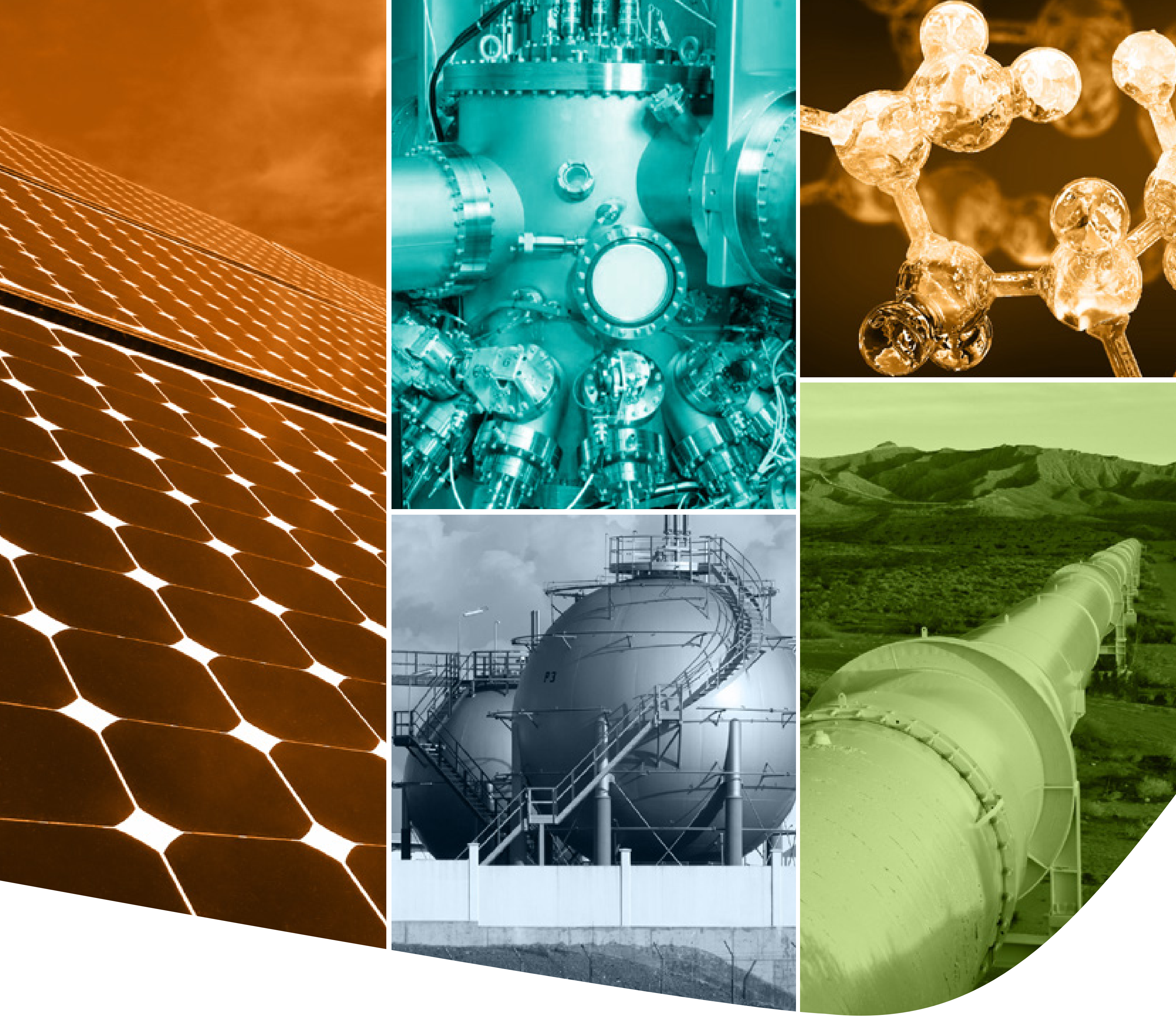

معهد قطر لبحوث
البيئة والطاقة
Qatar Environment & Energy
Research Institute

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The Qatar Environment and Energy Research Institute (QEERI)

is a member of Qatar Foundation for Education, Science and Community Development. QEERI's vision is to become a leading research center with global impact through addressing Qatar national needs. QEERI plays a key role in addressing the national energy and water security grand challenges, catalyzing the industrial ecosystem through local and international partnerships and developing local capabilities to boost Qatar's knowledge economy.

QEERI seeks to address these grand challenges by assisting and expediting the research and development by providing scientific, engineering and technological solutions in areas of solar energy, energy storage, smart grids, water desalination and reuse, and aquifer recharge.

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www.qeeri.org.qa

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WELCOME

On behalf of The Minerals, Metals & Materials Society (TMS) and the congress organizers, I am pleased to welcome you to the first MEMA Congress on Energy and Infrastructure Systems. Materials for energy extraction, conversion and storage, and sustainable infrastructure systems are critical research areas for the future of the Middle East and Mediterranean region. This congress is a part of ongoing efforts to build synergy and establish collaboration among materials researchers in the Middle East and Mediterranean region and the rest of the world.

We have assembled experts on materials for energy and infrastructure to cover a broad range of research topics, including infrastructure materials and their sustainability; computational materials science; multiscale materials modeling; materials for the conversion of one form of energy into another through solid phase energy conversion; energy storage; lightweight materials for energy efficiency; and materials issues for the oil and gas industries. Attendees will have the opportunity to exchange ideas, share new techniques and results, and move the field forward through collaborative efforts.

We look forward to an exciting meeting of dynamic discussions, outstanding speakers and an interactive poster session, and we thank you for your participation in MEMA 2015!

Warmest regards on behalf of the MEMA 2015 Organizing Committee,

Ibrahim Karaman, Texas A&M University

TMS would like to thank our GOLD SPONSORS for their gracious support of the event.

QAPCO
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معهد قطر لبحوث البيئة والطاقة
Qatar Environment & Energy Research Institute
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- **M. Enokizono**, Oita University
- **Tasneem Pervez**, Sultan Qaboos University

ABOUT THE CONGRESS

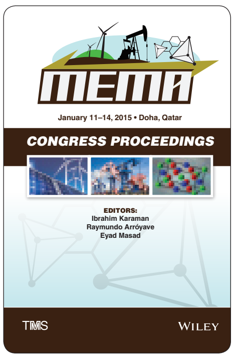
REGISTRATION

Your congress registration includes one copy of the proceedings disk. Your badge ensures admission to each of these events:
- Technical and Poster Sessions
- Sunday Welcome Reception
- Monday Poster Session
- Monday Dinner Event (*Sponsored by Texas A&M University of Qatar*)
- Tuesday Congress Banquet

Registration Hours
The registration desk will be located in Fateh Al Khair.

Sunday	16:00 to 19:30
Monday	07:00 to 17:00
Tuesday	07:30 to 17:00
Wednesday	07:30 to 17:00

Technical Sessions
Oral presentations will be held in the Al Wosail and Mukhtassar rooms. The poster session will be held in the Al Wosail Foyer. See the Technical Program Session Listing section on pages 8-16 for room locations.



Proceedings
Full conference registrants receive one copy of the proceedings as part of the registration fee. Additional copies may be purchased for $149.95 at **www.wiley.com** (TMS members receive a 35% discount). Approximately six weeks after the meeting, individual papers will be available through the Wiley Online Library: **http://onlinelibrary.wiley.com**.

POLICIES

BADGES

All attendees must wear a registration badge at all times during the congress to ensure admission to events included in the paid registration fee such as technical sessions and receptions.

REFUNDS

The deadline for all refunds was December 1, 2014. No refunds will be issued at the congress. Fees and tickets are nonrefundable.

PHOTOGRAPHY NOTICE

By registering for this congress, all attendees acknowledge that they may be photographed by meeting personnel while at events and that those photos may be used for promotional purposes.

AUDIO/VIDEO RECORDING POLICY

Recording of sessions (audio, video, still photography, etc.) intended for personal use, distribution, publication, or copyright without the express written consent of TMS and the individual authors is strictly prohibited. Attendees violating this policy may be asked to leave the session.

U.S. AMERICANS WITH DISABILITIES ACT

The U.S. Americans with Disabilities Act (ADA) prohibits discrimination against, and promotes public accessibility for, those with disabilities. In support of, and in compliance with ADA, we ask those requiring specific equipment or services to contact TMS Meeting Services at mtgserv@tms.org in advance.

CELL PHONE USE

In consideration of attendees and presenters, we kindly request that you minimize disturbances by setting all cell phones and other devices on "silent" while in meeting rooms.

NETWORKING & SOCIAL EVENTS

WELCOME RECEPTION

The Welcome Reception will be held on Sunday, January 11 from 18:00 to 19:30 in the Fountain Courtyard.

Sponsored by معهد قطر لبحوث البيئة والطاقة Qatar Environment & Energy Research Institute عضو في مؤسسة قطر Member of Qatar Foundation

A FUN EVENING OUT IN DOHA

The Evening Out in Doha will be held on Monday, January 12 from 19:00 to 21:00. Buses will depart from the Ritz-Carlton at 18:30.

Sponsored by TEXAS A&M UNIVERSITY at QATAR

POSTER SESSION

The Poster Session is planned for Tuesday, January 13 from 15:20 to 16:30 following the technical sessions in Al Wosail Foyer. Don't miss this great networking opportunity!

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CONGRESS BANQUET

The Congress Banquet will be held on Tuesday, January 13 from 18:00 to 20:00 at the Ritz-Carlton, in the Fountain Courtyard.

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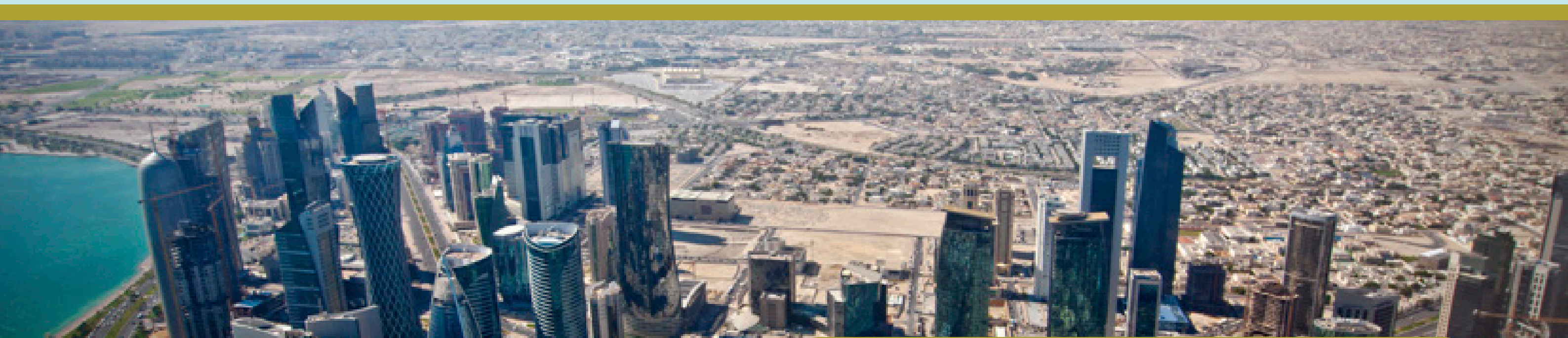
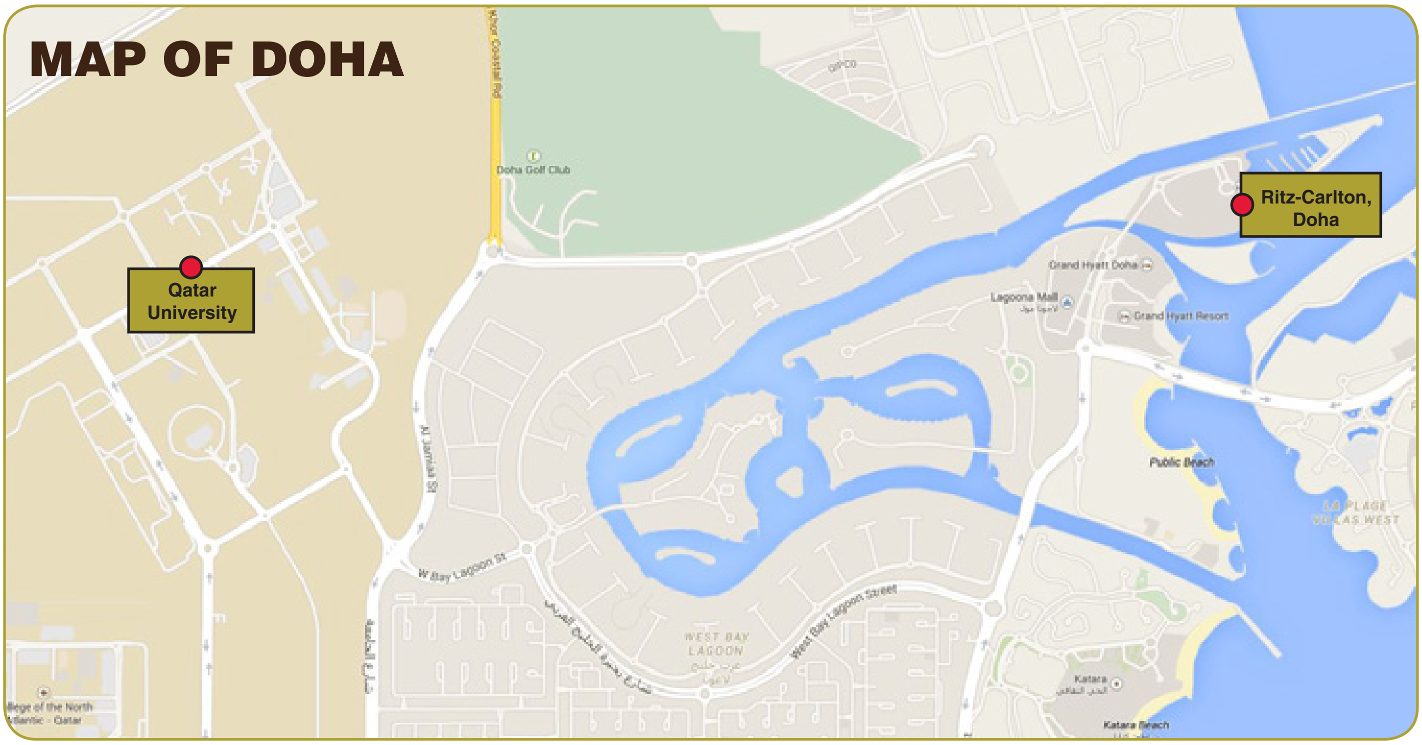
ABOUT THE VENUE



Discover the Ritz-Carlton, Doha hotel and experience the breathtaking beauty of the Gulf. From the city's traditions and culture to its modern amenities and exciting attractions, this stunning luxury hotel in Qatar provides guests with convenient access to everything this unforgettable destination has to offer.

For more information, visit www.ritzcarlton.com/Doha.

MAP OF DOHA



For more information on getting around Qatar, visit **www.qatartourism.gov.qa/en-us/home.aspx.**

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TECHNICAL PROGRAM

TECHNICAL SESSION LISTING

Monday, January 12, 2015

Plenary 1 - Room: Mukhtassar	
08:00	Introductory Comments
08:20	Keynote Computational Modeling of Deformation Mechanisms in Mg and Mg Alloys: W. Curtin[1]; M. Ghazisaedi[2]; A. Luque[3]; Z. Wu[3]; [1]EPFL; [2]Ohio State University; [3]Ecole Polytechnique Federale de Lausanne
09:05	Break
1-1: Cemenetitious Materials, Composites - Room: Mukhtassar	
09:20	Invited Computational Materials Science to Enable Sustainable Concrete Material Design: Zachary Grasley[1]; Xiaodan (Sonia) Li[1]; [1]Virginia Tech
10:00	Vertical Scanning Interferometry: A New Method to Quantify Solute-solvent Reaction Dynamics in Cementitious Environments: Gaurav Sant[1]; [1]University of California, Los Angeles
10:20	Effect of Interface and Interphase Regions on the Elasticity of Nanocomposite Cement: Ala Abu Taqa[1]; Ahmed Senouci[1]; Rashid Abu Al-Rub[2]; [1]Qatar University; [2]Masdar Institute of Science and Technology
10:40	Finite Element Simulation of the Response of No-Tension Materials: Alieh Alipour[1]; Tom Scarpas[1]; [1]Delft University of Technology
11:00	Investigation and Modeling of the Damage Evolution in Natural Fiber Composites: Habiba Bougherara[1]; Zia Mahboob[1]; Fodil Meraghni[2]; Laurent Peltier[3]; [1]Ryerson University; [2]ENSAM - Arts et Métiers ParisTech; [3]
11:20	Lunch (Al Wosail 2&3)
2-1: Ferrocaloric Materials - Room: Al Wosail 1	
09:20	Invited The Direct Conversion of Heat to Electricity Using Multiferroic Materials: Richard James[1]; [1]University of Minnesota
10:00	Invited Origin of Hysteresis in Multicaloric Materials: Sebastian Fähler[1]; [1]IFW Dresden
10:40	Approaches to Analyze Cycle Efficiency in Magnetocaloric Materials: Patrick Shamberger[1]; T.D. Brown[1]; J. Murley[1]; J.H. Chen[1]; J. Ross[1]; N. Bruno[1]; I. Karaman[1]; [1]Texas A&M University
11:00	The Tunable Microstructure and its Influence on the Giant Magnetocaloric Effect in Magnetic Shape Memory Alloys: Nickolaus Bruno[1]; Yujin Huang[2]; Ibrahim Karaman[1]; Joseph Ross[1]; Jianguo Li[2]; [1]Texas A&M University; [2]Shanghai JiaoTong University
11:20	Studies of Magnetic Properties of Ni-Mn-In-Co Heusler-type Glass-coated Microwires: Valentina Zhukova[1]; Mihail Ipatov[1]; Alexandr Aronin[2]; Galina Abrosimova[2]; Alexandr Kiselev[2]; Arcady Zhukov[3]; [1]Basque Country University; [2]Insitute of Solid State Physics; [3]Basque Country University and Ikerbasque
11:40	Lunch (Al Wosail 2&3)
3-1: Ab-Initio Approaches - Room: Al Wosail 4	
09:20	Invited Ab Initio Thermodynamics: A Novel Route to Design Structural Materials with Superior Mechanical Properties: Jörg Neugebauer[1]; Blazej Grabowski[1]; Fritz Kormann[1]; Tilmann Hickel[1]; [1]Max-Planck-Institut für Eisenforschung GmbH
10:00	A DFT Based Molecular Dynamics Study of $PbI_3(CH_3NH_3)$: Marcelo Carignano[1]; [1]QEERI - Qatar Foundation
10:20	Thermal Expansion Coefficient of Two Dimensional Materials: Cem Sevik[1]; [1]Anadolu University
10:40	Strong Stacking Between Organic and Organometallic Molecules as the Key for Material Design: Snezana Zaric[1]; Dusan Malenov[2]; Dragan Ninkovic[2]; [1]Texas A&M University at Qatar; [2]Innovation Centre of the Department of Chemistry
11:00	Calculation of Electronic Structure and Field Induced Magnetic Collapse in Ferroic Materials: Raymundo Arroyave[1]; P. Entel[2]; N. Singh[3]; M. Gruner[2]; A. Grünebohm[2]; V. V. Sokolovskiy[4]; V. D. Buchelnikov[4]; [1]Texas A&M University; [2]University, Duisburg-Essen; [3]University of Houston; [4]Chelyabinsk State University
11:20	Lunch (Al Wosail 2&3)
1-2: Cementitious Materials Sustainability - Room: Mukhtassar	
13:30	Introductory Comments

13:40	Invited Utilising Fine and Coarse Recycled Aggregates from the Gulf Region in Concrete: Roderick Jones[1]; Judith Halliday[1]; Laszlo Csetenyi[1]; Li Zheng[1]; Nikolaos Strompinis[1]; Moray Newlands[1]; [1]University of Dundee
14:20	Multiwalled Carbon Nanotubes Aspect Ratio, Functionalization, Weight Fraction & Surfactant Effect on the Mechanical Properties of Cementitious Materials: Mohamed Mohsen[1]; Rashid Abu El Rub[2]; Ahmed Senouci[1]; Nasser Alnuaimi[1]; Khaldoon Bani Hani[3]; [1]Qatar University; [2]Masdar Institute of Science and Technology; [3]Jordan University of Science and Technology
14:40	Defined Polymers as Candidates for Pavement Subgrade Soil Stabilization: Chandramohan Ayyavu[1]; Srinath R. Iyengar[1]; Howard J. H. M. Hanley[1]; Hassan S. Bazzi[1]; Dallas Little[1]; [1]Texas A&M University at Qatar
15:00	Break
2-8: Lightweight and High Performance Materials I - Room: Mukhtassar	
15:20	Nanomaterials for "Smart" Membrane Pretreatment and RO Desalination Technologies: Khaled Mahmoud[1]; [1]QEERI-QF
15:40	3D Nanotubular Surfaces for Energy Storage and Conversion: Tolou Shokuhfar[1]; [1]Michigan Technological University
16:00	Mechanical Properties of Al-Zr-Sc Alloys with Si and Er Micro-additions: Nhon Vo[1]; Nick Barta[2]; Georges Ayoub[3]; Ibrahim Karaman[2]; David Dunand[1]; [1]Northwestern University; [2]Texas A&M University; [3]Texas A&M University at Qatar
16:20	Development of High Strength and Ductile Al-xMg Alloys for Sustainable Applications: Min Zha[1]; Hans Roven[2]; Chris Devadas[3]; [1]Norwegian University of Science and Technology; [2]Qatar University; [3]Hydro Aluminium QSTP Qatar
16:40	Microstructural and Mechanical Characterization of Friction-Stirred Welded (FSW) TRC AZ31B Magnesium Alloy Sheets: Abdelhakim Dorbane[1]; Georges Ayoub[1]; Bilal Mansoor[1]; Ramsey Hamade[2]; Ghassan Kridli[3]; Abdellatif Imad[4]; [1]Texas A&M University at Qatar; [2]American University of Beirut; [3]University of Michigan-Dearborn; [4]Ecole Polytech'Lille
2-2: Energy Storage Materials - Room: Al Wosail 1	
13:30	Introductory Comments
13:40	Invited Nanomaterial Design Strategies for Capacitive Energy Storage Applications: Husam Alshareef[1]; [1]King Abdullah University for Science & Technology (KAUST)
14:20	Rechargeable Batteries: Lessons from Real Time Observation of Lithiation/Delithiation in Nanoscale Anode Materials: Reza Shahbazian-Yassar[1]; [1]Michigan Technological University
14:40	Electrode Materials Based on Phosphates for Lithium Ion Batteries as Efficient Energy Storage System: Saadoune Ismael[1]; Lasri Karima[1]; Bezza Ilham[1]; Ehrenberg Helmut[1]; Indris Sylvio[1]; Daniel Brandell[2]; [1]University Cadi Ayyad Marrakech; [2]Uppsala University
15:00	Break
15:20	Interfacial Stresses and Degradation of Oxide Scale and Substrate Interface at High Temperatures: Mohammed Khaleel[1]; E. Stephens[2]; J. Stevenson[2]; [1]Qatar Foundation; [2]Pacific Northwest National Laboratory
15:40	Predicting Acoustic Emission and Electrochemical Impedance Spectra for Damage Stochastics in Energy Materials: Pallab Barai[1]; Chien-Fan Chen[1]; Partha Mukherjee[1]; [1]Texas A&M University
16:00	Novel Organic Electrodes for Organic Rechargeable Batteries: Burak Esat[1]; Sumeyye Bahceci[1]; Sevda Akay[1]; Aliyu Bawa Abdullahi[1]; [1]Fatih University
16:20	$Na_2Fe_{0.5}Mn_{0.5}P_2O_7$ as Promising Cathode Material for Rechargeable Sodium Ion Batteries (NIBs): R. Shakoor[1]; Ramazan Kahraman[1]; Chanseon Park[2]; Soo Lim[2]; Jang Choi[2]; [1]Qatar University; [2]Korea Advanced Institute of Science and Technology (KAIST)
16:40	Nanomaterial-based Ultracapacitor for Power Integrated Circuits: Daniel Choi[1]; Waqas Gill[1]; Maarten Geest[1]; [1]Masdar Institute of Science and Technology
3-2: Energy Materials Simulation - Room: Al Wosail 4	
13:30	Introductory Comments
13:40	Invited Application of Phase-field Method to Modeling Microstructure Evolution in Li-ion Batteries: Long Qing Chen[1]; [1]Penn State University
14:20	Modeling of Thermal Behavior and Efficiency of Photovoltaic Panels: Said Ahzi[1]; [1]University of Strasbourg/Qatar Foundation

14:40	A Biomimetic-computational Approach to Optimizing the Quantum Efficiency of Photovoltaics: Andreas Holzenburg[1]; Lisa Perez[1]; [1]Texas A&M University
15:00	Break
15:20	Using Nonlinear Electret Effects to Design Piezolectricity and Magnetoelectricity in Soft Materials: Pradeep Sharma[1]; [1]University of Houston
15:40	Stability, Mechanical, Dielectric and Piezoelectric Properties of {AxA'(1-x)}{ByB'(1-y)}O_3 Ceramics: Berna Akgenc[1]; Çetin Tasseven[2]; Tahir Cagin[3]; [1]Kirklareli University; [2]Yildiz Technical University; [3]Texas A&M University
16:00	Revealing the Role of Organic Ligands in Hybrid Halid Perovskites for Phovoltaics Applications: Carlo Motta[1]; Fadwa El-Mellouhi[2]; Fahhad Alharbi[2]; Nouar Tabet[2]; Kais Sabre[2]; Stefano Sanvito[1]; [1]Trinity College Dublin and CRANN; [2]QEERI
16:20	Organic Molecule-Functionalized Zn_3P_2 Nanowires for Photochemical H_2 Production: DFT and Experimental Analyses: G. Ramos-Sanchez[1]; M. Albornoz[1]; Y-H. Yu[2]; Z. Cheng[1]; V. Vasiraju[3]; S. Vaddiraju[1]; Fadwa El-Mellouhi[4]; P. B. Balbuena[1]; [1]Artie McFerrin Department of Chemical Engineering; [2]Department of Materials Science & Engineering, Texas A&M University; [3]Department of Materials Science & Engineering, Texas A&M University; [4]QEERI
16:40	Tailoring Thermal Conductivity of Ge/Si Core-Shell Nanowires: Sevil Sarikurt[1]; Cem Sevik[2]; Alper Kinaci[3]; Justin Haskins[4]; Tahir Cagin[5]; [1]Dokuz Eylul University; [2]Anadolu University; [3]Argonne National Laboratory; [4]NASA Ames Research Center; [5]Texas A&M University

Tuesday, January 13, 2015

Plenary 2 - Room: Mukhtassar	
08:00	Introductory Comments
08:10	Keynote Materials Research for the Energy Industry Collaboration Opportunities between Energy Industry and Academia: Rustom Mody[1]; [1]Baker Hughes
08:55	Break

1-3: Multi-scale Characterization and Simulations of Infrastructure Materials - Room: Mukhtassar	
09:10	Invited Quantifying Material, Environmental, and System Variables Influencing the Structural Performance of Reinforced Concrete Structures Affected by Alkali Silica Reactions: David Trejo[1]; Joseph Bracci[2]; Paolo Gardoni[3]; [1]Oregon State University; [2]Texas A&M University; [3]University of Illinois at Urbana-Champaign
09:50	Invited Monitoring Concrete Infrastructure Condition Using Acoustic Sensing and Imaging: John Popovics[1]; [1]University of Illinois
10:30	Multiscale Design of Palm Natural Fiber Based Composite: Yehia Bahei-El-Din[1]; Taher Wahba[1]; Tarek Hatem[1]; [1]British University in Egypt
10:50	Mechanical Properties of Concrete Containing Qatar's Municipal Wastes: Nesibe Gozde Ozerkan[1]; Deniz Tokgoz[1]; Joseph Antony[2]; [1]Qatar University; [2]University of Leeds
11:10	Stochastic Framework for the Modeling and Propagation of Linear Viscoelastic Material Properties of Asphalt Mixtures in Pavement Structures: Loujaine Mehrez[1]; Eyad Masad[1]; [1]Texax A&M University at Qatar
11:30	Lunch (Al Wosail 2&3)

2-3: Nano-Engineered Materials for Energy Conversion - Room: Al Wosail 1	
09:10	Invited Challenges and Opportunities for Nano Engineered Materials: Pulickel Ajayan[1]; [1]Rice University
09:50	Towards Engineering Efficient Thermoelectrics: Large-scale Synthesis of Nanowires and their Assembly into Stable Welded Nanowire Networks: Sreeram Vaddiraju[1]; [1]Texas A&M University
10:10	Design of New Electroactive Materials Based on Nanoparticle-modified Polymers: Zoubeida Ounaies[1]; Nirmal Shankar Sigamani[1]; [1]The Pennsylvania State University
10:30	Active Nanocomposite Materials for Photo-mechanical Actuation: Igor Krupa[1]; Klaudia Czanikova[2]; Maria Omastova[2]; [1]Qatar University; [2]Polymer Institute SAV
10:50	Inherent Nonlinear Non-conservative Behavior of Resonant Piezoelectric Energy Harvesters: A Dynamical Systems Approach: Stephen Leadenham[1]; Alper Erturk[1]; [1]Georgia Institute of Technology

11:10	A Multiscale-Based Model for Composite Materials with Embedded PZT Filaments for Energy Harvesting: Yehia Bahei-El-Din[1]; Ahmed El-Etriby[1]; Mohamed Abdel-Meguid[1]; Khalid Shalan[1]; Tarek Hatem[1]; [1]British University in Egypt
11:30	Lunch (Al Wosail 2&3)
3-3: Modeling Materials Across the Scales - Room: Al Wosail 4	
09:10	Multiscale Modeling and Design of Advanced Interface Materials for High Energy Environments: Hussien Zbib[1]; [1]Washignton State University
09:30	Periodic Homogenization of SMA Composites under Isothermal Conditions: George Chatzigeorgiou[1]; Yves Chemisky[1]; Fodil Meraghni[1]; [1]Arts et Metiers ParisTech
09:50	Modeling the Deformation Mechanisms in Magnesium Single Crystals: Multiscale Dislocation Dynamics Analyses: Wassim Jaber[1]; Mutasem Shehadeh[1]; [1]American University of Beirut
10:10	Analysis of Solid State Bonding in the Extrusion Process of Magnesium Alloys -Numerical Prediction and Experimental Verification: Nabeel Alharthi[1]; Wojciech Misiolek[2]; Anthony Ventura[2]; [1]Lehigh University and King Saud University; [2]Lehigh University
10:30	Hydrogen Embrittlement in Pd: Binding Energetics and Structure at Grain Boundaries: Tahir Cagin[1]; [1]Texas A&M University
10:50	Multiscale Modeling of Discontinuous Precipitation in U-Nb: Thien Duong[1]; Alexander Landa[2]; Robert Hackenberg[3]; Patrice Turchi[2]; Raymundo Arroyave[1]; [1]Texas A&M University; [2]Lawrence Livermore National Laboratory; [3]Los Alamos National Laboratory
11:10	Lunch (Al Wosail 2&3)
1-4: Environmental Degradation - Room: Mukhtassar	
13:30	Introductory Comments
13:40	Invited Corrosion Challenges for the Oil and Gas Industry in the State of Qatar: Roy Johnsen[1]; [1]Norwegian University of Science and Technology
14:20	Effect of Electroless Co-P and Co-Ni-P Coatings on Cavitation Erosion-corrosion Resistance: Shemy Mohamed Ahmed Gaber Gaber[1]; Mohammed Aboraia[2]; Mohammed Doheim[2]; Salem Karrab. A[3]; [1]Majmaah University; [2]Assiut University.; [3]Misurata University
14:40	Prevention of Chloride Stress Corrosion Cracking (CSCC) using Thermally Sprayed Coating (TSC): Rehan Ahmed[1]; [1]Petronas Carigali
15:00	New Self-Healing Coatings Technique for Corrosion Protection: Eman Fayyad[1]; Mariam Al-Maadeed[1]; [1]Qatar University
2-4: Ferroelectric Materials in Energy Conversion - Room: Al Wosail 1	
13:30	Introductory Comments
13:40	Invited Insights into the Nature and Dynamics of Point Defects in Ferroelectric Materials: Clive Randall[1]; [1]Penn State University
14:20	Flexoelectricity and Nanoscale Energy Harvesting: Pradeep Sharma[1]; [1]University of Houston
14:40	Investigation of Electrical and Piezoelectricity of New Nanocomposites Based on Nanofibrillated Cellulose and Copolymers Containing Fluorinated and Nitrile Derivatives with Controlled Structure: Kaddami Hamid[1]; Kadimi Amal[1]; Ounaies Zoubeida[1]; Raihane Mustapha[1]; [1]Cadi Ayyad University
15:00	Novel Polymeric Materials for Mechanical Energy Harvesting: Miroslav Mrlík[1]; Mariam Al Maadeed[1]; [1]Qatar University, Center for Advanced Materials, P.O.BOX 2713, Doha, Qatar
3-4: Alloy and Microstructure Design - Room: Al Wosail 4	
13:30	Introductory Comments
13:40	Invited Discovery of Sustainable Magnesium Alloys: Pedro Rivera-Diaz-del-Castillo[1]; [1]University of Cambrdige
14:20	Alloy Design Strategies through Computational Thermodynamics and Kinetics Approaches: Raymundo Arroyave[1]; Shengyen Li[1]; Ruixian Zhu[1]; Ibrahim Karaman[1]; [1]Texas A&M University
14:40	Microstructure Design and Homogenization using Correlation Functions: Hamid Garmestani[1]; [1]Georgia Institute of Technology
15:00	Development of Tailored Residual Stress States Through Microstructurally Informed Modeling: Dimitris Lagoudas[1]; Brian Lester[1]; [1]Texas A&M University

15:20	**Poster Session - Room: Al Wosail Foyer**

P-1: A Durability Analysis of Super-Quiet Pavement Structures: Santosh Srirangam[1]; Kumar Anupam[1]; Tom Scarpas[1]; Cor Kasbergen[1]; Peter The[2]; [1]Delft University of Technology; [2]Directie Techniek en Technisch Management/afdeling Wegen en Geotechniek, Rijkswaterstaat ,Dienstonderdeel Grote Projecten en Onderhoud (GPO)

P-2: A New Test for Asphalt Binder Ductility and Intermediate Temperature: Alaedddin Mohseni[1]; Haleh Azari[2]; [1]Pavement Systems; [2]AASHTO

P-3: A New Test Method for Asphalt Mixture Fatigue Characterization: Alaedddin Mohseni[1]; Haleh Azari[2]; [1]Pavement Systems; [2]AASHTO

P-4: Active Composite Materials Undergoing Damage: A Homogenization Approach: George Chatzigeorgiou[1]; Fodil Meraghni[1]; Yves Chemisky[1]; Hassene Ben Atitallah[2]; Zoubeida Ounaies[2]; [1]Arts et Metiers ParisTech; [2]Pennsylvania State University

P-5: Alignment of Nanofibrillated Cellulose (NFC) in Silicone Oil by an Electrical Field: Impact on Effective Electrical Properties: Kaddami Hamid[1]; Kadimi Amal[1]; Raihane Mustapha[1]; Ounaies Zoubeida[2]; [1]Cadi Ayyad University; [2]The Pennsylvania State University

P-6: Boron Removal from Seawater Using ß-Cyclodextrin Modified Magnetic Nanoparticles Fixed on Cellulose Nanocrystals: Deema Almasri[1]; Tarik Rhadfi[1]; Khaled Mahmoud[1]; [1]QEERI

P-7: Computational Assessment of the Performance of Lead Halide Perovskite Solar Cells using Inorganic Layers as Hole Transport Materials: Mohammad Hossain[1]; Fahhad Alharbi[1]; Nouar Tabet[1]; [1]QEERI

P-8: Control of Grain Refinement of A356 Aluminum Alloy by Computer Aided Cooling Curve Analysis: Ahmad Sharifi[1]; Najmeddin Arab[1]; [1]Islamic Azad University

P-9: Controlled Growth of (1-D) ZnO Nanorod Supported Platinum Nanoparticle as Catalyst Materials: Sarim Dastgir[1]; Reem Al-Alawi[2]; Joydeep Dutta[2]; [1]Qatar Environment and Energy Research Institute; [2]Sultan Qaboos University

P-10: Coupled Turbulent Flow and Solidification Modeling in a Brass Slab Continuous Caster: Mandana Adeli[1]; M. Reza Aboutalebi[1]; [1]Iran University of Science & Technology

P-11: Damage Mechanisms of AZ31B Twin Roll Cast (TRC) at Different Strain Rates and Temperatures: Ana Rodriguez[1]; Georges Ayoub[2]; Amine Benzerga[1]; [1]Texas A&M University; [2]Texas A&M University at Qatar

P-12: Density Functional Theory Based Theoretical Calculations for Investigation of Highly Active Visible Light Driven TiO_2 Based Photocatalyst Photoelectrochemical Applications: Matiullah Khan[1]; Wenbin Cao[2]; Bilal Mansoor[1]; [1]Texas A & M University at Qatar; [2]University of Science and Technology Beijing

P-13: Design of Advanced Materials with Tailor-Made Properties Using Molecular Simulation: Ionic Liquids for the Chemical Process Industries: Ioannis Economou[1]; Eleni Androulaki[2]; Niki Vergadou[2]; [1]Texas A&M University at Qatar; [2]National Center for Scientific Research “Demokritos”

P-14: Development of a Redox Model for SOFC Anodes: Bora Timurkutluk[1]; Mahmut Mat[2]; [1]Nigde University; [2]Meliksah University

P-15: Different Approaches to Fabricate Doped-Graphene Composite Films and their Application as a Photovoltaic Transparent Electrode: Adnan Ali[1]; Khaled Mahmoud[1]; Marwan Khraisheh[1]; [1]Qatar Environment and Energy Research Institute

P-16: Direct Observation of Effects of Foam Density, Gating Design and Pouring Temperature on Mold Filling Process in Lost Foam Casting of A356 Alloy: Ahmad Sharifi[1]; Mehdi Mansouri Hasan Abadi[1]; Roholla Ashiri[1]; [1]Islamic Azad University

P-17: Discrete Element Simulation of Asphalt Mixtures Fracture: Enad Mahmoud[1]; Shadi Saadeh[2]; [1]UTPA; [2]CSLB

P-18: Effect of RE Elements on the Sorption Properties of Nanocrystalline Zr-Co Getters Prepared by Mechanical Alloying: Ali Heidary Moghadam[1]; Valiollah Dashtizad[2]; Ali Kaflou[2]; Hossein Yoozbashizadeh[3]; [1]Department of Materials Science and Engineering, Dezful Branch, Islamic Azad University; [2]Department of Advanced Materials and Renewable Energy, Iranian Research Organization for Science and Technology; [3]Department of Materials Science and Engineering, Sharif University of Technology

P-19: Efficient Route for Functionalization of Graphene Nanosheets with Catechol for Preparation of Performance Supercapacitor Electrodes: Efat Jokar[1]; Azam Iraji Zad[1]; Saeed Shahrokhian[1]; [1]Sharif University of Technology

P-20: Electrowinning of Aluminium Using a Depolarized Gas Anode: Geir Martin Haarberg[1]; [1]Norwegian University of Science and Technology and Qatar University

P-21: Evaluation of Asphalt Mixes Workability and Compactability Using Laboratory and Accelerated Field Testing: Samer Dessouky[1]; Manuel Diaz[1]; [1]University of Texas-San Antonio

P-22: Thermo-Mechanical Description of AISI4140 Steel at Elevated Temperatures: Farid Abed[1]; [1]American University of Sharjah

P-23: Fabrication of Bulk Nanocomposites by Mechanical Allying and Shock Compaction: Nikoloz Chikhradze[1]; Guram Abashidze[1]; Mikheil Chikhradze[1]; Akaki Gigineishvili[1]; George Oniashvili[1]; [1]Mining Institute/Georgian Technical University

P-24: Finite Element Analysis in Static and Dynamic Behaviors of Dental Prosthesis: Djebbar Noureddine[1]; [1]Université Djillali Liabes de Sidi Bel Abbes

P-25: Fluid Flow and Heat Transfer Modeling to NOx Characterization in Electric Arc Furnace (EAF): Ali Ershadi[1]; [1]Department of Mechanic Engineering, Dezful Branch, Islamic Azad University

P-26: Fracture Topography of Forged and Direct Quenched Ti/Nb/V HSLA Steels: Sikaddour Yacine[1]; Lebaili Soltane[1]; [1]USTHB

P-27: Graphene /TiO_2 Composite Electrodes Toward Oxygen Reduction Reaction: Halema Al-Kandari[1]; Aboubakr Abdullah[2]; Ahmad Mohamed[3]; Shekhah Al-Kandari[3]; [1]PAAET (Public Authority of Applied Education and Tranining; [2]Qatar University; [3]Kuwait University

P-28: High Haze Nano-Textured Aluminum Doped Zinc Oxide with Plasmonic Silver Nanoparticles for Enhanced Optical Absorption and Photocurrent of a-Si:H Thin Film: Hisham Nasser[1]; Engin Ozkol[1]; Alpan Bek[1]; Rasit Turan[1]; [1]Middle East Technical University (METU)/ The Center for Solar Energy Research and Application (GUNAM)

P-30: Influence of Joining Time on Microstructure and Mechanical Properties of TLP-joined IN-738LC to GTD-111: Mahdi Asgharzadeh Ghadi[1]; Mohammad Amin Amjadi[1]; Mohammad Saeed Shahriari[1]; Meysam Khakian[1]; [1]Mapna/ Mavadkaran

P-31: Mass Production and Large-scale Assembly of Degradation-resistant Nanowires: Venkata Vasiraju[1]; Yongmin Kang[1]; Sreeram Vaddiraju[1]; [1]Texas A&M University

P-32: Mechanical Response and Evolution of Damage of Al 6061-T6 Under Different Strain Rates and Temperatures: Abdelhakim Dorbane[1]; Georges Ayoub[1]; Bilal Mansoor[1]; Ramsey Hamade[2]; Ghassan Kridli[3]; Abdellatif Imad[4]; [1]Texas A&M University at Qatar; [2]American University of Beirut; [3]University of Michigan-Dearborn; [4]Ecole Polytech'Lille

P-33: Methane Production from Carbon Dioxide and Increasing Energy Investment -EROI in Shale Oil: Osama Akoubeh

P-34: Modeling of Carbon Dioxide Absorption Process by Solvent MEA & MEDA: Forough Kazemzadeh[1]; Mohammad Heidary Moghadam[1]; [1]Islamic Azad University

P-35: Molecular Dynamics Study on Physical Properties of Cu Nanoparticles: Hasan Kart[1]; Hüseyin Yildirim[2]; Sevgi Ozdemir Kart[1]; Tahir Cagin[3]; [1]Pamukkale University; [2]Karabuk University; [3] Texas A&M University

P-36: Multicomponent Pyrophosphate as a Promising Cathode Material for Rechargeable Lithium Ion Batteries (LIBs): R. Shakoor[1]; Ramazan Kahraman[1]; Chanseon Park[2]; Soo Lim[2]; Jang Choi[2]; [1]Qatar University; [2]Korea Advanced Institute of Science and Technology (KAIST)

P-37: Non-destructive Assessment of Concrete Mixtures at Cryogenic Temperatures: Towards Primary LNG Containment: Reginald Kogbara[1]; Srinath Iyengar[1]; Zachary Grasley[2]; Eyad Masad[1]; Dan Zollinger[2]; [1]Texas A&M University at Qatar; [2]Texas A&M University

P-38: Numerical Optimization of Lead Free Perovskite Solar Cell: Mohammad Hossain[1]; Ounsi Daif[1]; Nowshad Amin[2]; Fahhad Alharbi[1]; Nouar Tabet[1]; [1]QEERI; [2]National University of Malaysia

P-39: On the Effects of Plastic Anisotropy on the Ductile Fracture of Mg Alloys: Amine Benzerga[1]; S. Basu[1]; E. Dogan[1]; I. Karaman[1]; [1]Texas A&M University

P-40: Optimization of Soft Magnetic Properties in Nanocrystalline Glass-coated Microwires: Valentina Zhukova[1]; Ahmed Talaat[2]; Juan Blanco[2]; Mihail Ipatov[2]; Juan del Val[2]; Arcady Zhukov[3]; [1]Basque Country University, UPV/EHU ; [2]Basque Country University, UPV/EHU; [3]Basque Country University and Ikerbasque

P-41: Predictive Modeling For Sustainable Energy Solutions: Chaker El Amrani[1]; Othmane Bouhali[2]; [1]Abdelmalek Essaadi University, Tangier; [2]Texas A&M University at Qatar

P-42: Principles of Improvement the Energy Efficiency in Pyrometallurgy of Copper: Utilization the Secondary Heat Energy of Intermediate Products: Milorad Cirkovic[1]; Mile Bugarin[1]; Vlastimir Trujic[1]; Zeljko Kamberovic[1]; [1]Mining and Metallurgy Institute Bor, Serbia

P-43: Process Optimization of Seed Assisted Growth of Vertically Aligned ZnO Nanorods via Facile Solution Synthesis: Muhammad Aftab Akram[1]; Sofia Javed[1]; Mohammad Mujahid[1]; Mohammad Islam[2]; [1]National University of Sciences and Technology Pakistan; [2]Center of Excellence for Research in Engineering Materials (CEREM) Advanced Manufacturing Institute, College of Engineering, King Saud University

P-44: Pulsed Electrodeposition of Nano-Crystalline Ni with Uniform Co-Depostion of Micron Sized Diamond Particles on Annealed Copper Substrate: Prashant Kumar[1]; [1]Indian Institute of Technology Banaras Hindu University Varanasi

P-45: RAETEX Sustainable Pavement Technology: Michelle Ward[1]; Shayan Barmand[1]; [1]RAETEX Industries

P-46: Rejuvenation of Long-Term Exposed Nimonic 90 Made Turbine Blades: Mohammad Saeed Shahriary[1]; Mohammad Cheraghzadeh[1]; Ali Khanjani[1]; [1]Mavadkaran Engineering Company

P-47: Simulation of Solidification, Relaxation and Long-Term Behavior of a Borosilicate Glass: Nicolas Barth[1]; Daniel George[2]; Said Ahzi[1]; Yves Rémond[2]; Mohammad Ahmed Khaleel[3]; Frédéric Bouyer[4]; [1]University of Strasbourg/Qatar Foundation; [2]University of Strasbourg–CNRS; [3]Qatar Foundation; [4]CEA (French Alternative Energies and Atomic Energy Commission)

P-48: Storage and Release of Thermal Energy of Phase Change Materials Based on Linear Low Density Polyethylene, Paraffin Wax and Expanded Graphite Applicable in Building Industry: Patrik Sobolciak[1]; Mustapha Karkri[2]; Igor Krupa[3]; Mariam Al. Maadeed[3]; [1]Qatar University; [2]Université Paris-Est; [3]Qatar University

P-49: Structural Alloy AA6082 – Joining by Friction Stir Welding: Zhiui Zhang[1]; Christophe Herbelot[1]; Abdellatif Imad[1]; Rajashekhara Shabadi[1]; [1]University of Science and Technology of Lille

P-50: Towards Engineering Nanolaminated Ternary Carbides and Nitrides (MAX phases) and Their Composites for Extreme Environments: Miladin Radovic[1]; Liangfa Hu[1]; Rogelio Benitez[1]; Ankush Kothalkar[1]; Huli Gao[1]; Ibrahim Karaman[1]; [1]Texas A&M University

P-51: Martensitic Transformation of Ni_2FeGa Magnetic Shape Memory Alloy Studied by Density Functional Theory: Sevgi Özdemir Kart[1]; Cengiz Soykan[1]; Cem Sevik[2]; Tahir Çagin[3]; [1]Pamukkale University; [2]Anadolu University; [3]Texas A&M University

P-52: Surfactant Less Microwave Synthesis of Hierarchical Nanostructures of Titania and Their Application: Sofia Javed[1]; Mohammad Mujahid[1]; Muhammad Aftab Akram[1]; Mohammad Islam[2]; [1]National University of Sciences and Technology Pakistan; [2]Center of Excellence for Research in Engineering Materials (CEREM) Advanced Manufacturing Institute, College of Engineering, King Saud University

P-54: Phenomenological Model for Phase Transformation Characteristics of Textured Shape Memory Alloys: D. Chatziathanasiou[1]; Y. Chemisky[1]; F. Meraghni[1]; E. Patoor[1]; [1]Arts et Métiers ParisTech

P-55: Synthesis and Evaluation of Heterogeneous Nano-catalyst : Cr_2O_3 Loaded in to MCM-41: Ali Salemi Golezani[1]; [1]KIAU

P-56: The Effect of Using a Titanium Interlayer in Explosively Welded Cu/Al Plates: Majid Etminanbakhsh[1]; Mandana Adeli[2]; [1]Iran Research Center; [2]Iran University of Science & Technology

P-57: Thermal Analysis of Solar Panels: Nicolas Barth[1]; Joao Pedro de Magalhaes Correia[2]; Said Ahzi[1]; Mohammad Ahmed Khaleel[3]; [1]Qatar Foundation/University of Strasbourg; [2]University of Strasbourg; [3]Qatar Foundation

P-58: Thermo-mechanical Fatigue and Fracture of NiTiHf High Temperature Shape Memory Alloys: Ceylan Hayrettin[1]; Omer Karakoc[1]; Ibrahim Karaman[1]; [1]Texas A&M University

P-59: Toughness Improvement of Ferritic Mn Steels for Low Temperature Application: Il-Cheol Yi[1]; Yunik Kwon[1]; Yumi Ha[1]; Hakcheol Lee[2]; Nack J. Kim[1]; [1]POSTECH; [2]POSCO

P-60: Transport through Quantum Dots: Hamidreza Vanaie[1]; [1]Islamic Azad University

P-61: Warm Mix Asphalt: Microstructural, Chemical and Thermal Analyses: Ilaria Menapace[1]; Eyad Masad[1]; Dallas Little[2]; Emad Kassem[2]; Amit Bhasin[3]; [1]Texas A&M University at Qatar; [2]Texas A&M University; [3]The University of Texas at Austin,

P-62: Evaluation of Performance Characteristics of Warm Mix Asphalt in Qatar: Emad Kassem[1]; Lorena Garcia Cucalon[2]; Eyad Masad[3]; Dallas Little[2]; [1]Texas A&M Transportation Institute; [2]Texas A&M University; [3]Texas A&M University-Qatar

Wednesday, January 14, 2015

Plenary 3 - Room: Mukhtassar

08:00	Introductory Comments
08:10	Keynote Achievable Innovation in a Sustainable Infrastructure: Dallas Little[1]; [1]Texas A&M University
08:55	Break

1-5: Asphaltic Materials - Room: Mukhtassar

09:10	DEM Simulation of the Asphalt Concrete Flow Number Test: Thomas Papagiannakis[1]; Habatamu Zelelew; [1]University of Texas San Antonio
09:30	Assessment of the Benefits of Implementing Warm Mix Asphalt (WMA) for Roadways in Qatar: Yara Hamdar[1]; Ghassan Chehab[2]; Issam Srour[3]; [1]Graduate Research Assistant, Corresponding Author; [2]Associate Professor, Department of Civil and Environmental Engineering; [3]Assistant Professor, Engineering Management Program
09:50	Effect of Warm Mix Asphalt on Aging of Asphalt Binders: Ala Abbas[1]; Munir Nazzal[2]; Savas Kaya[2]; Sunday Akinbowale[1]; Bijay Subedi[1]; Lana Abu Qtaish[2]; [1]The University of Akron; [2]Ohio University
10:10	Investigation of Long- and Short-term Moisture Damage Characteristics of Warm Asphalt Mixtures Containing Reclaimed Asphalt: Aikaterini Varveri[1]; Stavros Avgerinopoulos[2]; Athanasios (Tom) Scarpas[1]; [1]Delft University of Technology; [2]De Montfort University
10:30	Improving Asphalt Mixtures Performance by Mitigating Oxidation Using Anti-Oxidants Additives: Samer Dessouky[1]; Manuel Diaz[1]; [1]University of Texas-San Antonio

10:50	An Innovative Concept for Testing Rutting Susceptibility of Asphalt Mixture: Alaedddin Mohseni[1]; Haleh Azari[2]; [1]Pavement Systems; [2]AASHTO
11:10	Structural Pavement Improvement Using SBS-Modified Binders: Robert Kluttz[1]; Willem Vonk[2]; Erica Jellema[2]; David Bell[3]; [1]Kraton Polymers; [2]Kraton Polymers Research B.V.; [3]Kraton Polymers U.S., LLC
11:30	Lunch (Al Wosail 2&3)

2-5: Shape Memory Alloys in Energy Conversion - Room: Al Wosail 1

09:10	On the Fracture Response of Shape Memory Alloy Actuators: Dimitris Lagoudas[1]; Theocharis Baxevanis[1]; [1]Texas A&M University
09:30	High-temperature Shape Memory Alloys for Actuation and Damping Applications – Functional Properties and Degradation Behavior: Thomas Niendorf[1]; Philipp Krooss[2]; Hans Maier[3]; [1]TU Bergakademie Freiberg; [2]University of Paderborn; [3]Leibniz Universität Hannover
09:50	Thermal Stability of Ni-rich Ni-Ti-Hf and Ni-Ti-Zr High Temperature Shape Memory Alloys Containing H-phase Precipitates: Aquilina Perez-Sierra[1]; Alper Evirgen[2]; Jaume Pons[1]; Ruben Santamarta[1]; Ibrahim Karaman[2]; Ronald Noebe[3]; [1]University of the Balearic Islands; [2]Texas A&M University; [3]NASA Glenn Research Center
10:10	Large Strains and Nondissipative Character of Superelastic Behavior of Ni-Fe-Ga(Co) Single Crystal: Volodymyr Chernenko[1]; Victor Lvov[2]; Elena Villa[3]; Jose Manuel Barandiaran[4]; [1]BCMaterials,UPV(EHU) & Ikerbasque; [2]Institute of Magnetism; [3]IENI-CNR; [4]BCMaterials & UPV(EHU)
10:30	Development of SMA Actuated Morphing Airfoil for Wind Turbine Blade Load Alleviation: Anargyros Karakalas[1]; Theodore Machairas[1]; Alexandros Solomou[1]; Vasilis Riziotis[2]; Dimitris Saravanos[1]; [1]University of Patras; [2]National Technical University of Athens
10:50	Identification of Model Parameter for the Simulation of SMA Structures using Full Field Measurements: Yves Chemisky[1]; F. Meraghni[1]; N. Bourgeois[2]; S. Cornell[3]; R. Echchorfi[1]; E. Patoor[1]; [1]Arts et Metiers ParisTech; [2]Université de Lorraine; [3]Texas A&M University
11:10	Comparison of the Work Output Values of Gradually Changing Porosity Samples and the Samples with Single Percent Porosity Level: Halil Tugrul[1]; Sule Cakmak[1]; Benat Kockar[1]; [1]Hacettepe University
11:30	Lunch (Al Wosail 2&3)

2-7: Materials Issues in Energy Conversion - Room: Al Wosail 4

09:10	Synthesis, Characterization and Environmental Impact Assessment of Graphene: Mariam AlAli AlMa'adeed[1]; Noorunnisa Khanam Patan[1]; Maryam Al-Aji[1]; Roda F. Al-Thani[1]; [1]Qatar University
09:30	Numerical Modeling of Cathode Contact Material Densification in SOFCs: Mohammed Khaleel[1]; Brian Koeppel[2]; Elizabeth Stephens[2]; [1]Qatar Foundation; [2]Pacific Northwest National Laboratory
09:50	Thin Film Coated Interconnectors Used in Solid Oxide Fuel Cells (SOFC) Via RF Magnetron Sputtering Method: Fatma Aydin[1]; Ali Özmetin[2]; Mahmut Mat[2]; [1]University of Nigde; [2]University of Meliksah
10:10	Perovskites of Type $LaBO_3$ Prepared by the Microwave-Assisted Method for Oxygen Production: Shimaa Ali[1]; Nada Atta[1]; Yasser Abd Al-Rahman[1]; Ahmed Galal[1]; [1]Cairo University, Faculty of Science
10:30	Nitrogen-Doped Carbon Nanofiber – Supported Nickel Oxide Composite for Methanol Oxidation: Aboubakr Abdullah[1]; Abdullah Al-Enizi[2]; Ahmed El-Zatahry[2]; Salem Al-Deyab[2]; [1]Qatar University; [2]King Saud University
10:50	Aluminum and Tin Doping Effect of ZnO Thin Films on the Photovoltaic Parameters of $CuIn1\text{-}xGaxS_2$/ß-$In2\text{-}xAlxS_3$/ZnO Solar Cells: Najoua Kamoun[1]; Mejda Ajili[1]; [1]Faculty of Science TUNIS/ Physics Condensed Matter Laboratory
11:10	Ammonia Borane (AB) as a Portable Source & Storage Material for Hydrogen: Muhammad Sohail[1]; [1]QEERI
11:30	Lunch (Al Wosail 2&3)

2-9: Lightweight and High Performance Materials II - Room: Mukhtassar

13:30	Introductory Comments
13:40	Sustainable Novel Technology for Producing New Generations of Structural Al-alloys and Al Containing Bi-metals: Hans Roven[1]; Kristian Skorpen[2]; Oddvin Reiso[3]; Chris Devadas[4]; [1]Qatar University; [2]Norwegian University of Science and Technology; [3]Hydro ASA; [4]Hydro Aluminium QSTP Qatar
14:00	Modification of Aluminium Surfaces with Metal Oxides: Rajashekhara Shabadi[1]; Vishweshvara Gudla[2]; Flemming Jensen[3]; Rajan Ambat[2]; Aude Simar[4]; [1]University of Science and Technology of Lille; [2]Department of Mechanical Engineering, Technical University of Denmark; [3]Bang & Olufsen Operations A/S; [4]Université Catholique de Louvain
14:20	Parametric Study for Crash Safety Improvement of a Car Bonnet Made from a Hybrid Aluminum and Natural Fiber Composite Structure: Sofiene Helaili[1]; Moez Chafra[1]; Yvon Chevalier[2]; [1]LASMAP; [2]SUPMECA

14:40	Adhesion Improvement Between Polyethylene and Aluminum Using Eco-friendly Plasma Treatment: Anton Popelka[1]; Igor Krupa[1]; Igor Novák[2]; Mabrouk Ouederni[3]; Fatima Abdulaqder[1]; Shrooq Al-Yazedi[1]; Taghreed Al-Gunaid[1]; Thuraya Al-Senani[1]; [1]Qatar University; [2]Slovak Academy of Sciences; [3]QAPCO
15:00	Break
15:20	The Effect of Tool Geometry on Material Mixing During Friction Stir Welding (FSW) of Magnesium AZ31B Welds: Zeina El-Chlouk[1]; Haig Achdjian[1]; George Ayoub[2]; Ramsey Hamade[1]; [1]American University of Beirut; [2]Texas A&M University at Qatar
15:40	Microstructural Design of Mg Alloys for Lightweight Structural Applications: Ebubekir Dogan[1]; Matthew Vaughan[1]; Ibrahim Karaman[1]; Gwénaëlle Proust[2]; Georges Ayoub[3]; Amine Benzerga[1]; [1]Texas A&M University; [2]School of Civil Engineering, The University of Sydney; [3]Texas A&M University at Qatar
16:00	Correlation of Magnetic Properties and Plastic Deformation Distribution in Steel Welds: Athanasios Mamalis[1]; Evangelos Hristoforou[2]; [1]PC-MAE; [2]National TU of Athens
16:20	Role of Multiscale Characterization to Examine the Mechanical Properties for Promoting New Material Developments: Application to Ni-base Superalloys: Bilal Mansoor[1]; Mustapha Jouiad[1]; [1]Masdar Institute of Technology

2-6: Photovoltaics and Solar-Thermal Energy Conversion - Room: Al Wosail 1

13:30	Introductory Comments
13:40	Sponge-like Silicon Nanostructures for Third Generation Photovoltaic Solar Cells: Rasit Turan[1]; Serim Ilday[1]; Emel Ozen[2]; Sinan Gundogdu[2]; Atilla Aydinli[2]; [1]Middle East Technical University; [2]Bilkent University
14:00	Mono-crystalline Bulk Silicon Based High-Efficiency Flexible Solar Cell: Rabab R. Bahabry[1]; Jhonathan P. Rojas[1]; Aftab Hussain[1]; Muhammad M. Hussain[1]; [1]Integrated Nanotechnology Lab, King Abdullah University of Science and Technology
14:20	Hole Mobility and Stresses in PECVD a-Si Thin Films: Nouar Tabet[1]; [1]QEERI
14:40	Sonochemical Synthesis of Cu_2ZnSnS_4 and $Cu_2ZnSnSe_4$ Nanocrystals for Absorber Layer Application in Thin Film Solar Cells: Mohammad Islam[1]; Syed Shah[2]; [1]King Saud University; [2]University of Delaware
15:00	Break
15:20	Electrochemical Deposition of High Purity Silicon from Molten Salts: Geir Martin Haarberg[1]; [1]Norwegian University of Science and Technology, and Qatar University
15:40	Cationic (V, Y)-codoped TiO_2 with Enhanced Visible Light Induced Photocatalytic Activity for Photoelectrochemical Applications: Matiullah Khan[1]; Wenbin Cao[2]; Bilal Mansoor[1]; [1]Texas A & M University at Qatar; [2]University of Science and Technology Beijing
16:00	Enhancement of the Kinetics of Heat Storage by Means of Cellular Metals: Olaf Andersen[1]; Jens Meinert[2]; [1]Fraunhofer-Gesellschaft; [2]Fraunhofer IFAM Dresden
16:20	Economic Technical Solutions for Enhancing the Efficiency of Thermal Solar Water Heating: Iman El Mahallawi[1]; Nagwa Khattab[2]; Ahmed Abdel- Rehim[3]; Sayed Akl[3]; [1]Cairo University; [2]National Research Centre; [3]British University in Egypt

3-5: Computational Approaches towards Mechanical Damage, Environmental Degradation - Room: Al Wosail 4

13:30	Introductory Comments
13:40	Invited Predicting Ductile Fracture Toughness: Alan Needleman[1]; [1]Texas A&M University
14:20	Investigation of Damage and Fracture in Two Magnesium Alloys: Amine Benzerga[1]; B. Kondori[1]; [1]Texas A&M University
14:40	Micromechanical Fatigue Visco-damage Model for Short Glass Fiber Reinforced Polyamide-66: Nicolas Despringre[1]; Yves Chemisky[1]; Gilles Robert[2]; Meraghni Fodil[1]; [1]ENSAM - Arts et Métiers ParisTech; [2]Solvay Engineering Plastics
15:00	Break
15:20	Crystal Plasticity and Fracture Simulations Using a New 2.5D Dislocation Dynamics Method: Shyam Keralavarma[1]; William Curtin[2]; [1]Indian Institute of Technology Madras; [2]Ecole Polytechnique Federale de Lausanne
15:40	Multiparadigm Modeling of Material Safety and Sustainability: Stress Corrosion Cracking: Tahir Cagin[1]; Hieu Pham[1]; Amine Benzerga[1]; [1]Texas A&M University
16:00	Understanding Dusting Corrosion in Iron from Kinetic Monte Carlo Simulations: Oscar Antonio[1]; Fadwa El-Mellouhi[2]; Othmane Bouhali[3]; Charlotte Becquart[4]; Normand Mousseau[1]; [1]Universite de Montreal; [2]QEERI; [3]Texas A&M University at Qatar; [4]École Nationale Supérieure de Chimie de Lille
16:20	Analysis of Thermo-Mechanical Rigidity of Continuously Cast Steel Slabs: Mostafa El-Bealy[1]; [1]Ain Shams University

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The TMS Middle East - Mediterranean Materials Congress on Energy and Infrastructure Systems 2015

TECHNICAL PROGRAM

TECHNICAL PROGRAM & ABSTRACTS

Plenary 1

Monday Morning
January 12, 2015

Room: Mukhtassar
Location: Ritz-Carlton Doha

Session Chair: Raymundo Arroyave, Texas A&M University

08:00 Introductory Comments

08:20 Keynote
Computational Modeling of Deformation Mechanisms in Mg and Mg Alloys: *W Curtin*[1]; M. Ghazisaedi[2]; A. Luque[3]; Z. Wu[3]; [1]EPFL; [2]Ohio State University; [3]Ecole Polytechnique Federale de Lausanne

Mg is the ultimate light-weight metal but, due to its hcp crystal structure and associated high plastic anisotropy, it has limited ductility and only moderate fracture toughness, making it difficult to use in industrial applications. A goal of computational materials design in Mg is to understand the fundamental dislocation structures and plastic deformation mechanisms in Mg and it alloys and, with this understanding, design new alloys with enhanced properties. Here we describe a suite of studies on Mg at quantum, atomistic, and discrete dislocation levels that elucidate the origins of competing deformation mechanisms and effects of alloying. First, we show first-principles density-functional theory (DFT) results on the basal <a> , pyramidal <c+a>, and twin dislocation core structures in Mg. Second, we present DFT results on the interactions of solutes with some of these dislocations. Third, we use these results in a new solute strengthening model and predict strengthening of basal slip and twinning in good agreement with experiments. Fourth, we introduce a new modified-embedded-atom-method interatomic potential for Mg, and show that it predicts dislocation core structures and Peierls stresses, and basal decohesion behavior, in good agreement with DFT results. Fifth, we develop a new model for twin growth in Mg and Mg solid solution alloys and explain a number of experimental observations associated with twinning. Finally, we show the results of molecular dynamics simulations of cracks in Mg, and correlate the crack tip deformation modes with the various dislocation structures and energetics. Collectively, this effort is building a fundamental base of quantitative and mechanistic understanding of deformation and fracture in Mg and its alloys that will complement experiments and aid in the design of new Mg materials.

09:05 Break

1-1: Cemenetitious Materials, Composites

Monday Morning
January 12, 2015

Room: Mukhtassar
Location: Ritz-Carlton Doha

Session Chairs: Yehia Bahei-El-Din, The British University of Egypt; Dallas Little, Texas A&M University

09:20 Invited
Computational Materials Science to Enable Sustainable Concrete Material Design: *Zachary Grasley*[1]; Xiaodan (Sonia) Li[1]; [1]Virginia Tech

Concrete is a complex composite on several length scales from nm to mm, consisting of various solid-like phases surrounded by gas and pore solution (with complex, evolving speciation) in the pore network. This complicated microstructure results in a nuanced interplay between physical processes, including chemical reactions, deformation, and structural evolution. The complicated nature of the interplay is a hindrance to informed material design for achieving sustainable concrete as it dissuades fundamentally sound material model development. Here, we show how computational materials science in combination with sound thermodynamics can be a useful tool to elucidate deformation mechanisms in reacting concrete, which can be used to help design concrete with controlled viscoelastic properties and predict the effect of changes in system chemistry on mechanical behavior. The research approach is quite general, and shows promise for improving our understanding of other coupled problems in concrete, including many durability problems.

10:00
Vertical Scanning Interferometry: A New Method to Quantify Solute-solvent Reaction Dynamics in Cementitious Environments: *Gaurav Sant*[1]; [1]University of California, Los Angeles

Reaction processes including: dissolution, precipitation and corrosion are critical in describing phase evolutions, microstructure formation and degradation in cementitious materials. In spite of their significance, the dynamics of such reactions remain slightly studied. New integrations of optical microscopy/laser profilometry, in the form of vertical scanning interferometry (VSI) are being used to quantify at the nanoscale, and in real-time, reaction dynamics relevant to cement, steel and the interactions of cement with chemical admixtures. New information provisioned using such methods accesses kinetic features of reactions, across a range of chemical and state variables (P,T) to: describe rate-controls on reactions, identify novel reaction manipulation strategies and provide inputs for computational simulation platforms. Such quantifications of mineral dissolution are helping cements react faster, and more efficiently, and quantify/mitigate steel corrosion. Such knowledge is critical to make concrete structures, last longer, perform better, and exert lower impacts on the environment.

10:20
Effect of Interface and Interphase Regions on the Elasticity of Nanocomposite Cement: *Ala Abu Taqa*[1]; Ahmed Senouci[1]; Rashid Abu Al-Rub[2]; [1]Qatar University; [2]Masdar Institute of Science and Technology

The elasticity of the nanocomposite cement has been investigated using axisymmetric model of a single aligned CNT embedded in cement matrix. The model, which has been built using Abaqus finite element software, consists of four phases; CNT, interface, interfacial transition zone (ITZ or interphase) and the cement matrix. Ignoring interphase region, the CNT and cement matrix were first assumed to be perfectly bonded at the interface and the results of the composite elastic modulus have been compared to those of the 3D models and to the upper and lower bounds of the mixtures theory for different CNT volume fractions. Moreover, using cohesive surface for modeling the interface, parametric study has been conducted to investigate the effect of interface and interphase properties on the overall composite elastic modulus for different CNT volume fractions and aspect ratios.

10:40
Finite Element Simulation of the Response of No-Tension Materials: *Alieh Alipour*[1]; Tom Scarpas[1]; [1]Delft University of Technology

Unbound granular materials that are used at base layer of flexible pavement cannot resist tensile forces. These materials are called no-tension materials. In this paper, a modified strain-energy function was used to describe the constitutive behavior of granular materials to simulate flexible pavement within the finite element framework CAPA3D .The constitutive model was defined such that the positive stresses in principal directions were zero. Comparisons between the no-tension materials and linear elastic materials for different boundary conditions and geometries were presented in this paper. The results of FE analysis show that effect of using no-tension model for base layer on pavement performance is significant. The deformation at top and horizontal strain at the bottom of asphalt concrete layer are higher when the no-tension model is used.

11:00
Investigation and Modeling of the Damage Evolution in Natural Fiber Composites: *Habiba Bougherara*[1]; Zia Mahboob[1]; Fodil Meraghni[2]; Laurent Peltier[3]; [1]Ryerson University; [2]ENSAM - Arts et Métiers ParisTech; [3]

The main objective of this investigation is to identify and characterize the damage mechanisms of flax-reinforced epoxy composites using an energy-based damage model combined with nanotomography observations. Four configurations of flax/epoxy composites layup were studied namely, unidirectional laminates [0]16 and laminates with different ply orientation (e.g., [90]16 , [+45]16 and [±45]16).The damage model's parameters for each configuration were determined from quasi-static and fatigue tests. The preliminary results showed that the energy-based damage model can predict accurately the damage rate in both longitudinal and transverse directions. The mechanism of damage initiation in the flax/epoxy composites and the damage evolution, during each test, were monitored using a nanotomograph. A direct correlation between the microstructure of the flax-reinforced epoxy composites and the damage was obtained.

2-1: Ferrocaloric Materials

Monday Morning — Room: Al Wosail 1
January 12, 2015 — Location: Ritz-Carlton Doha

Session Chairs: Dimitris Lagoudas, Texas A&M University; Volodymyr Chernenko, Universidad del Pais Vasco

09:20 Invited
The Direct Conversion of Heat to Electricity Using Multiferroic Materials: *Richard James*[1]; [1]University of Minnesota

Most power produced on earth relies on the phase transformation between water and steam. However, other phase transformations may have advantages such as convenient temperature regimes, simplicity, elimination of the electrical generator, elimination of heat exchangers and piping systems, efficiency, power density, or ease of capturing natural (solar thermal) or waste (from power plants, A/C systems, computers) sources of heat. We examine the use of first-order phase transformations in multiferroic materials. In these materials electricity is produced directly, without the need of a separate electrical generator, by induction or charge separation. A critical issue for energy conversion is the ability to pass back and forth through the phase transformation many times without significant hysteresis. We describe recent research that addresses this issue by strategies that achieve strong conditions of compatibility between phases. We discuss efficiency and power density, highlighting the importance of the first order nature of the phase transformation.

10:00 Invited
Origin of Hysteresis in Multicaloric Materials: *Sebastian Fähler*[1]; [1]IFW Dresden

Ferroic phase transitions driven by external magnetic, electric or stress fields promise more energy efficient solid state refrigeration. A key step towards this environmentally friendly technology was the use of first instead of second order phase transitions, which substantially increased the associated entropy change. However, a drawback of first order materials is the transformation hysteresis, which heats up the material and thus reduces or even eliminates the efficiency of a solid state cooling device. Despite this, hysteresis is often ignored when characterizing materials, e. g. by using the Maxwell relation or using only the first direct delta-T measurement instead of a complete cycle. I will sketch the structural and microstructural origin of hysteresis exemplarily for Heusler alloys.

10:40
Approaches to Analyze Cycle Efficiency in Magnetocaloric Materials: *Patrick Shamberger*[1]; T.D. Brown[1]; J. Murley[1]; J.H. Chen[1]; J. Ross[1]; N. Bruno[1]; I. Karaman[1]; [1]Texas A&M University

The principle motivation driving development of magnetocaloric effect materials is the promise of efficient magnetic refrigeration. However, the so-called "giant" magnetocaloric effect materials, which dominate the current magnetocaloric literature, are marked by hysteresis and kinetic effects which significantly detract from the efficiency of these materials. Here, we present an approach to analyze cycle efficiency based on 1) mapping of the entropy surface as a function of temperature (T) and magnetic field (H), and 2) integrating a hysteresis model to predict the state of the system as a function of some arbitrary T, H path. We will compare indirect measurements of entropy collected by two distinct methods and discuss experimental complications of the two approaches. Finally, we demonstrate combination of magnetic and entropy data with a hysteresis model to predict cycle efficiency of different cycles in a representative hysteretic material and discuss broad materials design guidelines for high performance magnetic refrigerants.

11:00
The Tunable Microstructure and its Influence on the Giant Magnetocaloric effect in Magnetic Shape Memory Alloys: *Nickolaus Bruno*[1]; Yujin Huang[2]; Ibrahim Karaman[1]; Joseph Ross[1]; Jianguo Li[2]; [1]Texas A&M University; [2]Shanghai JiaoTong University

The entropy and adiabatic temperature changes upon martensitic transformation induced by external magnetic fields were studied in various NiCoMn-X (X=Sn, In) magnetic shape memory alloys (SMAs). Their relative cooling power were determined using an extensive thermodynamic framework. Tunable materials parameters that lead to an improved caloric effect were identified, including magnetic-field sensitivities of martensitic transformation temperatures, transition ranges, and thermal hysteresis, and magnetization changes across the transition. These properties were determined experimentally from simple magneto-thermo-mechanical measurements before and after various annealing treatments and were identified to be related to microstructural features such as atomic ordering and grain size. The results indicated that large grain size and disordered austenite phases yield small transition ranges and hysteresis for the studied compositions. The improved microstructure after annealing also reduced the required driving force used to induce the temperature change, thereby revealing the possibility of using magnetic SMAs in room temperature solid state refrigeration.

11:20
Studies of Magnetic Properties of Ni-Mn-In-Co Heusler-type Glass-coated Microwires: Valentina Zhukova[1]; Mihail Ipatov[1]; Alexandr Aronin[2]; Galina Abrosimova[2]; Alexandr Kiselev[2]; *Arcady Zhukov*[3]; [1]Basque Country University; [2]Insitute of Solid State Physics; [3]Basque Country University and Ikerbasque

We report on magnetic properties and structure of Heusler-type NiMnIn(Co) glass-coated microwires with metallic nucleus diameters ranging from 13 up to 23 \956m and total diameters from 47 to 55 \956m prepared by the Taylor-Ulitovsky technique. We measured temperature dependence of magnetization of as-prepared and annealed glass-coated microwire. As-prepared glass-coated microwires are paramagnetic at room temperature exhibiting ferromagnetic ordering below 260K. Annealed NiMnIn sample present Curie temperature about 280K. At room temperature all studied samples present single cubic phase with a lattice constant lattice parameters: 0.5913 nm for $Ni_{50}Mn_{35}In_{15}$, 0.5888 nm for $Ni_{42.5}Mn_{37.5}In_{12.5}Co_{7.7}$ and 0.5884 nm for $Ni_{45}Mn_{36.5}In_{13.5}Co_{5}$. Both as-prepared and annealed microwires exhibit unusual magnetization growth in vicinity of Curie temperature and considerable difference in M(T) for field cooled and zero-field cooled dependences. Considerable dependence of magnetization on magnetic field below and in vicinity of Curie temperature can be related with two-phase structure or with the Hopkinson effect.

3-1: Ab-Initio Approaches

Monday Morning — Room: Al Wosail 4
January 12, 2015 — Location: Ritz-Carlton Doha

Session Chairs: Ioannis Economou, Texas A&M University Qatar; Raymundo Arroyave, Texas A&M University

09:20 Invited
Ab Initio Thermodynamics: A Novel Route to Design Structural Materials with Superior Mechanical Properties: *Jörg Neugebauer*[1]; Blazej Grabowski[1]; Fritz Kormann[1]; Tilmann Hickel[1]; [1]Max-Planck-Institut für Eisenforschung GmbH

A key requirement in developing computational tools to design structural materials with superior mechanical properties is the availability of accurate yet efficient methods that allow to compute and predict the phase and rate determining energies not only at T = 0 K but also under realistic conditions, i.e., at finite temperature. Combining accurate first principles calculations with mesoscopic/macroscopic thermodynamic and/or kinetic concepts allows now to address this issue and to determine free energies and derived thermodynamic quantities with an accuracy that often rivals available experimental data. The flexibility and the predictive power of these approaches to determine/predict defect and microstructure properties and the impact they can have in developing new strategies in achieving tailored microstructures will be discussed: Examples will address modern high-manganese steels that combine high strength with excellent formability (ductility), ultra-high strength pearlitic steels and understanding the mechanisms behind H embrittlement in high-strength steels.

10:00

A DFT Based Molecular Dynamics Study of $PbI_3(CH_3NH_3)$: *Marcelo Carignano*[1]; [1]QEERI - Qatar Foundation

Hybrid organic-inorganic perovskites are attracting the attention of the photovoltaic research world due to a remarkable succession of improvement in efficiency since their introduction in 2009. $PbI_3(CH_3NH_3)$, which is the prototypical example, has reached a conversion efficiency just shy of 20 % in five years of research efforts. From a computational point of view, the understanding of the material's properties poses many challenges. For example, even though these perovskites are in solid state at room temperature, the organic molecule is able to rotate at a relatively fast pace and therefore the system belong to the plastic crystal category. In this work we present a molecular dynamics simulation of $PbI_3(CH_3NH_3)$ based on forces calculated using DFT methods. In this way we properly consider the rotational dynamic of the methylammonium and investigate how that influences the overall structure of the perovskite and its optical properties, like the energy gap for electronic excitation.

10:20

Thermal Expansion Coefficient of Two Dimensional Materials: *Cem Sevik*[1]; [1]Anadolu University

The successful isolation of graphene has triggered the exploration of two-dimensional (2D) materials with different physical and chemical properties. Among them, h-BN, and semiconductor transition-metal dichalcogenides (TMDC), have attracted significant research interest due to their high potential for nanoelectronic and nanophotonic applications. The linear thermal expansion coefficients of these two dimensional honeycomb structures are systematically studied by using first-principles based quasi harmonic approximation. Our simulations show that the linear thermal expansion coefficients of graphene and h-BN are more negative than that of their multi-layered counterparts graphite and white graphite [1]. Contrary to graphene and h-BN, lattice thermal expansion coefficient of TMDCs are always positive and the values are comparable with those predicted for diamond [2]. [1] C. Sevik, Phys. Rev. B 89, 035422 2014[2] D. Cakir, F. M. Peeters, C. Sevik, Appl. Phys. Lett. 104, 203110 2014

10:40

Strong Stacking Between Organic and Organometallic Molecules as the Key for Material Design: *Snezana Zaric*[1]; Dusan Malenov[2]; Dragan Ninkovic[2]; [1]Texas A&M University at Qatar; [2]Innovation Centre of the Department of Chemistry

Very attractive properties of organic-inorganic materials consisting of planar molecules, namely magnetism, conductivity, non-linear optics and catalysis, are highly dependent on the stacking interactions. Metal-chelate rings and aromatic molecules are very common constituents of these materials. The search of Cambridge Structural Database has shown that stacking interactions ofchelates and aromatic molecules occur very often in crystal structures; these interactions are of very similar geometries to stacking between two aromatic molecules. The energies of these interactions have been calculated at high theoretical levels, showing much stronger stacking of six-membered chelate with benzene that stacking of two benzene molecules. The stacking interaction between two benzene molecules is -2.73 kcal/mol, while the interaction between benzene and chelate ring dependent on the metal type, being stronger for copper(II)-chelate (-6.08 kcal/mol) than for nickel(II)-chelate (-4.68 kcal/mol). The energies of interactions are calculated at CCSD(T)/CBS level and the benchmark study was performed to find Minnesota functionals that can reproduce this data.

11:00

Calculation of Electronic Structure and Field Induced Magnetic Collapse in Ferroic Materials: Raymundo Arroyave[1]; *P. Entel*[2]; N. Singh[3]; M. Gruner[2]; A. Grünebohm[2]; V. V. Sokolovskiy[4]; V. D. Buchelnikov[4]; [1]Texas A & M University; [2]University, Duisburg-Essen; [3]University of Houston; [4]Chelyabinsk State University

We have performed ab inito electronic structure calculations and Monte Carlo simulations of FeRh, Mn_3GaC and Heusler intermetallics alloys such as Ni-Co-Cr-Mn-(Ga, In, Sn) which are of interest for solid refrigeration and energy systems, an emerging tehnology involving such solid-solid systems. The calculations reveal that the important magnetic phase diagrams of these alloys which show the magnetic collapse and allow predictions of the related magnetocaloric effect which they exhibit at finite temperatures, can be obtained by the ab initio computations alone. This is a one-step procedure from theory to alloy design of ferroic functional devices.

1-2: Cementitious Materials Sustainability

Monday Afternoon — Room: Mukhtassar
January 12, 2015 — Location: Ritz-Carlton Doha

Session Chair: Srinath Iyengar, Texas A&M University at Qatar

13:30 Introductory Comments

13:40 Invited

Utilising Fine and Coarse Recycled Aggregates from the Gulf Region in Concrete: *Roderick Jones*[1]; Judith Halliday[1]; Laszlo Csetenyi[1]; Li Zheng[1]; Nikolaos Strompinis[1]; Moray Newlands[1]; [1]University of Dundee

This paper explores the feasibility in utilising materials generated from C&DW to produce a 'green' concrete. The two materials that are considered here are, (i) up-sizing silt-size material generated from recycled aggregates to produce a synthetic silt-sand and (ii) processed recycled coarse aggregates (RA) sourced from a Gulf Region landfill site. The work has demonstrated that there is potential for utilising silt wastes into foamed concrete, which can then be crushed to a sand-sized material suitable for use in concrete, however the porous nature of the material has highlighted that the water demand of this RA is high. RAs were characterised to BS EN 12620 and found suitable for use in concrete. The effect of RA on concrete properties is minimal when used up to 35% replacement levels, provided that they are pre-soaked.

14:20

Multiwalled Carbon Nanotubes Aspect Ratio, Functionalization, Weight Fraction & Surfactant Effect on the Mechanical Properties of Cementitious Materials: *Mohamed Mohsen*[1]; Rashid Abu El Rub[2]; Ahmed Senouci[1]; Nasser Alnuaimi[1]; Khaldoon Bani Hani[3]; [1]Qatar University; [2]Masdar Institute of Science and Technology; [3]Jordan University of Science and Technology

Carbon nanotubes (CNTs) present extraordinarily properties such as high strength and stiffness. These properties make them attractive candidates to be used in the design of cement composites materials. However, obtaining the targeted properties is related to a good dispersion of the nano filaments in the matrix. To solve the dispersion issue, methods such as sonication of CNTs in aqueous solution and functionalization are applied. These methods however are affected by several factors such as the aspect ratios, CNT/surfactant ratio, functionalization rate, surfactant type, CNT/Cement ratio, enduring dispersion in cement mix, sonication time and energy. In this paper, the effect of the aspect ratio, functionalization, weight fraction, and the surfactant on the mechanical strength of cement paste specimens is studied. Short, medium and long treated and non treated CNTs are tested at 0.03%, 0.08% and 0.15% weight fractions of cement. Furthermore, the microstructures are analyzed using SEM images.

14:40

Defined Polymers as Candidates for Pavement Subgrade Soil Stabilization: *Chandramohan Ayyavu*[1]; Srinath R. Iyengar[1]; Howard J. H. M. Hanley[1]; Hassan S. Bazzi[1]; Dallas Little[1]; [1]Texas A&M University at Qatar

The subgrade soil stabilization has a major influence on pavement construction and durability. Failure to chemically alter certain subgrades in Qatar has resulted in early pavement failures. Previous studies on synthesizing defined polymers as stabilizers for Qatar subgrades, have shown encouraging practical results, which, in some cases, demonstrated quantifiable engineering advantages over traditional stabilizers like Portland cement. Hence, investigation was expanded for different soil types, in order to tailor a polymer to be compatible with a subgrade soil of defined material characteristics. Accordingly, laboratory mechanical testing under realistic curing conditions was carried out with the variants of the polymer binders. In addition, the ionic microstructure of the polymer was modified to investigate how such changes relate to the polymer efficiency as a stabilizer. The results of the study indicate a definite correlation between the relative anionic and cationic make-up of the polymer and the chemical characteristics of the subgrade soil.

15:00 Break

2-8: Lightweight and High Performance Materials I

Monday Afternoon — Room: Mukhtassar
January 12, 2015 — Location: Ritz-Carlton Doha

Session Chairs: Ghassan Kridli, University of Michigan - Dearborn; David Dunand, Northwestern University

15:20
Nanomaterials for "Smart" Membrane Pretreatment and RO Desalination Technologies: *Khaled Mahmoud*[1]; [1]QEERI-QF

Seawater desalination has been the primary source of drinking water for Qatar. Recently, reverse osmoses (RO) has been demonstrated as a feasible desalination technology for Qatar. However, the main limitations of SWRO are the membrane fouling associated with particulate matter/colloids, organic/inorganic compounds, and biological growth. Nanomaterials have emerged as a smart additive for more efficient membrane-based water purification and desalination technologies. Emerging nanomaterials such as cellulose nanocrystals (CNCs) and graphene oxide (GOx) are exceptionally beneficial for membrane modification due to their mechanical properties and amenable surface functionalization. This would impart new functionality to the membrane such as selective ion penetration, hydrophilicity, antimicrobial properties, high water permeation, and impede bio-fouling. This talk proposes new schemes for implementing "smart" nanomodification to the membranes that decrease the adhesion or increase the release of adsorbed particulates and organic molecules and therefore mitigate fouling, added chemicals toxicity, and increase salt rejection efficiency.

15:40
3D Nanotubular Surfaces for Energy Storage and Conversion: *Tolou Shokuhfar*[1]; [1]Michigan Technological University

3D nanotubular surfaces can be produced on the surface of variety of so called 'Valve' metals. In this process, first a metal oxide layer will be produced on the surface and after careful control of anodization parameters such as applied voltage, current, pulse, and time, a self-organized nanotubes can be created for applications in solar cells, Li-ion batteries, and gas conversion reactions. In this talk we show how the manufacturing process can affect the energy performance of such surfaces.

16:00
Mechanical Properties of Al-Zr-Sc Alloys with Si and Er Micro-additions: Nhon Vo[1]; Nick Barta[2]; Georges Ayoub[3]; Ibrahim Karaman[2]; *David Dunand*[1]; [1]Northwestern University; [2]Texas A&M University; [3]Texas A&M University at Qatar

High-conductivity 1000-series (Al-<0.4Fe-<0.1Si, wt.%) and high-strength 6000-series (Al-(0.2-3)Mg-(0.2-1.8)Si, wt.%) aluminum alloys are used for high voltage cables, whose current-carrying capacity is limited by the maximum temperature of ~200 ºC, beyond which creep is rapid. Here, we report on a new creep- and coarsening-resistant, high-conductivity, high-purity ~99.7 (wt.%) aluminum alloy with temperature capability of ~400ºC. Micro-alloying additions of Zr, Sc, Er and Si result in nanoscale trialuminide precipitates which strengthen these alloys very efficiently. The mechanical properties of the alloy - with and without extreme deformation by equi-channel angular extrusion - are measured and compared with those of similar alloys with higher Sc content (and thus higher price).

16:20
Development of High Strength and Ductile Al-xMg Alloys for Sustainable Applications: Min Zha[1]; *Hans Roven*[2]; Chris Devadas[3]; [1]Norwegian University of Science and Technology; [2]Qatar University; [3]Hydro Aluminium QSTP Qatar

Binary Al-xMg alloys have been developed by severe plastic deformation and annealing, e.g., multiple pass ECAP combined with inter-pass annealing, achieving a simultaneous high strength and high ductility. The superior combination of mechanical properties was mainly attributed to high work hardening ability primarily originating from a bimodal grain structure and a high level of Mg in solid solution. In the bimodal structure, larger grains accommodate relative high numbers of dislocations hence promoting higher ductility. The ultrafine grains need higher local flow stress to continue deformation, i.e. thereby contributing to higher strength. In addition, the materials have a relatively high thermal stability and reasonable good electrical conductivity. In particular, the developed Al-7Mg alloy is attractive in view of the high strength, reasonably good ductility, relatively high thermal stability, good thermal conductivity and in a recycling perspective. All these properties are attractive for future sustainable infrastructure applications.

16:40
Microstructural and Mechanical Characterization of Friction-Stirred Welded (FSW) TRC AZ31B Magnesium Alloy Sheets: *Abdelhakim Dorbane*[1]; Georges Ayoub[1]; Bilal Mansoor[1]; Ramsey Hamade[2]; Ghassan Kridli[3]; Abdellatif Imad[4]; [1]Texas A&M University at Qatar; [2]American University of Beirut; [3]University of Michigan-Dearborn; [4]Ecole Polytech'Lille

The microstructural and mechanical evolution of friction-stirred welded twin roll cast AZ31B magnesium alloy was characterized. The joints were obtained with FSW process using tool rotation speed of 1200 rpm and displacement speed of 150 mm/min. Uniaxial tensile testing was performed on the as received material and the FS welded material cut with their major axis parallel to the welding direction. The tensile tests were conducted at 0.1s-1 and 0.001s-1 strain rates under variable temperatures ranging between room temperature to 300°C. It was observed that both strain rate and temperature has an influence on both mechanical and microstructural properties of the joint. Micro-hardness tests were performed on the joint showing a variation of hardness values between 70 HV and 50 HV.

2-2: Energy Storage Materials

Monday Afternoon — Room: Al Wosail 1
January 12, 2015 — Location: Ritz-Carlton Doha

Session Chairs: Mohammed Khaleel, The Qatar Environment and Energy Research Institute; Sreeram Vaddiraju, Texas A&M University

13:30 Introductory Comments

13:40 Invited
Nanomaterial Design Strategies for Capacitive Energy Storage Applications: *Husam Alshareef*[1]; [1]King Abdullah University for Science & Technology (KAUST)

The talk will focus on strategies that we have been developing to improve electrode material performance in capacitive energy storage devices. Conventional pseudocapacitors, hybrid supercapacitors, and microfabricated supercapacitors will be covered. The talk will cover the development of organic and inorganic electrodes that offer both macroporosity and mesoporosity using in-situ nucleation on current collectors. The resultant morphologies of such electrodes facilitate electrolyte permeation, reduce device resistance, and provide large surface areas for faster reaction kinetics at the electrode surface, thereby increasing device capacitance. Development of negative electrode materials for the fabrication of hybrid and asymmetric capacitive devices, which work at higher voltage, will also be covered. Finally, recent development in flexible and microfabricated supercapacitors for self-powered device applications will be highlighted.

14:20
Rechargeable Batteries: Lessons from Real Time Observation of Lithiation/Delithiation in Nanoscale Anode Materials: *Reza Shahbazian-Yassar*[1]; [1]Michigan Technological University

Electrodes in rechargeable batteries undergo complex electrochemically-driven phase transformations upon driving Li ions into their structure. Such phase transitions in turn affect the reversibility and stability of the battery. It is of prime importance to better understand how Li ions transport within the host electrodes and what phase transitions are triggered during such interaction. This presentation gives an overview of the PI's research program on in situ transmission electron microscopy (TEM) of battery materials. Various anode materials including SnO_2, Zn-Sb were subjected to lithiation process and the transport of Li ions was visualized within their atomic structure. For SnO_2 nanowires, it was observed that the Li ion transport preferably happens along (200) or (020) plans and [001] crystallographic directions. Zn-Sb alloys also exhibit a new cubic alloying phase LiZnSb that form by intermixing of the ABAB atomic ordering in hexagonal LiZnSb due to Li inclusion in their lattices.

14:40

Electrode Materials Based on Phosphates for Lithium Ion Batteries as Efficient Energy Storage System: *Saadoune Ismael*[1]; Lasri Karima[1]; Bezza Ilham[1]; Ehrenberg Helmut[1]; Indris Sylvio[1]; Daniel Brandell[2]; [1]University Cadi Ayyad Marrakech; [2]Uppsala University

At the present time, considerable effort is applied for the development of new electric energy sources and improvement of the already known systems. In particular, great attention is focused on rechargeable Li-ion batteries. Lithium transition metal phosphates are promising candidates as positive electrode materials for Li-ion batteries. The existence of $Mn(PO_4)y$ framework provides an excellent stability and long term cycling to this type of cathode in comparison to lithium transition-metal oxides, leading to safe energy storage system. In our group, many new phosphates were prepared by soft chemistry methods. According to their low electronic conductivities, the synthesized phosphates were coated by a thin layer of carbon leading to a great enhancement of the electrochemical properties in terms of energy storage efficiency and electrochemical cycling. The recently obtained results on $M_{0.5}TiOPO_4$ (M:Fe, Ni) oxyphosphates and $LiFe_{0.4}Mn_{0.6}PO_4$ olivine will be presented in this conference. The relationship between: structure-energy storage will be discussed.

15:00 Break

15:20

Interfacial Stresses and Degradation of Oxide Scale and Substrate Interface at High Temperatures: *Mohammed Khaleel*[1]; E. Stephens[2]; J. Stevenson[2]; [1]Qatar Foundation; [2]Pacific Northwest National Laboratory

Interfacial analysis utilizing interfacial indentation methodology (where micro/nano indentation is performed at the oxide scale/substrate interface to create and propagate cracks at the interface) was completed for the 14,000 and 20,000 hour, 800°C surface modified specimens. The localized oxide thickness and crack lengths were measured after applying loads ranging from 0.2 to 1.8 N. Post-processing of the results to date indicate that the critical load for surface blasted (SB) surface modified specimens is greater than the equivalent surface grind (SG) surface modified specimens which is indicative of a ~25% increase in interfacial strength in the SB specimens in comparison to the SG specimens. However, more data is needed to further quantify the interfacial strength and to reduce any uncertainty due to the approach applied.

15:40

Predicting Acoustic Emission and Electrochemical Impedance Spectra for Damage Stochastics in Energy Materials: Pallab Barai[1]; Chien-Fan Chen[1]; *Partha Mukherjee*[1]; [1]Texas A&M University

Electrochemical corrosion, hydrogen embrittlement, diffusion induced stress are different forms of degradation mechanisms observed in various energy and structural materials. Due to the underlying mechano-physicochemical interactions, the materials are subject to formation of microscopic cracks. Nucleation of these microcracks may lead to fracture formation, material isolation and debonding. Electrochemical impedance and acoustic emission spectroscopic methods have been used extensively to characterize mechano-chemical degradation of such materials. Computational methodologies have been developed to characterize the electrochemical impedance response and capture the propagation of acoustic waves within the material. Here we present the computational prediction of acoustic emission and electrochemical impedance spectra in order to understand the mechano-electrochemical interactions and corresponding stochasticity of damage evolution in intercalating materials for lithium-ion battery electrodes. These computational methodologies are applicable to understanding degradation phenomena in different energy and structural materials e.g. in corrosion, and solid oxide fuel cells.

16:00

Novel Organic Electrodes for Organic Rechargeable Batteries: *Burak Esat*[1]; Sumeyye Bahceci[1]; Sevda Akay[1]; Aliyu Bawa Abdullahi[1]; [1]Fatih University

The ever-increasing demand for high-performing, light weight, economical, and safe power storage for high–tech portable devices and electric vehicles leads to augmented research efforts in the field of organic or organic/hybrid materials to be used as electrodes in energy storage devices. There has been an increasing number of studies toward the development of novel pure or composite materials containing redox polymers with pendant organic electro-active groups which may be used as cathode- or anode-active material in batteries. These efforts may eventually lead to totally organic batteries with improved properties such as light weight, flexibility, improved environmental safety, low cost of manufacturing. We hereby represent novel polymers and carbon nanotubes with pendant electroactive groups such as TEMPO, benzimidazole-1-oxyl-3-oxides, quinones.

16:20

$Na_2Fe_{0.5}$ $Mn_{0.5}P_2O_7$ as Promising Cathode Material for Rechargeable Sodium Ion Batteries (NIBs): *R. Shakoor*[1]; Ramazan Kahraman[1]; Chanseon Park[2]; Soo Lim[2]; Jang Choi[2]; [1]Qatar University; [2]Korea Advanced Institute of Science and Technology (KAIST)

In the present study, we herein, report a novel multicomponent pyrophosphate ($Li_2Fe_1/3Mn_1/3Co_1/3P_2O_7$) cathode material for lithium rechargeable batteries that demonstrates decent electrochemical behavior and excellent thermal stability. Electrochemical measurements confirm that a reversible capacity of 100 mAh/g is obtained at C/20 rate with decent capacity retention and high rate performance. Ex situ analyses verify that the intercalation/de-intercalation of lithium into/from the host structure is associated with one phase reaction rather than a biphasic reaction with negligible volume change (~0.7%) in contrast to its single component ($Li_2FeP_2O_7$). TGA/DTA and thermal Insitu XRD analyses (25-550 C) confirm the excellent thermally stable of this material up to 550 C even in the delithiated state ($LiFe_1/3Mn_1/3Co_1/3P_2O_7$) with negligible weight loss (~2%) which is superior to delithiated $LiFeP_2O_7$ and many other reported cathodes. The promising properties of this novel cathode material can be mainly attributed to its unique crystal structure.

16:40

Nanomaterial-based Ultracapacitor for Power Integrated Circuits: *Daniel Choi*[1]; Waqas Gill[1]; Maarten Geest[1]; [1]Masdar Institute of Science and Technology

Some aging effects limit current supply to the Integrated Circuit (IC) due to the instable switching power supply, requiring an additional specific circuit board for supplying and regulating electric power to the main circuit board. It can be solved by depositing a capacitance layer on top of circuitry substrate. Copper (Cu) nanotube (NT)-based micro-chip capacitors fabricated onto an IC can be used to compensate the power requirement in regulating electric power to a circuit board. In this work, a process for fabricating NTs electrodes which may be compatible with complementary metal-oxide-semiconductor (CMOS) is presented. Cu NTs were used as the electrode materials for the on-chip capacitors. Anodized Oxide aluminum (AAO) templates integrated on SiO2/Si substrates were used for fabrication of a vertical array of Cu NTs. The surface area of the capacitor was increased by adding Cu NTs which enable a high density of capacitance for the devices.

3-2: Energy Materials Simulation

Monday Afternoon — Room: Al Wosail 4
January 12, 2015 — Location: Ritz-Carlton Doha

Session Chairs: Tahir Cagin, Texas A&M University; Cem Sevik, Anadolu University

13:30 Introductory Comments

13:40 Invited

Application of Phase-field Method to Modeling Microstructure Evolution in Li-ion Batteries: *Long Qing Chen*[1]; [1]Penn State University

Phase-field method is the method of choice for modeling microstructure evolution in many different processes. This presentation will discuss its applications to microstructural processes during Li-plating and Li-insertion into and extraction from electrodes in Li-ion batteries. The focus will be on Li_xFePO_4, one of the most-studied cathode materials in Li-ion batteries. The thermodynamics of the $FePO_4$-$LiFePO_4$ two-phase system and the effect of coherent stress on the miscibility gap and two-phase morphology will be discussed. A three-dimensional phase field model for modeling the morphological evolution during the intercalation/extraction of Li-ions into a host electrode will be described. It incorporates the effects of anisotropic diffusional mobility of Li-ions in the electrode host lattice, flux of Li-ions across the electrode/electrolyte interface, and coherency strains arising from the lattice parameter mismatch between the lithiated and unlithiated phases. Implementation of spectral methods to solving the systems of equations under non-periodic boundary conditions will be presented.

14:20
Modeling of Thermal Behavior and Efficiency of Photovoltaic Panels: *Said Ahzi*[1]; [1]University of Strasbourg/Qatar Foundation

In this work, we propose to analyze the thermal behavior of PV panels using finite element simulations. We applied this analysis to compute the temperature distribution in a PV panel BP 350 subjected to different atmospheric conditions. This analysis takes into account existing formulations in the literature. The results of the different formulations were analyzed using the NOCT conditions, meteorological data from Ajaccio, France, and a parametric study that incorporates variations in the ambient temperature, the global and beam radiations and the wind speed. The electrical performance of the PV panel was also studied. The analysis consisted in implementing two different one-diode models. Both approaches required the calculation of two important parameters hardly found in the literature, the series and shunt resistances. A parametric study was then performed to test the behavior of the I-V curve under different ambient temperatures and solar radiation

14:40
A Biomimetic-computational Approach to Optimizing the Quantum Efficiency of Photovoltaics: *Andreas Holzenburg*[1]; Lisa Perez[1]; [1]Texas A&M University

The most advanced low-cost organic photovoltaic cells have a quantum efficiency of ~10%. This is in stark contrast to plant/bacterial light-harvesting systems which offer quantum efficiencies close to unity. Of particular interest is the highly effective quantum coherence-enabled energy transfer. Noting that quantum coherence is promoted by charged residues and local dielectrics, classical atomistic simulations and time-dependent density functional theory (DFT) are used to identify charge/dielectric patterns and electronic coupling at exactly defined energy transfer interfaces. The calculations make use of structural information obtained on photosynthetic protein-pigment complexes while still in the native membrane making it possible to establish a link between supramolecular organization and quantum coherence in terms of what length scales enable fast energy transport and prevent quenching. Calculating energy transfer efficiencies between components based on different proximities will permit the search for patterns that enable defining material properties suitable for advanced photovoltaics.

15:00 Break

15:20
Using Nonlinear Electret Effects to Design Piezolectricity and Magnetoelectricity in Soft Materials: *Pradeep Sharma*[1]; [1]University of Houston

Piezoelectricity and magnetoelectricity are contradictory properties with a rather limited set of natural (often hard) materials that exhibit both. Composite materials—almost always restricted to hard ones---provide a limited recourse with the attendant limitations of small strains, fabrication challenges among others. In this article, using the concept of electrets, we propose a simple scheme to design soft, highly deformable materials that simultaneously exhibit piezoelectricity and magnetoelectricity. We demonstrate that merely by embedding charges and ensuring elastic heterogeneity, the geometrically nonlinear behavior of soft materials leads to an emergent piezoelectric and magnetoelectric behavior. We find that, an electret configuration made of sufficiently soft (non-piezoelectric and non-magnetic) polymer foams can exhibit simultaneous magnetoelectricity and piezoelectricity with large coupling constants that exceed the best-known ceramic composites.

15:40
Stability, Mechanical, Dielectric and Piezoelectric Properties of {AxA'(1-x)}{ByB'(1-y)}O_3 Ceramics: *Berna Akgenc*[1]; Çetin Tasseven[2]; Tahir Cagin[3]; [1]Kirklareli University; [2]Yildiz Technical University; [3]Texas A&M University

ABO_3 ceramics and their alloys form the basis of piezoelectricity based energy harvesting, actuators and electromechanical sensing for material health monitoring. Enhancing their electromechanical response is crucial for these technological applications. In this study we investigate the phase stability, anisotropic mechanical, dielectric, piezoelectric properties of various {AxA'(1-x)}{ByB'(1-y)}O_3 alloys using ab initio density functional theory methods. The effects of composition, order, oxygen vacancies, site-defects on structure, energetics, elastic stiffness, dielectic, and piezoelectric susceptibility tensors are systematically investigated within the generalized-gradient approximation for A, A'=Ba, Sr, Pb, K, Ag;. B, B'=Ti, Zr, Nb using supercells with 2x2x2 unit cells, for cubic, tetragonal, in some cases orthorhombic and rhombohedral lattice structures. In the present work, we have used Linear Response Theory as well as homogeneous field methods to provide an assessment of the performance of these methods for determination of properties.

16:00
Revealing the Role of Organic Ligands in Hybrid Halid Perovskites for Phovoltaics Applications: Carlo Motta[1]; *Fadwa El-Mellouhi*[2]; Fahhad Alharbi[2]; Nouar Tabet[2]; Kais Sabre[2]; Stefano Sanvito[1]; [1]Trinity College Dublin and CRANN; [2]QEERI

Solar cells based on the hybrid halide perovskite, $CH_3NH_3PbI_3$, have now reached an efficiency of about 17%, demonstrating a pace for improvements with no precedents in the solar energy arena. Despite such explosive progress, the microscopic origin behind the success of such material is still debated and in particular it is not clear what role the organic ligands play in the light-harvesting process. The high-temperature cubic phase of $CH_3NH_3PbI_3$ allows the molecules to assume different high-symmetry configurations within the crystal, inducing uniaxial distortion in the inorganic matrix. Such distortion is the direct result of van der Waals interactions and has drastic consequences on the electronic structure. We perform a comprehensive characterization of such material, including a description of the phonon properties and of the electrical conductivity as a function of the chemical potential. Finally, our results suggest possible design strategies for novel high-efficiency hybrid halide perovskites.

16:20
Organic Molecule-Functionalized Zn_3P_2 Nanowires for Photochemical H_2 Production: DFT and Experimental Analyses: G. Ramos-Sanchez[1]; M. Albornoz[1]; Y-H. Yu[2]; Z. Cheng[1]; V. Vasiraju[3]; S. Vaddiraju[1]; *Fadwa El-Mellouhi*[4]; P. B. Balbuena[1]; [1]Artie McFerrin Department of Chemical Engineering; [2]Department of Materials Science & Engineering, Texas A&M University; [3]Department of Materials Science & Engineering, Texas A&M University; [4]QEERI

Hydrogen production via photochemical reactions in water/methanol solutions containing Zn_3P_2 nanowires functionalized with an organic molecular layer is shown to be between 217 and 405 times higher than that obtained in absence of the molecular layer. Combined surface characterization and theoretical analyses are used to elucidate aspects of the photochemical reaction process. It is found that the protective layer exerts a passivation role decreasing the rate of nanowire degradation, while facilitating electron transfer for the hydrogen evolution reaction.

16:40
Tailoring Thermal Conductivity of Ge/Si Core-Shell Nanowires: *Sevil Sarikurt*[1]; Cem Sevik[2]; Alper Kinaci[3]; Justin Haskins[4]; Tahir Cagin[5]; [1]Dokuz Eylul University; [2]Anadolu University; [3]Argonne National Laboratory; [4]NASA Ames Research Center; [5]Texas A&M University

Low-dimensional nanostructured materials show large variation in their thermal transport properties. Here, we investigate the influence of core-shell architecture on nanowire (NW) thermal conductivity using molecular dynamics with Tersoff potentials Si-Ge, to design structures with desired thermal conductivity for thermoelectric device applications. To explore the parameter space, we have calculated thermal conductivity values of Ge/Si core-shell NWs having different lengths, cross-section sizes and Ge concentrations at several temperatures. We have found that (1) increasing the cross-sectional area of pure Si NW causes an increase in thermal conductivity (2) increasing the Ge core size in the Ge/Si structure results in a decrease in the thermal conductivity values at 300 K (3) there is no significant variation in the thermal conductivity of Si NW for temperature values larger than 300 K (4) the predicted thermal conductivity around 10 W m^{-1}K^{-1} is still larger than the value convenient for thermoelectric applications.

Plenary 2

Tuesday Morning
January 13, 2015

Room: Mukhtassar
Location: Ritz-Carlton Doha

Session Chair: Ibrahim Karaman, Texas A&M University

08:00 Introductory Comments

08:10 Keynote
Materials Research for the Energy Industry Collaboration opportunities between Energy Industry and Academia: *Rustom Mody*[1]; [1]Baker Hughes

Improving sustainability, reliability, and productivity are major themes of current critical Research in the upstream oil and gas industry. Although some of the pressure on supply forhydrocarbons has been addressed via the recent advancement of hydraulic fracturing, the industry's ability to meet ever-growing long-term global demand for energy will require materials, products, and services to access and produce oil and gas trapped in ultra-high-pressure and –temperature environments. For all downhole equipment technologies, new demands present new challenges for the industry. The development, characterization, modeling, and simulation of fluid systems, metallurgy, and sealing materials that can reliably withstand increasingly harsh downhole environments are examples of ongoing research that will remain a strategic priority, gaining commercial importance as conventional energy resources are consumed. The oil field industry must lead the development of new ultra-high-performance metal alloys, sealing materials and systems to meet the world's future demand for energy while it continuously improves the reliability and efficiency of oil and gas recovery from less demanding environments. Both of these tasks require the sustained ability for industry leaders, engineers, and scientists to innovate unceasingly.

08:55 Break

1-3: Multi-scale Characterization and Simulations of Infrastructure Materials

Tuesday Morning
January 13, 2015

Room: Mukhtassar
Location: Ritz-Carlton Doha

Session Chairs: Said Mansour, Qatar Environment and Energy Research Institute; Rashid Abu El Rub, The Masdar Institute of Science and Technology

09:10 Invited
Quantifying Material, Environmental, and System Variables Influencing the Structural Performance of Reinforced Concrete Structures Affected by Alkali Silica Reactions: *David Trejo*[1]; Joseph Bracci[2]; Paolo Gardoni[3]; [1]Oregon State University; [2]Texas A&M University; [3]University of Illinois at Urbana-Champaign

Contractors use high cement contents in concrete to accelerate the strength gain and reduce project construction time. Higher cement contents result in higher early strengths (HES). HES can result in earlier form removal, economic benefits to the contractor, and reduced project duration. Although the short-term benefits can be positive, longer-term challenges have arisen when high cements contents have been used. On a recent project owners recognized longitudinal cracking in columns. Investigations indicated that columns were exhibiting alkali silica reactions (ASR), likely a result of higher cement contents. Limited information is available on predicting performance and service life of structures exhibiting ASR. Therefore, this research investigated the structural performance of large-scale columns subjected to different levels of ASR. The researchers also assessed the performance of smaller-scale laboratory specimens. This paper reports on the influence of material characteristics, exposure conditions, and design parameters on the system performance and models are developed.

09:50 Invited
Monitoring Concrete Infrastructure Condition Using Acoustic Sensing and Imaging: *John Popovics*[1]; [1]University of Illinois

The development and implementation of effective mechanical wave-based nondestructive evaluation (NDE) methods for concrete infrastructure elements are described here. Such methods enable effective material maintenance procedures that promote more sustainable infrastructure. Fundamental background information is reviewed, followed by a description of our work to enhance bridge deck inspection capability using a contactless acoustic impact-echo scanning system. The data collected are presented in the form of 3-dimensional "cloud" images and 2-dimensional peak frequency plot images, which together indicate the location and characteristics of delamination defects. Next, work on fully contactless (air-coupled) ultrasonic surface wave tests and ultrasonic scanning robots is described. These ultrasonic data are used to characterize concrete with regard to distributed micro-cracking and discrete damage. Finally, work on through-thickness ultrasonic tomography to image steel-reinforced concrete columns is described. The resulting tomographs are used to detect damage that developed inside the concrete column during simulated seismic loading tests.

10:30
Multiscale Design of Palm Natural Fiber Based Composite: *Yehia Bahei-El-Din*[1]; Taher Wahba[1]; Tarek Hatem[1]; [1]British University in Egypt

In recent years, attempts have been made to use natural based fiber that is available in the local environment in order to decrease cost, decrease weight and increase availability. Furthermore, natural fiber-based composites are recyclable, non-hazardous and biodegradable. The current study suggests a major departure from present approaches for production of composite materials that use artificial fibers to utilize natural based fibers, namely; date palm fiber-polyethylene composites. In the current study, the mechanical properties of palm-based fiber composites are discussed relative to several parameters that include; laminate layup; fiber weight ratio; matrix materials; fiber treatment; etc. The analysis utilize multiscale experimental and numerical approaches for design, modelling and testing of palm fiber-based composites.

10:50
Mechanical Properties of Concrete Containing Qatar's Municipal Wastes: *Nesibe Gozde Ozerkan*[1]; Deniz Tokgoz[1]; Joseph Antony[2]; [1]Qatar University; [2]University of Leeds

Because of a dramatic increase in the solid waste production in Qatar, which is established as 2.5 million tons/year, solid waste management is one of the pillars of Qatar National Development Strategy. Besides, Qatar also has the highest cement consumption rate in the world with 4.24 tons which will increase in the following years due to 2022 Qatar World Cup construction facilities. In this study, polyethylene wastes obtained from Qatar's municipal solid waste and municipal solid waste incineration fly ash were utilized to develop high quality concrete as partial replacement of aggregates and cement, respectively. The initial results of the study showed that these wastes can successfully be used in concrete without having adverse effect on the mechanical properties. This developed concrete would not only help in solving some of the solid waste problem of Qatar but also reduce CO_2 emission due to cement production and hence saves energy.

11:10
Stochastic Framework for the Modeling and Propagation of Linear Viscoelastic Material Properties of Asphalt Mixtures in Pavement Structures: *Loujaine Mehrez*[1]; Eyad Masad[1]; [1]Texax A&M University at Qatar

The behavior of asphalt mixtures in pavement structures exhibit variability in the field as well as in lab tests. This variability could be attributed to the highly variable composition of asphalt mixtures at finer scales due to the complexity and heterogeneity of constituent materials. Robust modeling of pavement structures is vital for reliable response prediction and assessment. Asphalt mixtures exhibit time- and temperature-dependent viscoelastic and viscoplastic behavior. However, this behavior has not been addressed comprehensively within a stochastic framework. Thus, this study proposes a stochastic framework to model variability and uncertainties of spatially-dependent viscoelastic properties of asphalt mixtures, which in turn is propagated to predict the strain response of a pavement structure in a computational model. Spectral stochastic approaches have been implemented for the modeling and propagation of uncertainty. Statistical quantification of the spatial strain response is carried out using the constructed spectral stochastic reduced model.

2-3: Nano-Engineered Materials for Energy Conversion

Tuesday Morning Room: Al Wosail 1
January 13, 2015 Location: Ritz-Carlton Doha

Session Chairs: Mabrouk Ouederni, QAPCO - Qatar Petrochemical Company; Saadoune Ismael, Cadi Ayyad University

09:10 Invited
Challenges and Opportunities for Nano Engineered Materials: *Pulickel Ajayan*[1]; [1]Rice University
There has been much interest in the past two decades to create nanoscale building blocks from a diverse set of materials. Creation of scalable materials via nanoengineering has met with limited success due to several intrinsic and extrinsic factors. This talk will discuss our recent efforts in the design and engineering of nanomaterials, using building blocks that range in size, dimensionality and properties. Several nanoscale building blocks, spanning nanoparticles, nanowires, carbon nanotubes, graphene, and other emerging 2D atomic layers will be considered to demonstrate the challenges and opportunities in this field. Several application of these nanoengineered materials will be considered including low density multifunctional structures, composites, electronic devices, energy storage, and coatings.

09:50
Towards Engineering Efficient Thermoelectrics: Large-scale Synthesis of Nanowires and their Assembly into Stable Welded Nanowire Networks: *Sreeram Vaddiraju*[1]; [1]Texas A&M University
The lack of a pathway for precisely tuning the thermal and electrical transport through materials employed in the fabrication of thermoelectrics is a primary bottleneck preventing their deployment in terrestrial applications. The suggestion by recent studies that nanomaterials, such as nanowires, offer an opportunity to overcome this difficulty is promising. As thermoelectrics is a bulk application, then, there is a need for strategizing mass production and large-scale assembly of nanowires into bulk thermoelectric modules. This talk will summarize some of the work my group has been performing in this field. Specifically, the implementation of vapor phase schemes for the production of kilogram quantities of Zn_3P_2 nanowires, in-situ functionalization schemes for obtaining conjugated molecule functionalized nanowires and bulk-processing schemes for assembling nanowires in an interface-engineered manner into thermoelectric devices will be presented. The enhancement of the thermoelectric performance achieved through the use of materials in nanowire form will be discussed.

10:10
Design of New Electroactive Materials Based on Nanoparticle-modified Polymers: *Zoubeida Ounaies*[1]; Nirmal Shankar Sigamani[1]; [1]The Pennsylvania State University
Despite many advantages of electronic electroactive polymers (EAPs), there are major obstacles facing their transition to application. Notably they require high actuation voltages, have low blocked stresses and low operating temperatures. The goal of this project is to induce significant electromechanical coupling in nanoparticle-modified EAPs by exploiting the increasingly dominant role of interfaces at the nanoscale. In our previous research, we developed SWNT-based nanocomposites and demonstrated an electrostrictive response. However, due to the high electrical conductivity and dielectric loss, their operating voltage and electromechanical strains were limited. In this study, we synthesize and characterize other carbon nanostructure-modified and metal oxide-modified polymers as potential next generation EAPs. To synthesize and process the nanocomposites, we follow two routes, one relying on chemical dispersion and other focused on physical dispersion. After comparing dispersion for various volume content of particles, we characterize breakdown strength, effective mechanical and electrical properties as well as electromechanical performance.

10:30
Active Nanocomposite Materials for Photo-mechanical Actuation: *Igor Krupa*[1]; Klaudia Czanikova[2]; Maria Omastova[2]; [1]Qatar University; [2]Polymer Institute SAV
The light-driven actuation has a number of critical advantages, being noncontact and -in the case of sunlight- having an unlimited resource capacity. A plastics-based component actuated by visible light could be switched safely and rapidly by an external light source. The design of dynamic photo-actuating polymeric materials has far-reaching implications for many devices; one of the most exiting applications of these materials is in a development of sun-driven rotary motor that would spin spontaneously when illuminated – and generate electricity in a usual reliable and efficient way (as in turbines) rather than using the photovoltaics. In such a motor, the reversible contraction/expansion cycle of our photo-actuating elastomers will be made to produce mechanical work leading to an alternative. In this presentation we will discuss various features of photo-actuators based on soft plastics (ethylene-vinylacetate copolymer) and functionalized carbon nanotubes. The characterization methods will be highlighted and photo-actuating behavior will be demonstrated.

10:50
Inherent Nonlinear Non-conservative Behavior of Resonant Piezoelectric Energy Harvesters: A Dynamical Systems Approach: Stephen Leadenham[1]; *Alper Erturk*[1]; [1]Georgia Institute of Technology
Over the past two decades, similar manifestations of softening nonlinearity in piezoelectric materials have been attributed to different phenomena, such as purely elastic nonlinear terms and coupling nonlinearity, by different research groups. Recently, we developed a unified nonlinear non-conservative distributed-parameter electroelastic modeling framework to explore inherently nonlinear and dissipative behavior of mechanically and electrically excited piezoelectric cantilevers with a focus on stiff bimorphs made of PZT-5A and PZT-5H for geometrically linear and materially nonlinear resonant vibrations. After experimentally validating the model for two-way excitation, the focus is placed on energy harvesting from base excitation, in which the electric field levels are well below the coercive field. It is unveiled that the primary source of nonlinearity is quadratic softening in stiffness, while the standard cubic softening or coupling nonlinearities become effective only at much higher excitation levels. Dissipative nonlinearities are also found to be very important even for moderate excitation levels.

11:10
A Multiscale-Based Model for Composite Materials with Embedded PZT Filaments for Energy Harvesting: *Yehia Bahei-El-Din*[1]; Ahmed El-Etriby[1]; Mohamed Abdel-Meguid[1]; Khalid Shalan[1]; Tarek Hatem[1]; [1]British University in Egypt
Ambient vibrations are major source of wasted energy, exploiting properly such vibration can be converted to valuable energy. Accordingly, energy harvesting using smart structures with active piezoelectric ceramics has gained wide interest over the past few years. This paper provides numerical and experimental analysis of piezoelectric fiber based composites for energy harvesting applications proposing a multi-scale modeling approach coupled with experimental verification. The multi-scale approach suggested to predict the behavior of piezoelectric fiber-based composites use micromechanical model based on Transformation Field Analysis (TFA) to calculate the overall material properties of electrically active composite structure. Capitalizing on the calculated properties, single-phase analysis of a homogeneous structure is conducted using finite element method. The experimental work approach involves running dynamic tests on piezoelectric fiber-based composites to simulate mechanical vibrations experienced by a subway train floor tiles. Experimental results agree well with the numerical results both for static and dynamic tests.

3-3: Modeling Materials Across the Scales

Tuesday Morning Room: Al Wosail 4
January 13, 2015 Location: Ritz-Carlton Doha

Session Chair: Pedro Rivera, University of Cambridge

09:10
Multiscale Modeling and Design of Advanced Interface Materials for High Energy Environments: *Hussien Zbib*[1]; [1]Washington State University

Interfaces in metals, ceramics and alloys play a decisive role in determining the thermo-mechanical behavior under extreme loading and environmental conditions. To rationally design and accelerate discoveries of new material systems with novel thermo-mechanical properties-be it high temperature strength, corrosion resistance, fatigue life or any other mechanical property-the ability to predict the macroscopic properties on the basis of microstructure and interface structure is needed. In this work we develop a multiscale framework for designing metal/metal/ceramic nanocomposites with engineered nanolaminate structures that can exhibit high strengths, fracture and fatigue resistance, thermal stability and corrosion resistance under high energy environment. The framework is based on a computational material-by-design approach that includes a multiscale computational framework bridging molecular dynamics and dislocation dynamics (microscale) with crystal plasticity (mesoscale), to design nanolaminates and to study the thermo-mechanical properties, deformation, fracture and fatigue and corrosion resistance of a many possible combinations of these composites.

09:30
Periodic Homogenization of SMA Composites under Isothermal Conditions: *George Chatzigeorgiou*[1]; Yves Chemisky[1]; Fodil Meraghni[1]; [1]Arts et Metiers ParisTech

A homogenization framework is proposed for periodic composites with shape memory alloy (SMA) components under isothermal conditions. This homogenization approach identifies simultaneously the macroscopic and the microscopic response of the composite through an iterative approach that connects the mechanical problems in the overall body and the microstructure. The computational scheme contains three parts: the macroscale analysis, the representative volume element problem and the identification of the macroscopic tangent modulus. Numerical examples on multilayered SMA composites are presented and the complexity of the composite response and the SMA stress state is demonstrated. It is observed that, even in the case of uniaxial macroscopic boundary conditions, the SMA is under triaxial, highly non-proporsional, stress conditions, leading in some occasions to non-convex transformation surfaces for the composite.

09:50
Modeling the Deformation Mechanisms in Magnesium Single Crystals: Multiscale Dislocation Dynamics Analyses: *Wassim Jaber*[1]; Mutasem Shehadeh[1]; [1]American University of Beirut

Hexagonal-closed packed materials (HCP) materials has attracted interest recently due to their unique physical and mechanical properties. The low density and the high strength to weight ratio of such materials make them excellent candidate to save structural weight and consequently fuel consumption in automotive and aircraft fields. The deformation behavior of HCP metals is not completely understood as prior work still lacks a detailed understanding about the activation of slip planes and twinning. The work-hardening behavior and the effect of temperature and strain rate are not yet well-established. The overall objective of this work is study the deformation mechanisms in magnesium single crystals using multiscale dislocation dynamics plasticity (MDDP) model. Several Simulations are carried out to investigate the effects of crystal orientation, strain rate, and the grain size on the evolution of the dislocation density and microstructure, the slip systems activation, and hardening behavior

10:10
Analysis of Solid State Bonding in the Extrusion Process of Magnesium Alloys -Numerical Prediction and Experimental Verification: *Nabeel Alharthi*[1]; Wojciech Misiolek[2]; Anthony Ventura[2]; [1]Lehigh University and King Saud University; [2]Lehigh University

The automotive industry developments focused on increasing fuel efficiency are accomplished by weight reduction of vehicles, which consequently results in less negative environmental impact. Usage of low density material such as Magnesium alloys is an approach to replace heavier structural components. Many researchers have attempted to understand solid state bonding during deformation in different structural materials such as Aluminum, Copper and other metals and alloys. There is a lack of sufficient understanding of the extrusion welding in these materials. In this work a new criterion was established to evaluate the extrusion welding integrity based on microstructure characterization supported by mechanical testing of the extrusion welding regions in Magnesium alloy AM30 extrudate as well as numerical and physical simulations of AM30 extrudate. The proposed criterion and its analysis have provided better understanding of material response to processing parameters and assisted in selecting the processing windows for good practices in the extrusion process.

10:30
Hydrogen Embrittlement in Pd: Binding Energetics and Structure at Grain Boundaries: *Tahir Cagin*[1]; [1]Texas A&M University

We studied the fundamental process of hydrogen binding and embrittlement at interstitial, vacancy and grain boundary (GB) in palladium using Density-Functional Theory. Hydrogen occupy octahedral interstitial in bulk Pd bulk, however stable H-vacancy complexes with most H occupations have eight hydrogen located tetrahedral sites around vacancy. Furthermore, H presence leads to formation of vacancy pairs which in agreement with other experimentals. This observation implies hydrogen embrittlement (HE) mechanism through the connections of microvoid and cracks. Segregation of hydrogen at grain boundary, however, results in another way of possible ruptures. At GB, H-Pd bond length is the same as that in tetrahedral interstitial site and H atoms prefer locations of threefold bonding with Pd. High H accumulation results in grain boundary extension, which supports HE mechanism of grain decohesion observed by experiments.

10:50
Multiscale Modeling of Discontinuous Precipitation in U-Nb: *Thien Duong*[1]; Alexander Landa[2]; Robert Hackenberg[3]; Patrice Turchi[2]; Raymundo Arroyave[1]; [1]Texas A&M University; [2]Lawrence Livermore National Laboratory; [3]Los Alamos National Laboratory

Discontinuous precipitation (DP) and coarsening (DC) were experimentally observed in the uranium-niobium nuclear fuel. These reactions are undesirable as they degrade the fuel's corrosion resistance and ductility. To minimize the impacts, it is important to understand the fundamental mechanism of the reaction's characteristic discontinuity. In this study, we proposed to investigate such a mechanism using an integrated computational approach. In particular, three combinatorial methodologies including (1) first-principles calculations, (2) CALPHAD and (3) phase-field modeling were practiced; The coupling between first-principles calculations and CALPHAD was to assess self-consistent thermodynamic and kinetic descriptions of U-Nb system which were then utilized within the phase-field approach to simulate DP and DC reactions. Here, the interface dissipation model for non-equilibrium transformations was applied. Our diffusion-couple simulations showed that the U-Nb's characteristic discontinuity can be due to the fact that alpha forms two local equilibria (two common tangents) with gamma in this system at reacting conditions.

1-4: Environmental Degradation

Tuesday Afternoon Room: Mukhtassar
January 13, 2015 Location: Ritz-Carlton Doha

Session Chairs: Abdulaziz Almathami, Qatar Petroleum; Zachary Grasley, Texas A&M University

13:30 Introductory Comments

13:40 Invited
Corrosion Challenges for the Oil and Gas Industry in the State of Qatar: *Roy Johnsen*[1]; [1]Norwegian University of Science and Technology

In Qatar oil and gas has been produced from onshore fields in more than 60 years, while the first offshore field delivered its first crude oil in 1965. Due to the atmospheric conditions in Qatar with periodically high humidity, high chloride content, dust/sand combined with the temperature variations, external corrosion is a big treat to the installations and connecting infrastructure.

Internal corrosion in tubing, piping and process systems is also a challenge due to high H_2S content in the hydrocarbon mixture combined with water injection. To avoid corrosion different type of mitigations like application of coating, chemical treatment and material selection are important elements. This presentation will review the experiences with corrosion challenges for oil & gas installations in Qatar including some examples of corrosion failures that have been seen. The presentation will also include corrosion related challenges that still needs to be solved through research and development.

14:20
Effect of Electroless Co-P and Co-Ni-P Coatings on Cavitation Erosion-corrosion Resistance: *Shemy Mohamed Ahmed Gaber Gaber*[1]; Mohammed Aboraia[2]; Mohammed Doheim[2]; Salem Karrab. A[3]; [1]Majmaah University; [2]Assiut univ.; [3]Misurata University

In the present work, electroless Ni-Co-P and Cop coatings were produced on AISI 1045 steel with and without post-heat treatment. The properties of electroless coatings were characterized using an optical microscope, and microhardness tester. The cavitation erosion resistance of coatings was evaluated using a vibratory cavitation test. The test was carried out both in tap water and 3 wt.% NaCl solution, respectively. The electroless deposition characterized with low thickness films and it was higher for Ni-Co-P than for Co-P. The morphology of Ni–P and Co–P deposits were also dissimilar. Maximum hardness of heat treated samples was found to depend on the solution composition and occurs at temperature 400°C. The highest erosion resistance was observed in coatings after heat treatment at temperature of 650 °C, when measured in both tap water and 3 wt. % NaCl solution. However, the Co-P coatings specimens could not resist cavitation erosion in 3 wt.% NaCl solution. The results showed also that the cavitation erosion resistance is independent on surface hardness.

14:40
Prevention of Chloride Stress Corrosion Cracking (CSCC) using Thermally Sprayed Coating (TSC): *Rehan Ahmed*[1]; [1]Petronas Carigali

To prevent premature failure of traditional epoxy coatings on Austenitic Stainless Steel (SS) columns subjected to thermal cycling causing CSCC, it was recommended to replace the coating with a robust, sacrificially protecting TSC. The application of TSC was required to be carried out under strictly controlled conditions. This was achieved using a flameproof habitat constructed around the work site & by dehumidifying the air inside. The TSC was required to be carried out during a plant shutdown to ensure a stable surface to apply the TSC on and minimal disruption to production. We discuss the TSC design and methodology adopted to mitigate CSCC on SS columns, job requirements, job planning incorporating industry best practices, QA/QC regime followed, Safety health and environment aspects, the actual execution process, and subsequent lessons learnt. The paper will conclude on the merits of utilizing experienced personnel with effective work management processes to ensure optimal results.

15:00
New Self-Healing Coatings Technique for Corrosion Protection: *Eman Fayyad*[1]; Mariam Al-Maadeed[1]; [1]Qatar University

Coatings are used across many industries as a method to prevent corrosion. Cracks in the coating, caused by damage due to environmental effects or mechanical loading, will severely reduce effectiveness of the coating and allow the substrate to corrode. This study will explain the success of microencapsulation of Tung oil as a healing agent using urea-formaldehyde shell via in situ polymerization. The microcapsules had different diameters ranging from 100 to 250 μm with thickness from 2.5 to 1.5 μm, respectively. The epoxy coated samples with impeded capsules had the ability to heal the corrosion cracks as proved by Electrochemical impedance spectroscopy. It was found that the Tung oil microcapsules could heal the cracked area even after 168 hours immersed in 3.5 wt% NaCl solutions. The Smaller microcapsules had the better self-healing ability than the larger ones.

2-4: Ferroelectric Materials in Energy Conversion

Tuesday Afternoon — Room: Al Wosail 1
January 13, 2015 — Location: Ritz-Carlton Doha

Session Chair: Zoubeida Ounaies, Pennsylvania State University

13:30 Introductory Comments

13:40 Invited
Insights into the Nature and Dynamics of Point Defects in Ferroelectric Materials: *Clive Randall*[1]; [1]Penn State University

In any material, the defects can strongly perturb the properties, either electrical or mechanical. Point defects in ferroelectric materials are very important and often control performance and device limitations of capacitors and piezoelectrics. As we look forward into the future, the applications pulls on ferroelectric and dielectric material will demand higher electric fields and higher temperatures. Here we will discuss new insights into oxygen vacancy behavior in perovskite-based dielectrics. First, we will consider the defects that are established under equilibrium conditions that can be quenched in and are determined by partial Schottky reactions. Second, we will consider defect complexes that are resulting from acceptor and acceptor-donor pairs in the formulation. Third, we will consider the degradation process in multilayer ceramic capacitors and a new equation that predicts meantime to fail. Finally, we consider ferroelectric materials with very high oxygen vacancy concentrations and consider ferroelectrics under the

14:20
Flexoelectricity and Nanoscale Energy Harvesting: *Pradeep Sharma*[1]; [1]University of Houston

One of the most tantalizing applications of piezoelectricity is to harvest energy from ambient mechanical vibrations for powering micro and nano devices. However, piezoelectricity is restricted only to certain materials and is severely compromised at high temperatures. In this presentation, we present an overview of the phenomenon of flexoelectricity and its ramifications for energy harvesting. Aside from a review of experimental and atomistic simulation efforts of this phenomenon in a variety of nanostructures (such as graphne), we demonstrate that flexoelectricity based energy harvesting, at the nanoscale, is a viable alternative. Our results also pave the way for exploration of high temperature energy harvesting since unlike piezoelectricity, flexoelectricity persists well beyond the Curie temperatures of the high electromechanical coupling ferroelectrics that are often used.

14:40
Investigation of Electrical and Piezoelectricity of New Nanocomposites Based on Nanofibrillated Cellulose and Copolymers Containing Fluorinated and Nitrile Derivatives with Controlled Structure: *Kaddami Hamid*[1]; Kadimi Amal[1]; Ounaies Zoubeida[1]; Raihane Mustapha[1]; [1]Cadi Ayyad University

Aiming ultimately to study piezoelectricity of new nanocomposites based on nanofibrillated cellulose (NFC) and copolymers of controlled structures containing fluorinated and nitrile derivatives, the dielectric properties of these materials have been investigated. The Copolymers with different proportions were synthesized by emulsion polymerization and the NFC was extracted from the rachis of date palm tree by mean of TEMPO (2,2,6,6 téraméthylpipéridine-1oxyle) mediated oxidation. It was observed that the increase of percentage of AN in copolymers improve the dielectric constant and dielectric strength. Further improvement of these electrical properties was obtained after the incorporation NFC. The result of composites with 3wt% of NFCs in these copolymers will be presented.

15:00
Novel Polymeric Materials for Mechanical Energy Harvesting: *Miroslav Mrlík*[1]; Mariam Al Maadeed[1]; [1]Qatar University

This study will explain novel approach of new material preparation process and treatment with possible application as mechanical energy harvesters. These materials are able to produce electric output while they are mechanically stimulated. The amount of the harvested energy depend on the nature of the material and its structural properties. This study explain properties of different types of polymers including gamma-irradiated polypropylene (PP) polymer electret foams. Both, untreated PP foam as well as treated ones are investigated using various techniques such as differential scanning calorimetry (DSC), thermo-gravimetric analysis (TGA) and dynamical mechanical analysis (DMA). The impact of gamma-irradiation of various doses on morphology, microstructure and energy harvesting properties of PP polymer electret foams will be elucidated. Acknowledgement:This publication was made possible by NPRP grant # NPRP-6-282-2-119 from the Qatar National Research Fund (a member of Qatar Foundation). The statements made herein are solely the responsibility of the authors.

3-4: Alloy and Microstructure Design

Tuesday Afternoon — Room: Al Wosail 4
January 13, 2015 — Location: Ritz-Carlton Doha

Session Chair: Amine Benzerga, Texas A&M University

13:30 Introductory Comments

13:40 Invited
Discovery of Sustainable Magnesium Alloys: *Pedro Rivera-Diaz-del-Castillo*[1]; [1]University of Cambrdige

There is intensive activity in Europe on the discovery of new materials, especially from the point of view of combined properties optimisation, and elemental substitution towards more sustainable systems. This work presents a range of statistical techniques for alloy discovery: clustering, principal component analysis and neural networks; those tools aid in finding the compromise between properties, the "envelope" in materials design, and aid in identifying gaps to be filled by new alloys in property space. Those techniques are accompanied by physical models relating processing to microstructure and properties in magnesium alloys. Mechanical properties in over a hundred alloys reported in the literature are described, and the potential for substitution of rare earths is discussed. A methodology for the discovery of new magnesium alloys is presented.

14:20
Alloy Design Strategies through Computational Thermodynamics and Kinetics Approaches: *Raymundo Arroyave*[1]; Shengyen Li[2]; Ruixian Zhu[2]; Ibrahim Karaman; [1]Texas A & M University; [2]Texas A&M University

In this talk, I will discuss some examples in which computational thermodynamics and kinetics have been used in combination with computational optimization strategies have been used to optimize alloy performance under a wide range of constraints. First, I will discuss our recent work on Transformation Induced Plasticity Steels, where alloy and processing parameters constitute the degrees of freedom to be optimized in order to attain phase constitutions that result in superior combined strength and ductility. Experiments and computations are used to establish alloy/processing-microstructure-performance relations and the latter are used in the optimization scheme. A second example will be our more recent work on the development of alumina-forming, twinnable stainless steel alloys. In this case, thermodynamic and kinetic-based criteria are used to determine the conditions necessary for the formation of stable alumina protective layers as well as the the ability of the alloy to form deformation twins.

14:40
Microstructure Design and Homogenization using Correlation Functions: *Hamid Garmestani*[1]; [1]Georgia Institute of Technology

The field of materials and microstructure design has progressed significantly in the past two decades. There are two primary approaches involving top-down and bottom up approaches. In this presentation we will examine some of the efforts in top-down approaches as a basis for materials design on a nano and microscale. The basis for these techniques is the use of correlation functions as a means to represent microstructures. One of the major advantages is the direct representation of the evolution of microstructures in the form of processing path functions. Such functions can be used as a means for processing parameters optimization. Progress in this regards as related to Fuel Cells, solar cells and bio-materials are presented.

15:00
Development of Tailored Residual Stress States Through Microstructurally Informed Modeling: *Dimitris Lagoudas*[1]; Brian Lester[1]; [1]Texas A&M University

Microstructurally-informed composite design provides a valuable tool in the development of materials capable of addressing complex needs in industries including aerospace and energy. Such methodologies have previously been utilized to optimize material properties (e.g. yield, modulus) for different applications. Another powerful capability lies in designing microstructures to utilize combinations of inelastic constituents. Specifically, by tailoring microstructures to control the corresponding interactions, enhanced properties and functionalities may be observed in the effective response. One possibility lies in utilizing a recoverable response to generate permanent deformations thereby inducing controllable, tailored residual stress states. Such capability can be used to bias a phase and take advantage of desirable characteristics (e.g. improved mechanical response of a ceramic phase). To this end, the specific example of a shape memory alloy (SMA) – MAX phase ceramic composite will be explored here and the microstructure will be numerically designed to maximize the effect of the transformation-kinking response.

Poster Session

Tuesday Afternoon — Room: Al Wosail Foyer
January 13, 2015 — Location: Ritz-Carlton Doha

Session Chairs: Bilal Mansoor, Texas A&M University at Qatar; Srinath Iyengar, Texas A&M University at Qatar

P-1: A Durability Analysis of Super-Quiet Pavement Structures: *Santosh Srirangam*[1]; Kumar Anupam[1]; Tom Scarpas[1]; Cor Kasbergen[1]; Peter The[2]; [1]Delft University of Technology; [2]Directie Techniek en Technisch Management/afdeling Wegen en Geotechniek, Rijkswaterstaat ,Dienstonderdeel Grote Projecten en Onderhoud (GPO)

Poro Elastic Road Surfacings (PERS) as a substitute for conventional noise barriers or other traditional pavement surfacings like open graded mixes are currently attracting significant attention. Ascertaining the durability of PERS material itself and its bonding with the underlying pavement layer against high traffic and high load intensities is of primary importance. In this contribution, results are presented of nonlinear finite element simulations of a high volume pavement profile comprised of a PERS top layer bonded to a conventional open asphalt top layer. Traffic loading was applied by means of a simulated truck tire moving load for various operating conditions. The paper focuses on investigation of the influence on the structural pavement response of various loading conditions and material properties of PERS and adhesive layer. The study concludes with guidelines for the optimum combination of design parameters that lead to increased durability of pavements constructed with a PERS top layer.

P-2: A New Test for Asphalt Binder Ductility and Intermediate Temperature: *Alaedddin Mohseni*[1]; Haleh Azari[2]; [1]Pavement Systems; [2]AASHTO

The proposed testing procedure determines the ductility and intermediate temperature of asphalt binder. Due to the extensive use of modifiers for asphalt binders and the diversity of the additives (rejuvenators, polymers, rubber, warm mix, etc.), their fatigue performance have become increasingly more sophisticated than before. Current test methods have limitations for determining asphalt binder intermediate properties. Specific innovations are in two categories: • Mechanical Loading: A new concept for asphalt binder testing called incremental Repeated Load Permanent Deformation (iRLPD) is introduced which is borrowed from asphalt mixture testing. The damage-based test, performed on a DSR, allows repeating the fatigue test on the binder until it reaches flow. The stress is selected to cause similar damage as in the field.• Definition of Intermediate Temperature and Ductility: The test temperature at which the test reaches flow is considered to be Intermediate Temperature and the permanent strain at flow is "Ductility".

P-3: A New Test Method for Asphalt Mixture Fatigue Characterization: *Alaedddin Mohseni*[1]; Haleh Azari[2]; [1]Pavement Systems; [2]AASHTO

The proposed testing procedure determines the fatigue properties of asphalt mixture. Due to the extensive use of modifiers for asphalt binders and the diversity of the additives (rejuvenators, polymers, rubber, warm mix, RAP, RAS, etc.), the fatigue performance of asphalt mixtures have become increasingly more sophisticated than before. Specific innovations are in three categories: 1) Incremental Loading: A new concept for asphalt mixture testing called incremental Repeated Load Permanent Deformation (iRLPD) is introduced. The stress is selected to cause similar damage as in the field. 2) Realistic Field Loading: The test is performed in 300 cycle increments, each cycle consists of 0.1 s loading and 0.9 s rest period (repeated loading). This loading simulates the passing of a heavy wheel load at normal highway speed. 3) Fatigue Parameters: New fatigue parameters are proposed. Minimum Strain Rate (MSR), which is the test property of the iRLPD test

P-4: Active Composite Materials Undergoing Damage: A Homogenization Approach: George Chatzigeorgiou[1]; *Fodil Meraghni*[1]; Yves Chemisky[1]; Hassene Ben Atitallah[2]; Zoubeida Ounaies[2]; [1]Arts et Metiers ParisTech; [2]Pennsylvania State University

Active composite materials with periodic microstructure have gained much research interest the last decades due to their multifunctional capabilities, which make them excellent candidates for many engineering applications. Piezoelectric materials are frequently used as actuators due to their ability to transform a) electric field into stress and b) strain into electric displacement. Under large or multiple cycling mechanical loading, damage mechanisms are activated and they strongly infuence the electromechanical behavior of the composite. In this work we propose a homogenization framework, suitable for periodic piezoelectric media like uniaxial fiber composites, that accounts for mechanical damage. Numerical examples illustrate the influence of the debonding between fiber and matrix in the coupled electromechanical composite properties. Further experimental work will be performed to assess numerical resuls and mainly those related to coupling effects.

P-5: Alignment of Nanofibrillated Cellulose (NFC) in Silicone Oil by an Electrical Field: Impact on Effective Electrical Properties: *Kaddami Hamid*[1]; Kadimi Amal[1]; Raihane Mustapha[1]; Ounaies Zoubeida[2]; [1]Cadi Ayyad University; [2]The Pennsylvania State University

The purpose of the present study is twofold: the first goal is to investigate effect of electric field variables such as magnitude, frequency, time on alignment microstructure of two kinds of NFCs: oxidized for 5min (NFC-O-5 min) and oxidized for 2h (NFC-O-2h) dispersed in silicone oil (0.1wt% dospersion) using parallel electrodes . The second goal is to exhaustively investigate effect of such texturing on the dielectric properties. The NFCs response to electric field was a two-step process: Firstly NFCs rotate in the direction of electric field and secondly they interact with each other to form chains. The optimal parameters of alignment were found to be 5000Vpp/mm and 10 KHz for duration of 20 minutes for both kinds of NFCs. The impact of the alignment on the effective dielectric properties was illustrated. The highest increase on dielectric constant was achieved for the NFC-O-5 min at these optimum conditions.

P-6: Boron Removal from Seawater Using ß-Cyclodextrin Modified Magnetic Nanoparticles Fixed on Cellulose Nanocrystals: *Deema Almasri*[1]; Tarik Rhadfi[1]; Khaled Mahmoud[1]; [1]QEERI

High concentrations of boron in water could be detrimental to both humans and plants. The removal of boron from seawater by reverse osmosis (RO) is challenging due to the uncharged, naturally occurring, boric acid which can diffuse easily through the membranes resulting in poor rejection efficiency. Magnetic assisted adsorbents with chelating precursors provide a promising technology for the efficient removal of boron from seawater. This work highlights the synthesis of novel ß-cyclodextrin modified Fe3O4/ cellulose nanocrystal (CNC) magnetic composites and their application for the selective removal of boron from seawater. Cyclodextrin was used for the selective sorption of boron precursors. The particles were characterized with transmission electron microscopy (TEM), Fourier transform infrared spectroscopy (FTIR) and x-ray diffraction (XRD). The effect of magnetic sorbent dosage, initial pH, time and salinity on the sorption of boron was investigated by the quantification of final boron content using inductively coupled plasma mass spectrometry (ICP-MS).

P-7: Computational Assessment of the Performance of Lead Halide Perovskite Solar Cells using Inorganic Layers as Hole Transport Materials: *Mohammad Hossain*[1]; Fahhad Alharbi[1]; Nouar Tabet[1]; [1]QEERI

Hybrid perovskite solar cells emerged recently as cost effective alternative to conventional silicon devices. In this work, we analyze the potential of inorganic materials as hole transport materials in replacement of the expensive Spiro-OMETAD. Key cell factors like efficiency, fill factor, open circuit voltage, and short circuit current were calculated for devices including CuI, CuSCN, NiO, and Cu_2O as hole transport materials. Both defect free materials and structures including defect levels have been studied. Defect free n-TiO_2/$CH_3NH_3PbI_3$/p-Cu_2O structure shows the highest efficiency of 20.53%, whereas the efficiency is reduced to 17.60% in presence of a defect located at 0.45eV above the valance band of Cu_2O. The high open circuit voltage (1.13eV) for p-Cu_2O based structure suggests a minimized energy loss due to the charge transfer across the hetero-junctions. The results point out the possibility to develop high efficiency, low cost, and stable perovskite solar cells using Cu_2O as HTM.

P-8: Control of Grain Refinement of A356 Aluminum Alloy by Computer Aided Cooling Curve Analysis: *Ahmad Sharifi*[1]; Najmeddin Arab[1]; [1]Islamic Azad University

Computer aided cooling curve analysis is powerful technique in the foundry industries. By using this tool in evaluation of grain Refinement process in castings, quality control of those made easy. In this research, different types of inoculants were used to investigation of nucleation in A356 aluminum alloy. The cooling curve of each sample was recorded and by using a special computer program, the first derivative was calculated. By calculating zero curve and analyzing the cooling curve, it is possible to predict the quality of nucleation and calculation fraction of solids, latent heat and other information. The result of this research have shown that if maximum undercooling of nucleation was approximately 4 C, the quality of nucleation process will be more reliable.

P-9: Controlled Growth of (1-D) ZnO Nanorod Supported Platinum Nanoparticle as Catalyst Materials: *Sarim Dastgir*[1]; Reem Al-Alawi[2]; Joydeep Dutta[2]; [1]Qatar Environment and Energy Research Institute; [2]Sultan Qaboos University

Inorganic oxides are often used as catalyst supports due to their robust electrical, mechanical and material properties.[1] In recent years, nanostructured materials such as one-dimensional (1-D) Zinc oxide (ZnO) nanowires, nanorods and nanotubes have received increased attention due to their remarkable physical and chemical properties. These nanostructures with enhanced surface area serve as efficient, robust and thermally stable catalyst supports.[2] 1-D ZnO nanorods were epitaxially grown under various conditions on seeded glass substrates by a low temperature hydrothermal process. Platinum (Pt) nanoparticles were then grown directly on ZnO supports by using potassium hexachloroplatinate (IV) (K_2PtC_{l6}) as a source of Pt ions and their growth dynamics are studied. The ZnO support and ZnO-Pt catalysts were characterised by powder XRD, TEM, SEM, EDX, UV-Visible spectroscopy and ICP-OES. The catalytic activities of ZnO supported materials were evaluated for hydride transfer reactions using cyclohexanol as a model substrate.

P-10: Coupled Turbulent Flow and Solidification Modeling in a Brass Slab Continuous Caster: *Mandana Adeli*[1]; M. Reza Aboutalebi[1]; [1]Iran University of Science & Technology

In this research, a two-dimensional numerical modeling study was undertaken to account for coupled turbulent flow with solidification in a brass slab semi-continuous caster. The momentum and heat transfer equations have been solved simultaneously and interactions of fluid flow and energy have been taken into account. Solidification modeling was carried out using enthalpy method, while the mushy zone solidification was modeled using Darcy porosity approach. In order to verify the model the computed results were compared with the experimental data collected in a continuous casting plant, and a reasonable agreement was achieved. Case studies were performed using the model to evaluate the influence of some operational parameters on the process.

P-11: Damage Mechanisms of AZ31B Twin Roll Cast (TRC) at Different Strain Rates and Temperatures: *Ana Rodriguez*[1]; Georges Ayoub[2]; Amine Benzerga[1]; [1]Texas A&M University; [2]Texas A&M University at Qatar

The effects of temperature and strain rate on the fracture and damage of AZ31B were investigated. Special attention was paid to the work of fracture (W_f), which was found to exhibit a maximum at a specific strain rate and a specific temperature. Microstructural investigations at conditions of interest showed the marked effect of strain rate on the preferred sites of damage nucleation and development of micro-voids and micro-cracks. The findings point to the need for models for rate- and temperature-dependent damage in magnesium alloys.

P-12: Density Functional Theory Based Theoretical Calculations for Investigation of Highly Active Visible Light Driven TiO_2 Based Photocatalyst Photoelectrochemical Applications: *Matiullah Khan*[1]; Wenbin Cao[2]; Bilal Mansoor[1]; [1]Texas A & M University at Qatar; [2]University of Science and Technology Beijing

Solar fuel catalysis is one of the promising fields of photocatalysis which has taken considerable attentions from researchers during past several decades. The efficiency of a photocatalyst depends on, absorption of the solar energy photons generating electron-hole pairs, Interfacial charge transfer of the generated carriers to the reactive sites, and utilization of the photoexcited carriers in the oxidation/reduction process leading to the breaking of chemical bonds. Based on density functional theory (DFT), compensated and noncompensated V, Y codoped TiO_2 models were constructed and their structural, electronic and optical properties were calculated. The doped V and Y atoms exist in the form of substitutional point defects replacing Ti atom in the lattice. V, Y codoped TiO_2 possess stable configuration along with narrowed band gap. Codoping considerably shifted the absorption edge of TiO_2 towards visible regime which will drastically improve its photocatalytic response in waste water treatment for solar light applications.

P-13: Design of Advanced Materials with Tailor-Made Properties Using Molecular Simulation: Ionic Liquids for the Chemical Process Industries: *Ioannis Economou*[1]; Eleni Androulaki[2]; Niki Vergadou[2]; [1]Texas A&M University at Qatar; [2]National Center for Scientific Research "Demokritos"

Technological and economic development is based on the design and production of new advanced materials with tailor-made properties to satisfy the needs of end users. This design requires the fundamental understanding of the molecular structure and the development of appropriate models for the quantitative prediction of physical, mechanical and other properties based on the chemical constitution of the underlying materials. Molecular simulation using atomistic models has evolved in recent years as a powerful computational tool for the prediction of a broad range of properties of materials. Here, we will highlight research work on the development of new efficient simulation methods and models for Ionic Liquids (ILs), which is a new class of environment friendly solvents with a wide range of applications related to gas separation, catalysis and others. We will present application of new ILs toward carbon capture from industrial mixed gas streams.

P-14: Development of a Redox Model for SOFC Anodes: *Bora Timurkutluk*[1]; Mahmut Mat[2]; [1]Nigde University; [2]Meliksah University

A mathematical model is developed to represent the fluid flow, the heat transfer, the species transport and the electrochemical reaction in solid oxide fuel cells. In addition, a redox model representing the mechanical damage in the electrochemical reaction zones due to redox cycling is developed by defining a damage function as a function of strains and a damage coefficient. The differential equations are solved numerically with a commercial code which employs a finite element based approach. The model is validated with the experimental performance results. The effects of anode porosity and the electrolyte thickness on the cell performance and redox stability of the cells are numerically investigated.

P-15: Different Approaches to Fabricate Doped-Graphene Composite Films and their Application as a Photovoltaic Transparent Electrode: *Adnan Ali*[1]; Khaled Mahmoud[1]; Marwan Khraisheh[1]; [1]Qatar Environment and Energy Research Institute

Graphene based materials have strong presence in the solar cells applications, because of graphene unique 2D structure and exceptional properties. To date, graphene based conjugates have been applied in both OPVs and DSSCs as transparent electrodes, electron acceptors, or hole transporting layers aiming to enhance performances and higher the power conversion efficiency. In this work, we develop new graphene composites with improved optical and mechanical properties as effectual replacement of ITO layer in DSSCs. The films have been fabricated by electrospinning, electrohydrodynamic atomization and casting techniques. Transmittance of film has been measured by UV-visible spectroscopy. Morphology, structure and chemistry have been characterized by FESEM, XRD, Raman spectroscopy, XPS and FTIR techniques. Photocurrent-voltage (J-V) has been measured in each case. J-V curves have been used to derive calculate other parameters for DSSCs performance. The effect of graphene doping and the fabrication methods on the PCE of DSSCs has been discussed.

P-16: Direct Observation of Effects of Foam Density, Gating Design and Pouring Temperature on Mold Filling Process in Lost Foam Casting of A356 Alloy: *Ahmad Sharifi*[1]; Mehdi Mansouri Hasan Abadi[1]; Roholla Ashiri[1]; [1]Islamic Azad University

Mold filling sequence of A356 aluminum alloy was investigated with the aid of direct observation method (photography method). The results show that increase of the foam density causes decrease of the filling rate and increase of the filling time. Foam density has more pronounced effect on mold filling rate rather than pouring temperature. Gating design also affects the profile of molten metal advancement in the mold. The results show that the higher filling rate was obtained with G2 gating than with other gating system. Regarding the mold filling pattern, G3 gating system has more effective contact interface than G2 gating system and has lower filling time. Filling time in G4 gating and G1 gating system are nearly the same.

P-17: Discrete Element Simulation of Asphalt Mixtures Fracture: Enad Mahmoud[1]; *Shadi Saadeh*[2]; [1]UTPA; [2]CSLB

Fracture of asphalt mixtures was modeled using 2D-Discrete Element Method (DEM). A bilinear cohesive zone model was used to model crack initiation and propagation. Both homogeneous and heterogeneous models were developed. Image processing techniques were used to transfer planar images of SCB samples to a two-phase 2D-DEM model: mastic and coarse aggregates for the heterogeneous model. The sensitivity of the model to the cohesive zone model parameters, coarse aggregate properties, and bond strength was studied to facilitate the calibration process. Experimental data for semi-circular samples with three notch depths of 25.4, 31.8, and 38.0 mm were used. The model calibration had a very good agreement with the experimental results and the model successfully predicted the SCB testing results. Based on 2D-DEM results the crack propagation in SCB is mainly attributed to tensile stresses.

P-18: Effect of RE Elements on the Sorption Properties of Nanocrystalline Zr-Co Getters Prepared by Mechanical Alloying: *Ali Heidary Moghadam*[1]; Valiollah Dashtizad[2]; Ali Kaflou[2]; Hossein Yoozbashizadeh[3]; [1]Department of Materials Science and Engineering, Dezful Branch, Islamic Azad University; [2]Department of Advanced Materials and Renewable Energy, Iranian Research Organization for Science and Technology; [3]Department of Materials Science and Engineering, Sharif University of Technology

The effect of rare earth (RE) elements, including Ce and La, on the sorption properties of Zr-Co getters was investigated in this work. The nanocrystalline Zr_3Co intermetallic compound has been produced by mechanical alloying of the elemental powder. In all mechanical alloying experiments, the ball-to-powder weight ratio was 15:1. The phase evolution and microstructral change of powders during mechanical alloying and activation process were investigated by means of X-ray diffraction and scanning electron microscopy. The results showed that after an optimum mechanical alloying time of 16 h, the amorphous phase was produced. After the activation process, the studies revealed that Zr–Co–RE can be activated at lower temperature than Zr-Co getters and show better sorption properties.

P-19: Efficient Route for Functionalization of Graphene Nanosheets with Catechol for Preparation of Performance Supercapacitor Electrodes: *Efat Jokar*[1]; Azam Iraji Zad[1]; Saeed Shahrokhian[1]; [1]Sharif University of Technology

A novel and facile procedure for functionalization of graphene with some electroactive molecules is presented. The graphene has been functionalized by catechol-based molecules, which are electroactive molecules with electrochemically reversible properties. The functionalized graphene exhibits very effective seudocapacitor behavior for charge storage. For the first time, with the aim of an electrosynthesis procedure, catechol is covalently attached on graphene sheets. This attachment has been investigated by electrochemical, X-ray photoelectron spectroscopy and attenuated total reflectance methods. Catechol molecules have been attached via formation of etheric and esteric bonds on the surface of graphene. As a result, the functionalized graphene sheets show a reversible electrochemical behavior and can be used as pseudocapacitor electrodes with an excellent stability. The electrochemical results of the prepared electrodes reveal rather high specific capacity of 288 Fg-1 at a high current density of 28 A g-1, which shows remarkably enhanced performance for supercapacitor applications.

P-20: Electrowinning of Aluminium Using a Depolarized Gas Anode: *Geir Martin Haarberg*[1]; [1]Norwegian University of Science and Technology and Qatar University

Consumable carbon anodes are used in the electrowinning of aluminium by the Hall-Heroult process and in other proposed processes in molten salts. Emissions of CO_2 may be eliminated by introducing an inert oxygen evolving anode, which however will require a higher anode potential. By introducing natural gas or hydrogen to the anode the CO_2 emissions can be reduced and the anode potential can be lowered. Laboratory experiments were carried out in a modified Hall-Heroult electrolyte with excess AlF_3 at 850 ^oC. Anodes of platinum, tin oxide and graphite were tested during electrolysis at constant current, with the supply of argon, methane and hydrogen through the anodes. Laboratory studies showed that by introducing both hydrogen and methane separately through a porous SnO_2 anode in molten Na_3AlF_6-AlF_3-Al_2O_3 (4.5 wt%) at 850 ^oC the anode potential was found to be lowered by several hundred millivolts for a limited time during electrolysis.

P-21: Evaluation of Asphalt Mixes Workability and Compactability Using Laboratory and Accelerated Field Testing: *Samer Dessouky*[1]; Manuel Diaz[1]; [1]University of Texas-San Antonio

Polymer-modified asphalt have been proven to improve mechanical characteristics of asphalt mixes, however there are concerns that mixes become drier and more difficult to compact. This study aims to develop compaction indices using routine laboratory compaction procedure to evaluate the workability and compactability of hot and warm mixes prior to laydown. Workability is reflected in the ease of blending while compactability is reflected in the mixes' stability and resistance to densification. To quantify thresholds for the indices, laboratory and accelerated field testing were implemented. The workability index was tentatively found to be a minimum of 4.5 while the compactability indices were tentatively found to be a maximum of 0.5 and a minimum of 20. The compactability indices were capable of predicting mix resistance to permanent deformation.

P-22: Thermo-Mechanical Description of AISI4140 Steel at Elevated Temperatures: *Farid Abed*[1]; [1]American University of Sharjah

The recently increasing use of high strength steel in structural applications necessitates the need to understand the micro- and macro-structural behavior of the alloy at different loading conditions. The behavior of structural steel changes during deformation and the damage process may start in the form of micro-cracks and micro-voids leading at its latest stage to the development of macro-cracks and consequently material failure. This paper presents experimental results of the flow stress as well as SEM images to describe the microstructure of the alloy at different levels of strain rates (quasi-static) and temperatures. The main objective is to introduce a systematic understanding of the ductile failure mechanism due to accumulation of plastic deformation to enable proper structural design and hence provide better serviceability.

P-23: Fabrication of Bulk Nanocomposites by Mechanical Allying and Shock Compaction: *Nikoloz Chikhradze*[1]; Guram Abashidze[1]; Mikheil Chikhradze[1]; Akaki Gigineishvili[1]; George Oniashvili[1]; [1]Mining Institute/ Georgian Technical University

The results of a theoretical, experimental investigation and fabrication of multifunctional bulk nanostructured composite materials based on Ti-Al-B-C are presented in the paper. The elementary pure (at list 99%)crystalline Ti and Al, C and amorphous B powders were used as an precursors. The blend with different percentage ratio from precursors was prepared. The high energetic "Fritsch" Planetary premium line ball mill is used for mechanical alloying and nanopowder production. The optimal technological regimes for mechanical allying and nanopowder preparation are determined experimentally. Mechanically alloyed nano blend compacted by explosive consolidation technology and nanostructured bulk composite materials are fabricated. For shock wave generation the industrial explosives and new explosives obtained from decommissioned weapons are used in the experiments. The parameters of the explosive consolidation and their influence on structure-properties of obtained composites are also discussed in the paper.

P-24: Finite Element Analysis in Static and Dynamic Behaviors of Dental Prosthesis: *Djebbar Noureddine*[1]; [1]Université Djillali Liabes de Sidi Bel Abbes,

In recent years, implants have gained growing importance in all areas of medicine. The success of the treatment depends on many factors affecting the bone–implant, implant–abutment and abutment–prosthesis interfaces. In this paper, static and dynamic behaviors of the dental prosthesis are investigated. Three-dimensional finite element models of dental prosthesis were constructed. Dynamic loads in 5 sec applied on occlusal surface. Therefore, FEA was selected for use in this study to examine the effect of the static and dynamic loads on the stress distribution for an implant-supported fixed partial denture and supporting bone tissue.

P-25: Fluid Flow and Heat Transfer Modeling to NOx Characterization in Electric Arc Furnace (EAF): *Ali Ershadi*[1]; [1]Department of Mechanic Engineering, Dezful Branch, Islamic Azad University

A representative CFD model has been developed to simulate fluid flow and heat transfer in an electric arc furnace(EAF). Modeling aimed to characterize fluid flow, turbulence and heat transfer in different furnace aspect ratios, via 3D axisymmetric model, as well to identify the NOx formation mechanism inside the furnace and potential control facilities. Thermal mechanism of NOx formation is well studied in EAF, which assumed to be ordinary and main mechanism for NOx formation, and recognized that is very sensitive to temperature value. The maximum NOx concentration observed in the vicinity of Electrode, where the highest temperature measured and allows NOx formation sourcing air ingestion from slag door and its value correlates with N_2-O_2 levels in the furnace. All results show that reducing air entrance to the furnace via slag door, either velocity or surface reduction, minimize NOx formation which would be an important parameter in furnace design and operation.

P-26: Fracture Topography of Forged and Direct Quenched Ti/Nb/V HSLA Steels: *Sikaddour Yacine*[1]; Lebaili Soltane[1]; [1]USTHB

HSLA are widely used in construction , ships, automotive and petrolium industry for gas/oil transportation by pipelines. The demand for higher transportation capacity and sufficient safety, avoiding long running brittle or ductile cracks, has been one of the most relevant driving forces in the development of new kinds of Ti/Nb/V HSLA . Goals are fracture surface topographyc characterization of forged and direct quenched Ti/Nb/V HSLA steels by SEM. Effect of inclusions particles morphology and size on the form and size of dimples are investigated. Dimples with boat-shape and equiaxed form were observed with uniform orientation, also it on number, form, distribution and size of non-metallic inclusions particles. Also, Morphology, chemical composition, size and distribution of non-metallic inclusions particles are determined by EDX and SEM , the experiments revealed very complex and heterogeneous particles form with sulphides and oxides based, the same observation have been made in C/Mn steels.

P-27: Graphene /TiO_2 Composite Electrodes Toward Oxygen Reduction Reaction: *Halema Al-Kandari*[1]; Aboubakr Abdullah[2]; Ahmad Mohamed[3]; Shekhah Al-Kandari[3]; [1]PAAET (Public Authority of Applied Education and Tranining; [2]Qatar University; [3]Kuwait University

Graphene oxide (GO) was prepared from graphite using Hummers method. Then, GO was reduced either by H_2 gas or hydrazine hydrate (HH) in microwave. Several surface and bulk characterization techniques prove the successfulness of the oxidation and reduction processes of graphite and GO, respectively. FT-IR and XPS showed that, GO consists mainly of hydroxyl, epoxy, carbonyl and carboxylic groups. The reduction process using HH or H_2 is not 100% completed as shown in XPS and XRD. Go was loaded on commercial nanoparticles TiO_2 and subjected to the reduction process using different methods. The electrocatalytic properties of commercial TiO_2, TiO_2-supported GO, HH-reduced GO and H_2 -reduced GO towards oxygen reduction reaction (ORR) in presence and absence of UV radiation were tested and compared to GC electrode. Different percentages of composite was also tested.

P-28: High Haze Nano-Textured Aluminum doped Zinc Oxide with Plasmonic Silver Nanoparticles for Enhanced Optical Absorption and Photocurrent of a-Si:H thin film: *Hisham Nasser*[1]; Engin Ozkol[1]; Alpan Bek[1]; Rasit Turan[1]; [1]Middle East Technical University (METU)/ The Center for Solar Energy Research and Application (GUNAM)

Textured Aluminum doped Zinc Oxide (Al:ZnO) and silver nanoparticles (AgNP) are used to enhance light absorption in thin film solar cells (SCs). Textured Al:ZnO has strong scattering properties of light. AgNPs serve as light scattering islands to enhance optical path length of light in the absorber layer, as they possess localized surface plasmons. In this work, we target the fabrication of optimally textured Al:ZnO using a single step HCl chemical etching. Our results show that the obtained textured Al:ZnO has up to 1- to 2-fold enhanced haze transmittance over all solar spectrum. Using the simple dewetting technique, AgNP were fabricated on flat and textured Al:ZnO. We observe that the AgNPs resonate in the visible and near infrared portion of the spectrum which is consequential for light trapping in thin film SC. As proved by experimental results, a-Si:H deposited on wet etched Al:ZnO combined with AgNP has the highest measured photocurrent.

P-30: Influence of Joining Time on Microstructure and Mechanical Properties of TLP-joined IN-738LC to GTD-111: *Mahdi Asgharzadeh Ghadi*[1]; Mohammad Amin Amjadi[1]; Mohammad Saeed Shahriari[1]; Meysam Khakian[1]; [1]Mapna/Mavadkaran

Influence of joining time on microstructural and mechanical characteristics of IN-738LC joined to GTD-111 using TLP process and with MBF-20 filler was studied. Joining process was performed at 1100°C in a vacuum condition and for various durations of 5, 30 and 60 minutes. Microstructural observations were performed using optical microscopy, SEM and EDS. It was shown when required time for isothermal solidification is not met, deleterious inter-metallic and eutectic compounds would form on the joining center-line. Moreover, the nature of eutectic structures formed during isothermal solidification process could be changed by varying bonding time. It was also found that the mechanical properties of the bond is highly dependent on the amount of inter-metallic and eutectic compounds formed in the joint area, so that when no inter-metallic compounds are formed, the highest strength values could be reached.

P-31: Mass Production and Large-scale Assembly of Degradation-resistant Nanowires: *Venkata Vasiraju*[1]; Yongmin Kang[1]; Sreeram Vaddiraju[1]; [1]Texas A&M University

Next generation energy conversion devices, such as photovoltaics and thermoelectrics, are expected to be fabricated from nanowire building blocks as recent theoretical and experimental studies on single nanowire energy conversion devices demonstrated that this format of materials offers good performance. However, the high surface-to-volume ratio of materials in nanowire form renders them unstable in aqueous and acidic environments. Typical techniques, such as conformal coating of the nanowires with barrier layers alter their properties significantly. Therefore, an alternate technique for stabilizing nanowires that involves non-conformal decoration of their surfaces with small inorganic molecules of BN was developed. This not only made the nanowire non-wettable to aqueous and acidic solution and rendered them stability, but also prevented major detriment in their useful electronic and electrical properties. In this presentation, use of this strategy for stabilizing Zn_3P_2, ZnO and Mg_2Si nanowires, without majorly altering their electrical and electronic properties, will be discussed.

P-32: Mechanical Response and Evolution of Damage of Al 6061-T6 Under Different Strain Rates and Temperatures: *Abdelhakim Dorbane*[1]; Georges Ayoub[1]; Bilal Mansoor[1]; Ramsey Hamade[2]; Ghassan Kridli[3]; Abdellatif Imad[4]; [1]Texas A&M University at Qatar; [2]American University of Beirut; [3]University of Michigan-Dearborn; [4]Ecole Polytech'Lille

The mechanical response and damage mechanisms of rolled Al 6061-T6 alloy subjected to tensile testing at different temperatures and various strain rates have been investigated in this paper. The evolution of the microstructure has been examined for the different testing conditions showing strain rate and temperature effects. The fracture surfaces of samples damaged at different uniaxial testing conditions were observed through Scanning Electron Microscope (SEM). Annealing tests at different temperatures have been performed and microstructure analyses for each condition have been achieved showing grain size evolution. Investigation of the fracture initiation sites has been achieved by conducting interrupted tests and observing the microstructure through SEM. Observations has pointed out that precipitates and iron rich phases are privilege cites for crack initiation.

P-33: Methane Production from Carbon Dioxide and Increasing Energy Investment -EROI in Shale Oil: *Osama Akoubeh*

Hydrogenation of CO_2 or the reduction to methane has studied by Paul Sabatier in 1910 using Ni catalyst and later different type of catalyst replaced to reduce cost ,even though the value of hydrogen in energy market much higher than natural gas to adapt this process in addition to that fact the net energy after subtracting energy required to produceHydrogen from water electrolysis make this method not commercially considered and adapted. The different types of hydrocarbons other than methane such as methanol , ethers ..etc has put the Sabatier methanation in research only. New study discovered to convert CO_2 to methane and water vapor only under 40 bar of pressure with additional energy , meaning that the net energy not zero as the thermal energy of reactions after subtracting energy for hydrogen from water splitting still negative.

P-34: Modeling of Carbon Dioxide Absorption Process by Solvent MEA & MEDA: *Forough Kazemzadeh*[1]; Mohammad Heidary Moghadam[1]; [1]Islamic Azad University

In this study, solubility of carbon dioxide in monoethanolamine(MEA) and methyldiethanolamine(MDEA) is measured by using one or two parameters Peng Robinson state equation (P.R-EOS) and using MATLAB programming software, and optimal values of binary interaction parameters with P.R-EOS in liquid phase are measured. The solubility data are measured over temperature 303, 313 and 323 k and different pressure 100 to 1000 kpa for the three different concentration of MEA & MDEA (6%MDEA, 24%MEA-18% MDEA, 12% MEA-6%MEA , 24% MDEA) . The obtained results show that over the range of tested pressure, temperature and concentration, if the temperature increases in a constant pressure, Co2 solubility in MEA & MDEA decreases. this solubility increases at a constant temperature with an increases in pressure. Also by increasing concentration of MDEA more than MEA solubility increases.

P-35: Molecular Dynamics Study on Physical Properties of Cu Nanoparticles: *Hasan Kart*[1]; Hüseyin Yildirim[2]; Sevgi Ozdemir Kart[1]; Tahir Cagin[3]; [1]Pamukkale University; [2]Karabuk University; [3] Texas A&M University

Thermodynamical, structural and dynamical properties of Cu nanoparticles are investigated by using Molecular Dynamics (MD) simulations at various temperatures. MD simulations of the Cu-nanoparticles are performed by means of the MPiSiM codes by utilizing from Quantum Sutton-Chen (Q-SC) many-body force potential to define the interactions between the Cu atoms. The diameters of the copper nanoparticles are varied from 2 nm to 10 nm. Simulation results such as melting point, radial distribution function are compared with the available experimental bulk results. Radial distribution function, mean square displacement, diffusion coefficient, Lindeman index and Honeycutt- Andersen index are also calculated for estimating the melting point of the Copper nanoparticles.

P-36: Multicomponent Pyrophosphate as a Promising Cathode Material for Rechargeable Lithium Ion Batteries (LIBs): *R. Shakoor*[1]; Ramazan Kahraman[1]; Chanseon Park[2]; Soo Lim[2]; Jang Choi[2]; [1]Qatar University; [2]Korea Advanced Institute of Science and Technology (KAIST)

In the present study, we herein, report a novel multicomponent pyrophosphate ($Li_2Fe_1/3Mn_1/3Co_1/3P_2O_7$) cathode material for lithium rechargeable batteries that demonstrates decent electrochemical behavior and excellent thermal stability. Electrochemical measurements confirm that a reversible capacity of 100 mAh/g is obtained at C/20 rate with decent capacity retention and high rate performance. Ex situ analyses verify that the intercalation/de-intercalation of lithium into/from the host structure is associated with one phase reaction rather than a biphasic reaction with negligible volume change (~ 0.7%) in contrast to its single component ($Li_2FeP_2O_7$). TGA/DTA and thermal Insitu XRD analyses (25-550 ° C) confirm the excellent thermally stable of this material up to 550°C even in the delithiated state ($LiFe_1/3Mn_1/3Co_1/3P_2O_7$) with negligible weight loss (~2%) which is superior to delithiated $LiFeP_2O_7$ and many other reported cathodes. The promising properties of this novel cathode material can be mainly attributed to its unique crystal structure.

P-37: Non-destructive Assessment of Concrete Mixtures at Cryogenic Temperatures: Towards Primary LNG Containment: *Reginald Kogbara*[1]; Srinath Iyengar[1]; Zachary Grasley[2]; Eyad Masad[1]; Dan Zollinger[2]; [1]Texas A&M University at Qatar; [2]Texas A&M University

A number of non-destructive techniques were used to assess the suitability of different concrete mixtures for primary containment of liquefied natural gas (LNG). Concrete mixtures were prepared using limestone, traprock, sandstone and lightweight coarse aggregates, with siliceous river sand and limestone sand as fine aggregates. The mixtures were cured under water for at least 28 days and then cooled from ambient (20°C) to cryogenic temperatures (-165°C). The coefficient of thermal expansion and damage evolution of the concrete mixtures were measured with strain gages and acoustic emission sensors during the cooling process. Changes in porosity and pore size distribution were measured using 1H nuclear magnetic resonance; while changes in microstructure were examined using scanning electron microscopy and x-ray computed tomography, before and after cryogenic freezing. Damage consisted of well-distributed microcracks rather than macrocracks. Limestone and traprock mixtures showed better damage resistance during cooling to cryogenic temperatures than sandstone and lightweight mixtures.

P-38: Numerical Optimization of Lead Free Perovskite Solar Cell: *Mohammad Hossain*[1]; Ounsi Daif[1]; Nowshad Amin[2]; Fahhad Alharbi[1]; Nouar Tabet[1]; [1]QEERI; [2]National University of Malaysia

Alternative perovskite solar cells are emerging rapidly to compete with other conventional photovoltaic materials. However, toxic lead content of organic-inorganic perovskite is an issue to be addressed briefly. In this work, we propose to use organo-tin halide perovskite absorber layer to replace toxic Pb-based light harvester. We perform a numerical optimization of the layer thicknesses both from the optical and electrical points of view, using SCAPS (Solar Cell Capacitance Simulator) and analytical calculations. We study two types of electron conducting materials (n-ZnO and n-TiO_2). Both $ZnO/CH_3NH_3SnI_3$/Spiro-OMETAD and $TiO_2/CH_3NH_3SnI_3$/Spiro-OMETAD structures show the conversion efficiencies above 15% of (respectively 15.44% and 15.64%). Accordingly, we present a fully optimized device architecture. The analyzed results indicate the feasible fabrication of high efficiency Pb-free perovskite solar cells.

P-39: On the Effects of Plastic Anisotropy on the Ductile Fracture of Mg Alloys: Amine Benzerga[1]; *S. Basu*[1]; E. Dogan[1]; I. Karaman[1]; [1]Texas A&M University

Plastic anisotropy is often invoked to rationalize the low formability of strongly anisotropic materials. Analysis based on homogenization theory suggests however that certain forms of plastic anisotropy may hinder void growth under any triaxial stress state. This paper reports on our recent efforts to engineer the anisotropy of Mg alloy AZ31 by means of severe plastic deformation. Processing routes are carefully guided by simulations based on a self-consistent viscoplastic model. Deformation anisotropy and damage accumulation are investigated at room temperature. Plastic flow anisotropy is characterized using cylindrical geometries in order not to bias the intrinsic material behavior with structural effects. Damage accumulation is investigated using round notched bars with different notch radii to vary the stress triaxiality. A suite of analytical measurements and observations are carried out to characterize the microstructure in the as-received, post-processing and post-deformation states. A simple model is proposed to rationalize the trends.

P-40: Optimization of Soft Magnetic Properties in Nanocrystalline Glass-coated Microwires: Valentina Zhukova[1]; Ahmed Talaat[2]; Juan Blanco[2]; Mihail Ipatov[2]; Juan del Val[2]; *Arcady Zhukov*[3]; [1]Basque Country University, UPV/EHU ; [2]Basque Country University, UPV/EHU; [3]Basque Country University and Ikerbasque

We studied magnetic properties, structure and Giant magnetoimpedance (GMI) effect, of Finemet-type FeCuNbSiB microwires. We observed that GMI effect and magnetic softness of glass-coated microwires produced by the Taylor-Ulitovski technique can be tailored either controlling magnetoelastic anisotropy of as-prepared FeCuNbSiB microwires or controlling their structure by heat treatment. We observed considerable magnetic softening of studied microwires after annealing. This magnetic softening correlates with the devitrification of amorphous samples. Amorphous Fe-rich microwires exhibited low GMI effect (GMI ratio below 1%). Considerable enhancement of the GMI effect (GMI ratio up to 100%) has been observed in heat treated microwires with nanocrystalline structure. Some of as-prepared Fe-rich exhibited nanocrystalline structure and GMI ratio up to 45%. We believe that FINEMET-type glass-coated microwires with higher saturation magnetization are good candidates for GMI sensor and metacomposites applications.

P-41: Predictive Modeling For Sustainable Energy Solutions: *Chaker El Amrani*[1]; Othmane Bouhali[2]; [1]Abdelmalek Essaadi University, Tangier; [2]Texas A&M University at Qatar

Sustainable energy solutions such as wind and solar power are the key to energy security and economic progress. They are also the best way to reduce carbon emissions and preserve a healthy environment. Modeling these solutions is necessary to compute parameters governing the energy production. In this paper we describe the use of the Weather Research and Forecasting (WRF) Model, to estimate annual energy output from distributed wind turbines and solar panels. The WRF is a numerical weather prediction system designed to serve the atmospheric research with spatial resolution ranging from a few meters to thousands of kilometers. The WRF predicts temperature, humidity, wind speed, etc. for short and long period of time, which can be used to calculate the energy generation by sustainable systems. The WRF is an intensive processing model. The paper discusses as well its porting to high performance computing platform to accelerate the application run-time.

P-42: Principles of Improvement the Energy Efficiency in Pyrometallurgy of Copper: Utilization the Secondary Heat Energy of Intermediate Products: *Milorad Cirkovic*[1]; Mile Bugarin[1]; Vlastimir Trujic[1]; Zeljko Kamberovic[1]; [1]Mining and Metallurgy Institute Bor, Serbia

Having in mind that the energy is more and more expensive and that the natural energy resources are smaller and smaller, this research presents a contribution to the use of renewable thermoenergetic resources in terms of improving the economy and ecology in the pyrometallurgical copper production. Pyrometallurgical copper production is a big consumer of energy resources of all kinds. The process products are holders of large energy amount that is lost uncontrollably in the environment, thereby affecting adversely the economic and environmental effects. This paper presents the results of research the renewable thermoenergetic resources from metallurgical products. Using the comparative method, the consumption of energy resources is determined in the modern technological processes and standard pyrometallurgical process of copper production in Bor (Serbia) and, based on the heat balance, the amount of the secondary energy is defined and the method of its evaluation is proposed.

P-43: Process Optimization of Seed Assisted Growth of Vertically Aligned ZnO Nanorods via Facile Solution Synthesis: Muhammad Aftab Akram[1]; Sofia Javed[1]; Mohammad Mujahid[1]; *Mohammad Islam*[2]; [1]National University of Sciences and Technology Pakistan; [2]Center of Excellence for Research in Engineering Materials (CEREM) Advanced Manufacturing Institute, College of Engineering, King Saud University

In this paper optimization of seed assisted growth of vertically aligned ZnO nanorods by facile solution synthesis is being reported. Effect of seed layer characteristics such as orientation and thickness and effects of growth conditions such as precursor solution concentration, growth temperature and growth time were investigated. Optical properties were studied by UV-VIS spectrometer while Hall Effect was used for electrical characterization and SEM gave information about morphology. XRD was also used for structural characterization.

P-44: Pulsed Electrodeposition of Nano-Crystalline Ni with Uniform Co-Depostion of Micron Sized Diamond Particles on Annealed Copper Substrate: *Prashant Kumar*[1]; [1]Indian Institute of Technology Banaras Hindu University Varanasi

Nanocrystalline nickel was deposited on annealed copper substrate of unit surface area (1 cm2) via pulsed electrodeposition technique using potentiostat (model 263A, Princeton Applied Research, USA) from Watts bath. Diamond particles of three different dimensions, viz., 1, 3, and 6 micron were added separately (5 g/L). . The temperature was kept constant at 55 °C. Depositions were carried out at different current densities, viz., 50, 100,150 and 200 mA/ cm2 for different durations, i.e.7, 14 and 21 minutes and best results are optimized for 200mA/cm2. Scanning electron micrographs show uniform deposition of microstructure of micron diamond on the surface of copper embedded in the nickel matrix. Elemental mapping confirmed uniform deposition of nickel and diamond with almost no cracks or pits. Mechanical properties of the sample such as, Vicker's microhardness & corrosion resistance increased abruptly after the electrodeposition.

P-45: RAETEX Sustainable Pavement Technology: Michelle Ward[1]; *Shayan Barmand*[1]; [1]RAETEX Industries

RAETEX Doha's sustainable pavement technology, Crumb Rubber Polymer Modified Bitumen (CR-PMB), introduces a polymer-based bitumen modification process using recycled tire rubber with equal to or better performance than conventional modification methods used today. RAETEX's CR-PMB technology reclaims the polymer, styrene-butadiene-rubber and Natural Rubber latex from tires and disperses them in their original state into the bitumen, thereby improving the rheological properties of the pavement. Temperatures used in this process are significantly lower than those used in conventional asphalt-rubber processes, therefore preventing the destruction of the polymers and maintaining a quality-controlled environment. The elemental sulfur and carbon black dispersed from the tires add strength and UV resistance. Additional benefits of CR-PMB include reduced post-consumer waste materials, improved pavement safety, noise reduction and protection against Urban Heat Island effect.

P-46: Rejuvenation of Long-Term Exposed Nimonic 90 Made Turbine Blades: *Mohammad Saeed Shahriary*[1]; Mohammad Cheraghzadeh[1]; Ali Khanjani[1]; [1]Mavadkaran Engineering Company

In first part, the effect of internal service damages on the microstructure of a second stage gas turbine blade, which is made of Nimonic 90 superalloy was evaluated. Formation of network grain boundary carbides and huge amount of carbides, because of service exposure, and also significant change in gamma prime structure were shown in the microstructure. According to mentioned degradation in the microstructure of the blade, in the second phase, blades are subjected to rejuvenation treatment. By using proper heat treatment, one can resuscitate the microstructure of degraded blade and mechanical properties. To obtain this, blades were solution treated at 1080ºC for 8hr, and different treatments were carried out on them. Finally, by comparing the obtained microstructures, the most suitable rejuvenation heat treatment was chosen and mechanical properties of the rejuvenated blades were tested. Results showed that appropriate heat treatment can restore the tensile and creep properties of the blades.

P-47: Simulation of Solidification, Relaxation and Long-Term Behavior of a Borosilicate Glass: *Nicolas Barth*[1]; Daniel George[2]; Said Ahzi[1]; Yves Rémond[2]; Mohammad Ahmed Khaleel[3]; Frédéric Bouyer[4]; [1]University of Strasbourg/Qatar Foundation; [2]University of Strasbourg–CNRS; [3]Qatar Foundation; [4]CEA (French Alternative Energies and Atomic Energy Commission)

High-level radioactive waste (HLW) vitrification is a manufacturing process designed to dispose of nuclear energy fission products over long-term timescales. We studied and modeled the thermomechanical phenomena occurring during the processing of the glass blocks, e.g. during their solidification and their cooling down. The thermomechanical modeling takes place in 3D FEM simulations. The relaxations of the borosilicate glass are to be taken into account through scripted algorithms. They allow us to describe accurately the evolution of the glass properties over its phase transition (the glass transition temperatures are non-uniform in the HLW package). A damage behavior within the frame of Continuum Damage Mechanics is also used to predict the glass cracking surface area.

P-48: Storage and Release of Thermal Energy of Phase Change Materials Based on Linear Low Density Polyethylene, Paraffin Wax and Expanded Graphite Applicable in Building Industry: *Patrik Sobolciak*[1]; Mustapha Karkri[2]; Igor Krupa[3]; Mariam Al. Maadeed[3]; [1]Qatar University; [2]Université Paris-Est; [3]Qatar university

Thermal energy storage systems are crucial for reducing dependency on fossil fuels and also for minimize CO_2 emissions. In this contribution, the phase change materials based on linear low density polyethylene paraffin wax and expanded graphite were used as new energy storage system to study the heat transfer characteristics of paraffin wax during melting and solidification processes. Pronounced increase of thermal conductivity with increasing of expanded graphite content has been observed. Differencial scanning calorimetry was used for an estimation of the specific enthalpy of melting and crystallization and for a determination of the specific heat capacity. A dramatic increase of the specific heat capacity has been observed in the vicinity of melting point of paraffin wax.The sensible heat and the ability to store and release the thermal energy of Phase Change Materials were investigated by specific home-made equipment based on the transient hot guarded plane method.

P-49: Structural Alloy AA6082 – Joining by Friction Stir Welding: Zhiui Zhang[1]; Christophe Herbelot[1]; Abdellatif Imad[1]; *Rajashekhara Shabadi*[1]; [1]University of Science and Technology of Lille

Aluminium alloy 6082 in T6 condition finds vast applications as structural members in various applications. Apart from its medium strength characteristics, it also exhibits excellent corrosion resistance and mostly applied in the form of plates. Often, such plates require an efficient joining of plates which produce minimum distortions and be readily applicable. Friction Stir Welding (FSW) being a solid state joining method offers an efficient and cost effective means of joining. Present study reports, the influence of processing parameters on the evolution and morphology of the welding zones and mechanical properties of 6086 Aluminium Alloys. 6082 alloy sheets in T6 condition were welded in butt joints using FSW. An in-situ observation using the acoustic emission was carried out during the welding procedure. A correlation between the acoustic emission and the mechanical properties will be reported.

P-50: Towards Engineering Nanolaminated Ternary Carbides and Nitrides (MAX phases) and Their Composites for Extreme Environments: *Miladin Radovic*[1]; Liangfa Hu[1]; Rogelio Benitez[1]; Ankush Kothalkar[1]; Huli Gao[1]; Ibrahim Karaman[1]; [1]Texas A&M University

A new class of carbides and nitrides with nanolaminated structure - known as the MAX phases - has recently emerged that has challenged their typical description. The main reason for growing interest in the MAX phases lies in the unusual, and sometimes unique, set of properties that the MAX phases possess. Like typical ceramics, the MAX phases are elastically stiff, good thermal and electrical conductors, resistant to chemical attack, and have relatively low thermal expansion coefficients. Mechanically, however, the MAX phases cannot be more different when compared to typical ceramics because they are relatively soft and most readily machinable, thermal shock resistant and damage tolerant. Some of the MAX phases – notably Ti_2AlC and Ti_3SiC_2 - are refractory and oxidation, fatigue and creep resistant. At room temperature, they can be compressed to stresses as high as 1 GPa and fully recover upon removal of the load, while dissipating ~ 25% of the mechanical energy. From more than 60 different MAX phases, Ti_2AlC is considered to be one of the best candidates for applications in extreme environments because of its excellent corrosion/oxidation resistance in air and water vapor at high temperatures, due to the formation of spallation-resistant layer of Al_2O_3 with crack healing capabilities. In this paper the emphasis will be given to the engineering of Ti_2AlC and its composites for application in extreme environments. The effect of microstructure on mechanical properties (stress-strain response, brittle-to-plastic transition temperature and creep resistance) and oxidation resistance is discussed in more detail in this paper. In addition, different methods of processing Ti_2AlC and its composites with desired microstructure and properties are discussed.

P-51: Martensitic Transformation of Ni_2FeGa Magnetic Shape Memory Alloy Studied by Density Functional Theory: *Sevgi Özdemir Kart*[1]; Cengiz Soykan[1]; Cem Sevik[2]; Tahir Çagin[3]; [1]Pamukkale University; [2]Anadolu University; [3]Texas A&M University

Ni_2FeGa is a new magnetic shape memory alloy which shows desirable properties including low transformation stress, high reversible strains and small hysteresis. The structural stabilities, mechanic, magnetic and electronic properties of Ni_2FeGa alloys are obtained by performing spin-polarized energy calculations based on density functional theory. It is found that L21 austenitic phase and martensitic phases of NM and 5M have the minimum energy at a=5.76 A, c/a=1.33 and c/a=0.99, respectively. We found that the magnetic moment of Ni increases, but that of Fe diminishes through martensitic transformation (MT), indicating that the electrons transfer from Ni to Fe. Some significant differences in the minority spin states of DOS take place over MT, leading to stabilize the final structure. Tetragonal shear elastic constant takes considerably small value in the parent phase, reflecting that the elastic instability leads to MT. The results calculated are comparable with those of previous calculations and the experiments.

P-52: Surfactant Less Microwave Synthesis of Hierarchical Nanostructures of Titania and Their Application: Sofia Javed[1]; Mohammad Mujahid[1]; Muhammad Aftab Akram[1]; *Mohammad Islam*[2]; [1]National University of Sciences and Technology Pakistan; [2]Center of Excellence for Research in Engineering Materials (CEREM) Advanced Manufacturing Institute, College of Engineering, King Saud University

Heirarchical nanostructures of titania are of great importance for light driven applications. The present work is about an environment friendly microwave synthesis of hierarchical titania nanoflowers in DI water. Submicron sized hierarchical nanoflowers are obtained without any surfactants or hydrofluoric acid. FESEM, TEM, BET, XRD and raman spectroscopy were utilized to understand the structures. Mechanism of formation of nanoflowers is also studied. The application of the synthesized nanostructures in dye sensitized solar cells is presented.

P-54: Phenomenological Model for Phase Transformation Characteristics of Textured Shape Memory Alloys: *D. Chatziathanasiou*[1]; Y. Chemisky[1]; F. Meraghni[1]; E. Patoor[1]; [1]Arts et Métiers ParisTech

In the present study, a new phenomenological model that accounts for the effect of texture on phase transformation characteristics is developed. A new transformation criterion that includes the effect of tension-compression asymmetry and anisotropy linked to texture is proposed and combined with a thermodynamical model to describe the thermomechanical behavior of polycrystalline shape memory alloys. Accordingly, an altered Prager criterion has been developed, introducing a general transformation of the axes in the stress space. The thermodynamical parameters of the model are identified based on a polycrystalline self-consistent micromechanical model previously developed by Patoor et al. (1995) for several loading cases on isotropic, rolled and drawn textures. Transformation surfaces in the stress space and transformation strain space are obtained and compared with the micromechanical model. It is shown that a suitable description of the evolution equation for transformation strain is necessary to obtain a good agreement between the macroscopic and the microscopic polycrystalline simulations.

P-55: Synthesis and Evaluation of Heterogeneous Nano-catalyst : Cr_2O_3 Loaded in to MCM-41: *Ali Salemi Golezani*[1]; [1]KIAU

In this study a nano-composite catalyst was synthesized by incorporation of chromium precursor in to MCM-41 as a base catalyst. First MCM-41 mesoporous material was synthesized using hydrothermal route which was accompanied by pH adjusting. Then achieved MCM-41was impregnated by chromium nitrate aqueous solution for several time under water aspiration. Raw powder was cured by heat treatment in vacuum furnace at 500°c. Phase formation, morphology and gas absorption properties of resulted materials were characterized by XRD, HRTEM and BET analysis respectively. Investigation proved high quality hexagonal meso structure as a matrix and Cr_2O_3 as a second phase has been formed with a narrow size pore diameter distribution and high surface area in MCM-41/Cr_2O_3 nano-composite structure. Pores diameters and specific surface area of synthesized nano-composite was approximately determined 3.5 nm and 961.5 m2/g respectively.

P-56: The Effect of Using a Titanium Interlayer in Explosively Welded Cu/Al Plates: *Majid Etminanbakhsh*[1]; Mandana Adeli[2]; [1]Iran Research Center; [2]Iran University of Science & Technology

ETJs (Electrical Transition Joints) are widely used in electrochemical industries such as aluminum smelters and zinc electrolysis plants. Explosive welding is a relatively easy and cost-effective method for fabrication of copper/aluminum clads used as ETJs. The problem is the probability of formation of numerous brittle intermetallic compounds between copper and aluminum according to Cu-Al phase diagram. This renders the joints susceptible to losing their strength especially when subjected to higher temperatures, e.g. during the process of welding. In the present research, the use of a titanium interlayer between copper and aluminum was studied. The two types of clad, i.e. , with and without titanium are characterized using optical and Scanning Electron Microscopy. It was found out that the presence of titanium retards the diffusion process between Cu and Al, yielding a joint with higher strength and bonding properties as the detrimental effect of temperature on the joints has been eliminated.

P-57: Thermal Analysis of Solar Panels: *Nicolas Barth*[1]; Joao Pedro de Magalhaes Correia[2]; Said Ahzi[1]; Mohammad Ahmed Khaleel[3]; [1]Qatar Foundation/University of Strasbourg; [2]University of Strasbourg; [3]Qatar Foundation

In this work, we propose to analyze the thermal behavior of PV panels using finite element simulations (FEM). We applied this analysis to compute the temperature distribution in a PV panel BP 350 subjected to different atmospheric conditions. This analysis takes into account existing formulations in the literature and, based on NOCT conditions, meteorological data was used to validate our approach for different wind speed and solar irradiance. The electrical performance of the PV panel was also studied. The proposed 2D FEM analysis is applied to different region's climates and was also used to consider the role of thermal inertia on the optimization of the PV device efficiency.

P-58: Thermo-mechanical Fatigue and Fracture of NiTiHf High Temperature Shape Memory Alloys: *Ceylan Hayrettin*[1]; Omer Karakoc[1]; Ibrahim Karaman[1]; [1]Texas A&M University

Solid state actuators have attracted significant attention in aerospace, automotive and energy industries. Shape memory alloys (SMAs) are promising candidates for these actuator applications because SMAs have highest energy density among all active materials. One of the problems of SMAs is lack of data and understanding of fatigue during thermo-mechanical actuation. The aim of this study is to develop reliable methods to quantify thermo-mechanical fatigue and fracture behavior of SMAs. Thermo-mechanical fatigue tests were conducted by cycling temperature under constant stress until failure. Thermo-mechanical fracture tests were used to investigate crack growth under constant stress and temperature cycling. Here, precipitation hardenable NiTiHf SMAs were studied. Preliminary results showed that this material can generate up to 3% repeatable actuation strain and can lasts above 20000 cycles. The effect of different microstructures, in particular the effect of precipitate size and martensite morphology, on the fatigue and fracture behavior will be presented.

P-60: Transport through Quantum Dots: *Hamidreza Vanaie*[1]; [1]Islamic Azad University

We have investigated the electronic transport properties of a quantum dot constructed by MTX@C60 molecule that are coupled to two semi-infinite SWCNT electrodes using Keldysh nonequilibrium Green's function formalism and GW method. For the systems under investigation, we study effects of atom position and encapsulation into cage, contacts and gate and bias voltages. Our results indicate that the effects of displacement and the gate and bias voltages are important factors in the electron conduction.

P-61: Warm Mix Asphalt: Microstructural, Chemical and Thermal Analyses: *Ilaria Menapace*[1]; Eyad Masad[1]; Dallas Little[2]; Emad Kassem[2]; Amit Bhasin[3]; [1]Texas A&M University at Qatar; [2]Texas A&M University; [3]The University of Texas at Austin,

During the past two decades, Warm Mix Asphalts (WMA) have been used in pavement with good performance. The WMA macroscopic properties were addressed by several papers, while limited studies tried to comprehend the influence of WMA additives on asphalt composition and microstructural properties. This study intends to investigate the effect of two WMA additives, Advera® and Sasobit®, on asphalt properties. The microstructural changes were investigated with Atomic Force Microscopy (AFM), which in the past consented to identify the binder phases, such as "bee" structures. The AFM images outlined the influence of the WMA additives, particularly Sasobit®, on the binder phases. Furthermore, the appearance of phase discontinuities in the matrix indicates the different abilities of the phases to adjust stresses. Any chemical reactions between asphalt and WMA additives were excluded by Nuclear Magnetic Resonance. Thermal analyses were applied to highlight the effect of the WMA additives on the asphalt thermal properties.

P-62: Evaluation of Performance Characteristics of Warm Mix Asphalt in Qatar: *Emad Kassem*[1]; Lorena Garcia Cucalon[2]; Eyad Masad[3]; Dallas Little[2]; [1]Texas A&M Transportation Institute; [2]Texas A&M University; [3]Texas A&M University-Qatar

Multiple Warm Mix Asphalt (WMA) technologies have been recently developed to reduce mixing and laying temperatures, reduce energy consumption, lower emissions and fumes, reduce binder aging, and facilitate compaction of asphalt mixtures. The WMA technology has not been explored in the State of Qatar or in the Gulf region. This study aims to develop WMA using local materials used in road construction in Qatar and evaluate its performance characteristics. Several laboratory tests at the component level have been conducted to provide a fundamental understanding of individual interaction between each component of mixtures such as aggregates, asphalt binder, and water. The preliminary results showed that some WMA additives have enhanced the ability of asphalt binders to coat the microtextural features of the surface of aggregates which provides better mechanical interlocking between asphalt binder and aggregate particles. In addition, WMA mixtures have exhibited comparable performance to conventional asphalt mixtures in dry condition.

Plenary 3

Wednesday Morning
January 14, 2015

Room: Mukhtassar
Location: Ritz-Carlton Doha

Session Chair: Eyad Masad, Texas A&M University at Qatar

08:00 Introductory Comments

08:10 Keynote
Achievable Innovation in a Sustainable Infrastructure: *Dallas Little*[1]; [1]Texas A&M University

Constructing and maintaining a sustainable infrastructure is a daunting task to say the least. In order to help do so, innovative solutions have been proposed. These include recycling materials, smart materials that can "repair" or "heal" themselves and those that can even sense damage and signal the need for repair at a point in time that will optimize the effectiveness of such maintenance or repair. Although many innovative methods have been offered by the brightest of minds, for each, one must assess the efficacy of these methods. This keynote presentation discusses innovative methods that are founded in sufficient practicality to make them valid candidates for innovation in improving sustainability and cutting costs of our infrastructure. The presentation will address as examples innovative subgrade and subbase treatment for existing structures and self-healing materials and practical ways to promote such healing action.

08:55 Break

1-5: Asphaltic Materials

Wednesday Morning
January 14, 2015

Room: Mukhtassar
Location: Ritz-Carlton Doha

Session Chairs: Gaurav Sant, University of California, Los Angeles; Eyad Masad, Texas A&M University at Qatar

09:10
DEM Simulation of the Asphalt Concrete Flow Number Test: *Thomas Papagiannakis*[1]; Habatamu Zelelew; [1]University of Texas San Antonio

This paper presents simulation results of the behavior of asphalt concretes subjected to the Flow Number test (AASHTO TP 79-12). It utilizes the Discrete Element Method (DEM) to simulate the microstructure of 9 Asphalt Concrete (AC) mixtures captured using X-Ray Computed Tomography (CT). Advanced digital image processing techniques were utilized to process the X-ray CT images and to suitably input their microstructure into the DEM model. The viscoelastic rheological properties of the asphalt mastics (composed of binder and aggregate fines passing 0.075 mm sieve) were defined by fitting Burger model parameters on frequency sweep test data conducted at 60 °C. Each simulation was conducted under a confining pressure of 69 kPa. The results are presented in terms of plots of vertical axial strain versus number of loading cycles. The resistance of these three mixtures to permanent deformation is compared through the estimated Flow Number (FN).

09:30
Assessment of the Benefits of Implementing Warm Mix Asphalt (WMA) for Roadways in Qatar: Yara Hamdar[1]; *Ghassan Chehab*[2]; Issam Srour[3]; [1]Graduate Research Assistant, Corresponding Author; [2]Associate Professor, Department of Civil and Environmental Engineering; [3]Assistant Professor, Engineering Management Program

The long-term performance of WMA pavements and their performance in hot climates are not well known. Therefore, most tools that quantify the costs of WMA are restricted to early phases of the pavement life-cycle and consider only one impact category--financial cost or carbon footprint. This study aims to develop a comprehensive tool to quantify the overall cost of implementing WMA. The tool is based on life cycle assessment (LCA) and combines both environmental and economic costs in a single metric to simplify comparison of alternatives. This study uses the MEPDG (Mechanistic Empirical Design Guide) software to model long-term WMA pavement performance and incorporates it in the LCA tool. The tool, though tailored to fit any scenario, will be applied to Qatar by creating an inventory database that is particular to the country. The study aims to draw the line for when benefits of WMA outweigh costs as compared to HMA.

09:50
Effect of Warm Mix Asphalt on Aging of Asphalt Binders: *Ala Abbas*[1]; Munir Nazzal[2]; Savas Kaya[2]; Sunday Akinbowale[1]; Bijay Subedi[1]; Lana Abu Qtaish[2]; [1]The University of Akron; [2]Ohio University

This paper evaluated the rheological and chemical properties of asphalt binders recovered from short-term and long-term aged foamed warm mix asphalt (WMA) and traditional hot mix asphalt (HMA). AASHTO R 30 was utilized to simulate the short-term and long-term aging of the laboratory-prepared asphalt mixtures. The dynamic shear rheometer (DSR) was used to characterize the rheological properties of the unaged and aged asphalt binders. Fourier-transform infrared (FTIR) spectroscopy was used to identify and quantify the amount of functional groups present in these binders. Gel permeation chromatography (GPC) was utilized to determine the molecular size distribution within these binders. The asphalt binders recovered from short-term and long-term oven aged HMA mixtures exhibited slightly higher G*/sind and G*sind values than those recovered from foamed WMA mixtures. The FTIR and GPC test results agreed with those obtained in the DSR. This indicates that foamed WMA mixtures undergo less aging than traditional HMA mixtures.

10:10
Investigation of Long- and Short-term Moisture Damage Characteristics of Warm Asphalt Mixtures Containing Reclaimed Asphalt: *Aikaterini Varveri*[1]; Stavros Avgerinopoulos[2]; Athanasios (Tom) Scarpas[1]; [1]Delft University of Technology; [2]De Montfort University

The design of sustainable road infrastructure calls for construction of asphalt pavements with enhanced durability characteristics. A critical parameter that influences the long-term performance of pavements is moisture damage. In this paper, a moisture conditioning protocol which attempts to distinguish the contributions of long- and short-term moisture damage i.e. moisture diffusion and cyclic pore pressure generation, is utilized. Asphalt specimens produced with different technologies such as warm mix asphalt (WMA) and reclaimed asphalt (RA) were conditioned in various combinations of water bath immersion and cyclic pore pressures by means of the Moisture Induced Sensitivity Tester. The results show that the proposed conditioning protocol can be used to evaluate moisture susceptibility and distinguish among asphalt mixtures with different moisture damage characteristics. Moreover the protocol enables the quantitative determination of the individual short- and long-term contribution to the overall damage of the specimens.

10:30
Improving Asphalt Mixtures Performance by Mitigating Oxidation Using Anti-Oxidants Additives: *Samer Dessouky*[1]; Manuel Diaz[1]; [1]University of Texas-San Antonio

Oxidation in polymer-modified asphalt occurs due to exposure in air and high temperatures. The aging mechanism tends to alter the physical and chemical properties of asphalt as reflected by the change in their rheological properties. In this study, a blend of SBR and hindered phenols (HP) was used to improve the rheological characteristics of base and polymer-modified asphalt. The stiffening indices and the complex modulus indices were used to assess the effectiveness of the additives and its thermal stability, respectively. It was found that the additives were capable of increasing the stiffness at high temperature and reducing the hardening propensity of aged asphalt at intermediate and low temperatures. Asphalt morphology suggested that the degree of polymer network chains break-down was in less severity when the HP was used. Performance testing of hot-mix asphalt suggested that the HP additives enhanced the stripping resistance, improved rutting performance and extended the service life.

10:50
An Innovative Concept for Testing Rutting Susceptibility of Asphalt Mixture: *Alaedddin Mohseni*[1]; Haleh Azari[2]; [1]Pavement Systems; [2]AASHTO

The new innovation is regarding a new test and analysis method for evaluating the rutting resistance of asphalt mixtures using the Superpave Asphalt Mixture Performance Tester (AMPT). This new test method resolves several critical shortcomings of the current flow number (FN) test method (AASHTO TP 79). An innovative "incremental" loading approach is used. The loading is applied in several increments of varying stress levels. Instead of conducting the test at a fixed stress level as in the current practice, repeated loading is applied in four increments of 500 cycles each. In the first increment, the stress level is 200 kPa, which is used as a conditioning increment. The stress levels for the other 3 increments are 400, 600, and 800 kPa. A new more robust test parameter, referred to as Minimum Strain Rate (MSR), is introduced, which is the permanent strain due to the 500th load cycle.

11:10

Structural Pavement Improvement Using SBS-Modified Binders: Robert Kluttz[1]; Willem Vonk[2]; Erica Jellema[2]; *David Bell*[3]; [1]Kraton Polymers; [2]Kraton Polymers Research B.V.; [3]Kraton Polymers U.S., LLC

The most popular bitumen modifier styrene-butadiene-styrene block-copolymer (SBS; >70% of the global PMB market), does not have a great effect on the stiffness of the binder and thus the asphalt mix. From that perspective, it would not have a big impact on the design of a pavement, particularly if the design method does not take into account resilience and fatigue performance improvement. At the same time, modifying hard base bitumen is not obvious from a compatibility and workability perspective with the standard SBS polymers available, while there is a regional trend in the industry to use increasingly harder binders that increase the stiffness.

2-5: Shape Memory Alloys in Energy Conversion

Wednesday Morning — Room: Al Wosail 1
January 14, 2015 — Location: Ritz-Carlton Doha

Session Chairs: Sebastian Fähler, The Leibniz Institute for Solid State and Materials Research Dresden; Thomas Niendorf, Technical University of Freiberg

09:10

On the Fracture Response of Shape Memory Alloy Actuators: *Dimitris Lagoudas*[1]; Theocharis Baxevanis[1]; [1]Texas A&M University

The effect of thermo-mechanically-induced global phase transformation on crack initiation and growth in an SMA actuator is investigated by means of experimentation and the finite element method. Experiments on double U-notched and CT specimens were performed under nominally isobaric loading conditions. Crack initiation, growth and catastrophic failure were observed after just a few thermal cycles or even during the first thermal cycle depending on the level of the bias load and the material configuration. This behavior is characteristic of SMAs; conventional metallic materials do not display a similar response. Finite element analysis was employed to gain a further insight into the experimental results. Results showed that during cooling the energy release rate increase drastically, an order of magnitude for specific material systems. This in turn implies that crack growth may be triggered as a result of phase transformation, resulting eventually in the material's ultimate failure, in accordance with experimental evidence.

09:30

High-temperature Shape Memory Alloys for Actuation and Damping Applications – Functional Properties and Degradation Behavior: *Thomas Niendorf*[1]; Philipp Krooss[2]; Hans Maier[3]; [1]TU Bergakademie Freiberg; [2]University of Paderborn; [3]Leibniz Universität Hannover

For actuation and damping applications at elevated temperatures conventional shape memory alloys (SMAs) such as Ni-Ti are not suited due their low martensite start temperatures and fast degradation, respectively. In order to overcome these issues new alloys have been proposed. So far, the focus was mainly on ternary systems Ni-Ti-X containing large amounts of noble elements or refractory metals. Unfortunately, these alloys are either extremely expensive or hard to process. In the present study, alternative high-temperature shape memory alloys (HT-SMAs) containing cheaper base metals are investigated. The alloys under consideration are Ti-Ta-X for actuation and Co-Ni-Ga for damping applications. Both alloys show promising functional properties, but still, functional degradation is an issue. For both alloys mechanical testing has been conducted accompanied by microstructure analyses. Degradation mechanisms are revealed to be imposed by different mechanisms including micro-plasticity and diffusion. Based on the findings, treatments are proposed allowing for significant life extension.

09:50

Thermal Stability of Ni-rich Ni-Ti-Hf and Ni-Ti-Zr High Temperature Shape Memory Alloys Containing H-phase Precipitates: Aquilina Perez-Sierra[1]; Alper Evirgen[2]; *Jaume Pons*[1]; Ruben Santamarta[1]; Ibrahim Karaman[2]; Ronald Noebe[3]; [1]University of the Balearic Islands; [2]Texas A&M University; [3]NASA Glenn Research Center

Ni-rich NiTiHf and NiTiZr alloys have attracted attention due to their outstanding properties as high temperature shape memory alloys. The significant performance upgrading with respect to (Ti+Hf/Zr)-rich alloys has been attributed to the H-phase nanoprecipitates formed after selective thermal treatments. Indeed, the changes introduced by the precipitates depend on its size and volume fraction. Among other effects, these precipitates can increase the martensitic transformation temperatures, improve the dimensional stability and enhance the shape memory properties. Nevertheless, there is little information about the stability of these alloys when staying for long times at working temperatures. In this presentation, three Ni-rich alloys containing 20at% Hf, 20at% Zr and 25at% Hf are studied after different thermal treatments producing two distinctive sizes and densities of H-phase precipitates. The stability of the martensitic transformation and precipitate distributions after ageing just below and above the martensitic transformation range will be analyzed and discussed.

10:10

Large Strains and Nondissipative Character of Superelastic Behavior of Ni-Fe-Ga(Co) Single Crystal: *Volodymyr Chernenko*[1]; Victor Lvov[2]; Elena Villa[3]; Jose Manuel Barandiaran[4]; [1]BCMaterials,UPV(EHU) & Ikerbasque; [2]Institute of Magnetism; [3]IENI-CNR; [4]BCMaterials & UPV(EHU)

The superelastic behavior of $Ni_{50}Fe_{19}Co_4Ga_{27}$ (at.%)single crystal above martensitic transformation (MT)temperature (200 K)was studied in tensile mode. Two substantially different regimes of deformation behavior were observed: ordinary superelastic loops showing a pronounced hysteresis of the stress-induced MT were obtained at temperatures below 318 K, while giant almost anhysteretic deformation of 14% was observed in the temperature range above indicated temperature. A thermodynamic theory has been developed showing that the drastic change of transformation behavior of the studied alloy can be interpreted as being related to the presence of a critical point in the stress–temperature phase diagram. The critical temperature, T = 318 K, is the upper bound of the temperature range where the stress-induced MTs can occur. Above this temperature, a gradual deformation process characterized by the highly non-linear stress–strain dependencies is observed, reflecting a post-critical state of the alloy and abnormally low values of the elastic modulus.

10:30

Development of SMA Actuated Morphing Airfoil for Wind Turbine Blade Load Alleviation: Anargyros Karakalas[1]; Theodore Machairas[1]; Alexandros Solomou[1]; Vasilis Riziotis[2]; *Dimitris Saravanos*[1]; [1]University of Patras; [2]National Technical University of Athens

Wind turbine rotor upscaling has led to the point where the blade structure cannot sustain increased aerodynamic loads without novel load alleviation concepts introduction. Research on load alleviation using morphing blade sections is presented. Antagonistic shape memory alloy (SMA) actuators are implemented to deflect the section trailing edge (TE) to target shapes and target time trajectories using time-series relating TE movement with changes in lift coefficient. Challenges regarding the complex thermomechanical response of morphing section and the enhancement of SMA transient response to frequencies meaningful for aerodynamic load alleviation are addressed. Using a recently developed finite element for SMA actuators, new actuator configurations are considered for fast cooling and heating cycles. Numerical results quantify the attained ranges of TE angle movement, the moving time period and the developed stresses. Estimations of the attained variations of lift coefficient vs. time are also presented to assess the performance of the morphing section.

10:50

Identification of Model Parameter for the Simulation of SMA Structures using Full Field Measurements: *Yves Chemisky*[1]; F. Meraghni[1]; N. Bourgeois[2]; S. Cornell[3]; R. Echchorfi[1]; E. Patoor[1]; [1]Arts et Metiers ParisTech; [2]Université de Lorraine; [3]Texas A&M University

With the design of new complex devices in shape memory alloys (SMAs) and to take advantage of their large recoverable strains, SMA components are increasingly subjected to multiaxial loadings. The problem of the identification of such parameters remains crucial to be able to better design and predict the overall behaviour of such component. In this work, the model parameters are determined from multiaxial and heterogeneous tests carried out on specimens with the same thermomechanical loading history. Digital Image Correlation technique is employed to obtain the strain fields at the surface of the specimen. Finite Element Analysis provides the numerically evaluated strain fields using a thermodynamical constitutive model. The strain fields computed numerically are compared with experimental ones obtained by DIC to find the model parameters which best matches experimental measurements using a newly developed parallelized mixed genetic/gradient-based optimization algorithm. It is demonstrated that model parameters for the simulation of SMA structures are thus obtained based on a few heterogeneous tests at different temperatures.

11:10

Comparison of the Work Output Values of Gradually Changing Porosity Samples and the Samples with Single Percent Porosity Level: Halil Tugrul[1]; Sule Cakmak[1]; *Benat Kockar*[1]; [1]Hacettepe University

In this study, the work output values and superelasticity properties of the $Ni_{50.6}Ti_{49.4}$ samples having gradually changing porosity levels were compared. Porous NiTi samples were produced with space holder technique via using pure magnesium as a space holder. Uniaxially pressed NiTi+Mg green samples were conventionally sintered under controlled atmosphere. 36 % and 80% porosity levels were combined in one sample in order to achieve gradually changing porosity, at which a shell of 18mm outer diameter of 36% was combined with 10 mm core diameter of 80% porosity. Cyclic compression tests were conducted on all 36%, 80% and 36%+80% sintered samples in order to obtain the superelastic properties. Pore architecture and microstructures of the samples were investigated to understand the transformation and superelasticity behavior of all samples. These results were then compared to come up with a suitable actuator material.

2-7: Materials Issues in Energy Conversion

Wednesday Morning Room: Al Wosail 4
January 14, 2015 Location: Ritz-Carlton Doha

Session Chairs: Marwan Khraisheh, The Qatar Environment and Energy Research Institute; Pradeep Sharma, University of Houston

09:10

Synthesis, Characterization and Environmental Impact Assessment of Graphene: *Mariam AlAli AlMa'adeed*[1]; Noorunnisa Khanam Patan[1]; Maryam Al-Aji[1]; Roda F. Al-Thani[1]; [1]Qatar University

This paper presents the synthesis and characterization of graphene by using chemical and thermal reduction method. Graphene was synthesized from GO, which was prepared by modified hummers method. The obtained layers of graphene was confirmed by using different characterization methods such as FTIR, XRD, Raman spectroscopy, SEM and TGA. The environmental impact assessment has been carried out by using life cycle assessment (LCA) approach. Results indicated that the production of graphene by chemical method can have significant Eco-toxicity potential (MAEP) and global warming potential (GWP). Possible production of graphene by different new microorganisms will be discussed as an alternative environmentally approach.

09:30

Numerical Modeling of Cathode Contact Material Densification in SOFCs: *Mohammed Khaleel*[1]; Brian Koeppel[2]; Elizabeth Stephens[2]; [1]Qatar Foundation; [2]Pacific Northwest National Laboratory

Numerical modeling was used to simulate the constrained sintering process of the cathode contact layer during assembly of solid oxide fuel cells (SOFCs). A finite element model based on the continuum theory for sintering of porous bodies was developed and used to investigate candidate low-temperature cathode contact materials. Constitutive parameters for various contact materials under development were estimated from dilatometry screening tests, and the influence of processing time, processing temperature, initial grain size, and applied compressive stress on the free sintering response was predicted for selected candidate materials. The densification behavior and generated stresses within a 5-cell planar SOFC stack during sintering, high temperature operation, and room temperature shutdown were predicted. Insufficient constrained densification was observed in the stack at the proposed heat treatment, but beneficial effects of reduced grain size, compressive stack preload, and reduced thermal expansion coefficient on the contact layer densification and stresses were observed.

09:50

Thin Film Coated Interconnectors Used in Solid Oxide Fuel Cells (SOFC) Via RF Magnetron Sputtering Method: *Fatma Aydin*[1]; Ali Özmetin[2]; Mahmut Mat[2]; [1]University of Nigde; [2]University of Meliksah

Nowadays, due to the high expectations in energy efficiency, reliability, transportability and environmental impact, alternative energy sources has gained more importance to meet power demand instead of building new conventional power plants. Solid oxide fuel cells (SOFCs) are electrochemical devices which convert chemical energy of fuels directly into electricity and heat. However, due to the high operating temperature (800-1000oC) of solid oxide fuel cells only a limited number of materials can be used as interconnectors. In this sudy, Crofer22APU was chosen as the basic interconnector material and corrosion resistances of coupons of Crofer22APU coated with various materials under the operating conditions were investigated. The coupons were coated by Manganese Cobaltite Spinel (MnCoO), Lanthanum Strontium Manganite (LSM) and Lanthanum Strontium Ferrite (LSF) using a RF magnetron sputtering. Resistance measurements were performed using a standard four point probe technique. Microstructures of the coatings were determined by SEM/EDS. Coatings were confirmed using XRD analysis.

10:10

Perovskites of Type $LaBO_3$ Prepared by the Microwave-Assisted Method for Oxygen Production: Shimaa Ali[1]; Nada Atta[1]; Yasser Abd Al-Rahman[1]; *Ahmed Galal*[1]; [1]Cairo University, Faculty of Science

$LaBO_3$ (B = Ni, Mn, Cr and Co) were prepared by microwave-assisted citrate method. The electrocatalytic activity toward oxygen evolution reaction was investigated by dc linear polarization and electrochemical impedance measurements. XRD characterization showed that pure perovskite crystals were formed. FESEM images showed that changing the type of the B-site metal ion affected the morphology of the prepared perovskites. HRTEM images confirmed the formation of the orthorhombic phase LaCrO3 and the rhombohedral phases of $LaNiO_3$, $LaMnO_3$ and $LaCoO_3$. The order of the electrocatalytic activity was $LaNiO_3 > LaFeO_3 > LaMnO_3$, that was related to the calculated values of the activation energy 11.38, 20.13 and 22.01 kJ mol-1 for $LaBO_3$ (B = Ni, Fe and Mn), respectively. $LaCrO_3$ and $LaCoO_3$ showed no catalytic activity toward OER due to the dissolution and the formation of passive layer of Co_3O_4 when being tested in $HClO_4$ medium. The reaction order and mechanism were identified.

10:30

Nitrogen-Doped Carbon Nanofiber – Supported Nickel Oxide Composite for Methanol Oxidation: *Aboubakr Abdullah*[1]; Abdullah Al-Enizi[2]; Ahmed El-Zatahry[2]; Salem Al-Deyab[2]; [1]Qatar University; [2]King Saud University

Nitrogen-Doped Carbon Nanofiber – Supported NiO Composite was prepared by electrospinning a sol-gel mixture of graphene, polyaniline with aqueous solutions of Polyvinylpyrrolidone (PVP) followed by a high-temperature annealing process. The electrospun fiber was carbonized for 5 h at 800 oC after being stabilized for 2 h at 200 oC followed by loading it by 10% NiO. The electrocatalytic activities of the produced nanocomposite have been studied using cyclic voltammetry, and chronoamperometry. N-CNF characterized by X-ray diffraction (XRD), thermogravimetric analysis (TGA), Surface area (BET), X-ray photoelectron spectroscopy (XPS), Transmission electron microscope (TEM), and scanning-electron microscopy (SEM. The obtained N-doped carbon nanofiber has a nitrogen content of 1.9 atomic % with a diameter range of (110–450) nm, and a surface area (393.3 m2 g-1). The material with a loaded NiO prepared at different temperatures has a nitrogen content of 1.9 wt%. Also, it showed an excellent electrocatalytic properties towards methanol oxidation reaction.

10:50
Ammonia Borane (AB) as a Portable Source & Storage Material for Hydrogen: *Muhammad Sohail*[1]; [1]QEERI

Amine-boranes (H3BNHnR3-n; R=H, alkyl, aryl) are widely used as reducing and hydroboration reagents. Due to their high volumetric and gravimetric hydrogen content, these molecules have been extensively explored as portable hydrogen source and storage materials. In this context, B-H activation by transition metals is an area of active research as it provides an appealing method to release not only hydrogen from amine-boranes (dehydrogenation) but also obtain useful B-N polymeric materials at moderate temperatures and reasonable rates.Photolysis of $CpRe(CO)_3$ in the presence of H_3BNEt_3 yields the trans-$CpRe(CO)_2(H)_2$ complex. This preliminary finding presents a rare example of transition metal mediated dehydrogenation of a tertiary amine-borane and suggests that the abstracted hydrogens may be stored in the form of metal hydride complexes.

2-9: Lightweight and High Performance Materials II

Wednesday Afternoon — Room: Mukhtassar
January 14, 2015 — Location: Ritz-Carlton Doha

Session Chairs: Georges Ayoub, Texas A&M University at Qatar; Bilal Mansoor, Texas A&M University at Qatar

13:30 Introductory Comments

13:40
Sustainable Novel Technology for Producing New Generations of Structural Al-alloys and Al Containing Bi-metals: *Hans Roven*[1]; Kristian Skorpen[2]; Oddvin Reiso[3]; Chris Devadas[4]; [1]Qatar University; [2]Norwegian University of Science and Technology; [3]Hydro ASA; [4]Hydro Aluminium QSTP Qatar

The unique and novel process of metal screw-extrusion was applied for continuous compaction and extrusion of profiles, e.g. from rapidly solidified (RS) aluminium or mixed bi-metal granulated feedstock. Firstly, in-house and commercially produced RS granulates of AlMgSi alloys were fed to the screw-extruder in order to produce Ø10 mm extrusions in a continuous manner. The profiles were characterized and their properties and microstructures were compared to conventionally ram-extruded counterparts. Secondly, Al granulates were mixed with Ti or Mg feedstock in order to produce bi-metal or composite extrusions which were further analyzed. The preliminary results indicate that this novel technology has the potential to produce extrusions very efficiently as to energy savings and at low cost. Besides, new alloys can be produced directly from recycled granulates. Screw extruded profiles can in the future have integrated structural and advanced functional properties, i.e. not been available up to now.

14:00
Modification of Aluminium Surfaces with Metal Oxides: *Rajashekhara Shabadi*[1]; Vishweshvara Gudla[2]; Flemming Jensen[3]; Rajan Ambat[2]; Aude Simar[4]; [1]University of Science and Technology of Lille; [2]Department of Mechanical Engineering, Technical University of Denmark; [3]Bang & Olufsen Operations A/S; [4]Université Catholique de Louvain

Aluminium alloy sheets are finding vast applications as a part of the structural members as aesthetic building panels. Surfaces of such panels often require painting, polymer coatings and similar protective coatings to make them visually appeasing. Which often needs maintenance and hence not cost effective. In the present feasibility study, we report the possibility of bringing inherent colour to the surfaces by the incorporation of metal oxide particles of Ti, Y and Ce which scatter light differently when compared to the oxide free aluminium surfaces, hence the change in the appearance of the surfaces. This study presents our efforts to inherently change the appearance of the aluminium surfaces. In this presentation, we discuss the process of incorporating the oxide particles into the surfaces, their characterisations using SEM, HRTEM, GIXRD and the surface appearance was analysed using photospectrometry technique that measures the diffuse and total reflectance of the surface.

14:20
Parametric Study for Crash Safety Improvement of a Car Bonnet Made from a Hybrid Aluminum and Natural Fiber Composite Structure: *Sofiene Helaili*[1]; Moez Chafra[1]; Yvon Chevalier[2]; [1]LASMAP; [2]SUPMECA

There is a growing interest on pedestrian's protection in automotive safety standards. Pedestrians head impact is one of the most important tests. In this paper, a hybrid composite structure made from natural fiber and aluminum, which improve the head protection when impact is taken place, is presented. The structure is made from a honeycomb composite made from unidirectional and woven composites and a thin aluminum layer. A head impact model is developed and coupled with an optimization algorithm in order to identify the best suitable number of hexagonal layers and thickness of the aluminum layer of the honeycomb structure. Key words: Composites, vegetal fiber, homogenization, head impact, sandwich panel, crash, safety

14:40
Adhesion Improvement Between Polyethylene and Aluminum Using Eco-friendly Plasma Treatment: *Anton Popelka*[1]; Igor Krupa[1]; Igor Novák[2]; Mabrouk Ouederni[3]; Fatima Abdulaqder[1]; Shrooq Al-Yazedi[1]; Taghreed Al-Gunaid[1]; Thuraya Al-Senani[1]; [1]Qatar University; [2]Slovak Academy of Sciences; [3]QAPCO

Polyethylene (PE) belongs among the most widely used polymers in many industrial applications, such as in building, packaging or transport industry. Qatar is one of the largest producers of PE in the world. Composite laminates consisting of PE and metal materials, such as aluminum (Al) lead to an improvement of various mechanical and physical properties necessary for special applications in building industry. Aluminum composite panel (ACP) represents type of flat panel that consists of two thin aluminum sheets bonded to a non-aluminum core, often made from PE. ACPs are frequently used for external cladding or facades of buildings. The main problem relates the adhesion between both materials. In this research work the improvement of adhesion properties of composite laminates prepared from PE and Al using plasma treatment was investigated. This surface treatment led to the significantly increase of peel strength of PE-Al adhesive joints.

15:00 Break

15:20
The Effect of Tool Geometry on Material Mixing During Friction Stir Welding (FSW) of Magnesium AZ31B Welds: *Zeina El-Chlouk*[1]; Haig Achdjian[1]; George Ayoub[2]; Ramsey Hamade[1]; [1]American University of Beirut; [2]Texas A&M University at Qatar

In friction stir welding (FSW) material flow determines to a great extent the weld feasibility and, ultimately, quality. This work reports on the investigation of the effect of tool geometry on the mixing and material flow during FSW of magnesium AZ31B to magnesium AZ31B. The study involves both FEM simulations and experiments. Nondestructive X-ray imaging is used to pinpoint the location of several steel shots (beads) which were pre-placed within the joint prior to FSW. The experimental results were also augmented with finite element analyses using the commercial engineering FEM software Deform the results of which compare favorably with those of the experiments. Resulting mixing behavior was contrasted for several tools with different configurations and geometries including tool with round shoulder and straight pin and others with concave-shoulder with tapered pin.

15:40
Microstructural Design of Mg Alloys for Lightweight Structural Applications: *Ebubekir Dogan*[1]; Matthew Vaughan[1]; Ibrahim Karaman[1]; Gwénaëlle Proust[2]; Georges Ayoub[3]; Amine Benzerga[1]; [1]Texas A&M University; [2]School of Civil Engineering, The University of Sydney; [3]Texas A&M University at Qatar

Interest on Mg alloys has significantly increased in recent years for weight-critical applications. However, Mg alloys show poor formability and low strength especially at low temperatures, which limits its extensive usage as a structural material. Severe plastic deformation and detailed knowledge of multiple deformation mechanisms can be utilized to design microstructure, crystallographic texture, and flow anisotropy of magnesium alloys, subjected to equal channel angular processing (ECAP), for ultrahigh strength, ductility, and formability. Using a microstructure based visco-plastic self-consistent crystal plasticity model with detailed electron backscatter diffraction (EBSD) analyses, new ECAP processing methodologies were developed in order to control the flow anisotropy and achieve desired microstructure and grain refinement down to few hundred nanometers. These studies led to the ultrahigh strength levels in magnesium alloys without rare earth alloying, and significantly enhanced their low temperature formability which are otherwise impossible to process at low temperatures due to their inherent poor formability.

16:00

Correlation of Magnetic Properties and Plastic Deformation Distribution in Steel Welds: *Athanasios Mamalis*[1]; Evangelos Hristoforou[2]; [1]PC-MAE; [2]National TU of Athens

The current paper refers to the development of a non destructive technique able to predict the initiation of cracks and defects in pipelines and generally in critical magnetic steel structures, therefore aiming at the Steel Health Monitoring (SteHeMon). The proposed method is based on the correlation of magnetic properties with structure-microstructure of steels and may also be used for the detection of welding non-uniformities, impurities etc.

16:20

Role of Multiscale Characterization to Examine the Mechanical Properties for Promoting New Material Developments: Application to Ni-base Superalloys: Bilal Mansoor[1]; *Mustapha Jouiad*[1]; [1]Masdar Institute of Technology

The unique high temperature properties of Nickel-based superalloys under aggressive environment are a function of their unique microstructure. The synergy between mechanical testing and Electron Microscopy is crucial to better screen these complex materials and develop a better structure-property understanding. Here we present some data from creep tests performed on N18 Ni-based superalloy, which exhibit 3 scales of precipitation. We will explore the origins of failure and link it systematically to primary precipitates. This structure-property understanding has played a crucial role in the development of new classes of superalloys without the precipitates such as Udimet 720, Udimet 706, Inconel 718, Inconel 625. The main purpose of such development is to avoid early failures and increase the strength at higher temperature which can be mainly correlated to their finer secondary precipitates. In this talk, we will describe the microstructural origins of the high temperatures mechanical strength of these novel Ni-based superalloys.

2-6: Photovoltaics and Solar-Thermal Energy Conversion

Wednesday Afternoon Room: Al Wosail 1
January 14, 2015 Location: Ritz-Carlton Doha

Session Chairs: Mariam Al-Maadeed, Qatar University; Rasit Turan, Middle East Technical University

13:30 Introductory Comments

13:40

Sponge-like Silicon Nanostructures for Third Generation Photovoltaic Solar Cells: *Rasit Turan*[1]; Serim Ilday[1]; Emel Ozen[2]; Sinan Gundogdu[2]; Atilla Aydinli[2]; [1]Middle East Technical University; [2]Bilkent University

Third-generation solar cells are expected to utilize the quantum size effect occurring in the semiconductor quantum dots fabricated in an appropriate matrix and lead to increase in the solar cell device efficiency significantly. So far, a successful device realization has not been possible due to the difficulties in the electronic transport in the dielectric matrix that forms an insulating medium. Si nanosponge is composed of tiny interconnected Si nanostructures embedded in an oxide matrix. These nanostructures form an interconnected quantum structure where the charge transport does not require the tunneling current. The band gap of the material can still be engineered by process parameters for tandem solar cell fabrication. Si-nanosponge is then a promising candidate for the fabrication of third-generation photovoltaic (PV) solar cells. Here, we report on the fabrication of Si-based nanosponge structures using both thermal and CW laser annealing of the samples prepared by different techniques.

14:00

Mono-crystalline Bulk Silicon Based High-Efficiency Flexible Solar Cell: *Rabab R. Bahabry*[1]; Jhonathan P. Rojas[1]; Aftab Hussain[1]; Muhammad M. Hussain[1]; [1]Integrated Nanotechnology Lab, King Abdullah University of Science and Technology

In this era of strong and global push for sustainable future, researchers and technologists are focusing on enhancing clean and renewable energy solutions. However, there are still many concerns need to be addressed before renewable energy technologies become viable to be integrated into mainstream energy market. We report a novel flexible solar cell design incorporating key features: high efficiency, low cost, lightweight, flexible, and mono-crystalline silicon solar cell. Our fabrication process is CMOS compatible, uses bulk mono-crystalline Si (100) – the most widely used substrate for its low coat and exclusive electrical and mechanical properties. The resultant thin photoactive layers have high flexibility, periodic arrays of nano-structured junctions that dramatically amplify absorption while decreasing system parasitic resistance. We recycle the remaining bulk wafers (after releasing the top thin layer) by chemical mechanical polishing to reduce the cost further

14:20

Hole Mobility and Stresses in PECVD a-Si Thin Films: *Nouar Tabet*[1]; [1]QEERI

We describe how we can achieve stress engineering during the growth of amorphous silicon thin films by Plasma Enhanced Chemical vapor Deposition/ Then we discuss the hole mobility measurements obtained from time of Flight technique and discuss the observed correlation stress-hole mobility based on the analysis of the structural properties of the films generated by numerical simulations.

14:40

Sonochemical Synthesis of Cu_2ZnSnS_4 and $Cu_2ZnSnSe_4$ Nanocrystals for Absorber Layer Application in Thin Film Solar Cells: *Mohammad Islam*[1]; Syed Shah[2]; [1]King Saud University; [2]University of Delaware

Quaternary compositions based on Copper-Zinc-Tin-Sulfide/Selenide (CZTS/CZTSe) are promising alternatives to Cu-In-Ga-S-Se (CIGSSe) in thin film solar cells due to their non-toxic, earth-abundant constituents. Nanocrystals with precise size control and stoichiometry can be synthesized using sonochemical method for subsequent thin film deposition using inkjet printing or spin/dip/paste coating techniques. Using metal salts and large metallic particles (of the order of micrometers) in certain molar ratios, high intensity ultrasonication was carried out at room temperature to facilitate particle deagglomeration and dispersion, controllable reactions and faster reaction kinetics. The effect of processing parameters (precursor solution chemistry, sonication time, annealing conditions, etc.) on the particle morphology and composition was investigated using HR-TEM, FE-SEM and XRD techniques. The band gap energy and electrical properties of the films produced using these nanocrystals were also determined. The preliminary results from solar cells testing using these materials as absorber layer will be presented and discussed.

15:00 Break

15:20

Electrochemical Deposition of High Purity Silicon from Molten Salts: *Geir Martin Haarberg*[1]; [1]Norwegian University of Science and Technology, and Qatar University

Several approaches were tried in order to develop an electrochemical route for producing high purity silicon from molten salts. SiO_2, K_2SiF_6 and metallurgical silicon were used as the source of silicon. Molten electrolytes based on chloride ($CaCl_2$-NaCl) and fluoride (LiF-KF) at temperatures from 550 - 900^oC were used. The electrochemical behaviour of dissolved silicon species was studied. Electrolysis experiments were carried out to deposit silicon. Silicon could be cathodically deposited in molten chloride and fluoride electrolytes. High electrorefining efficiency was obtained for many elements by using a liquid Si-Cu anode. The challenge was to reduce the contents of boron and phosphorus. The energy consumption was estimated to be less than 3 kWh/kg Si. Such a low energy requirement suggests that electrorefining by using repeated steps may be a promising way to produce silicon of solar grade quality.

15:40

Cationic (V, Y)-codoped TiO_2 with Enhanced Visible Light Induced Photocatalytic Activity for Photoelectrochemical Applications: *Matiullah Khan*[1]; Wenbin Cao[2]; Bilal Mansoor[1]; [1]Texas A & M University at Qatar; [2]University of Science and Technology Beijing

To utilize the wide spectrum of solar irradiations, an effective co-doping approach is applied to modify the photoelectrochemical properties of TiO_2 by doping vanadium (transition metal) and yttrium (rare earth element). V and/or Y codoped TiO_2 was prepared using hydrothermal method without any post calcination for crystallization. V, Y codoped TiO_2 exhibited high absorption coefficient with enhanced visible light absorption compared to monodoped samples. All the prepared samples showed pure anatase phase and spherical morphology with uniform particle distribution. It is found that both the doped V and Y exist in the form of substitutional point defects replacing Ti atom in the lattice. The photocatalytic activity, evaluated by the degradation of methyl orange, displays that the codoped TiO_2 sample exhibits enhanced visible light photocatalytic activity. The synergistic effects of V and Y drastically improved the visible light absorption and electron-hole pair's separation leading to the enhanced visible light catalytic activity.

16:00

Enhancement of the Kinetics of Heat Storage by Means of Cellular Metals: *Olaf Andersen*[1]; Jens Meinert[2]; [1]Fraunhofer-Gesellschaft; [2]Fraunhofer IFAM Dresden

High power density heat storage is usually hindered by the low heat conductivity of techni-cally relevant storage materials (i. e. paraffines, zeolites, hydrides). For improved devices, the length of conductive paths within the storage material has to be minimised with as low cost as possible in terms of storage capacity. Moreover, the structure should couple nicely to the heat exchanger architecture. Cellular metals such as foams and fiber structures have been investi-gated with regard to their relevant thermophysical properties and manufacturing routes for suitable heat exchangers and heat storage devices. Additionally, performance results meas-ured in a laboratory environment are given. In particular, it could be demonstrated that it is possible to build simple, fast, and compact fiber-based phase change material storage devices with a heating power of several kilowatts and charging times in the range of a few minutes with negligible degradation in performance over the testing period.

16:20

Economic Technical Solutions for Enhancing the Efficiency of Thermal Solar Water Heating: *Iman El Mahallawi*[1]; Nagwa Khattab[2]; Ahmed Abdel-Rehim[3]; Sayed Akl[3]; [1]Cairo University; [2]National Research Centre; [3]British University in Egypt

In this work we show that there is a great option for enhancing the efficiency of low temperature (< 100 0C) thermal solar heaters by the development of a new economic material based on a commercial locally available black painting (PACEN code 10382 colour 890) modified to be used as a selective absorber material. The results presented in this work show that using nano particles or carbon-nanotubes dispersed polymers causes an enhancement in the total solar energy absorbed by the solar collector (measured by gain in water temperature) by more than 33 % compared to Polyvinyl Alcohol alone, and an enhancement from 34.6% to 52.5% after applying the developed black coating painting loaded with 1% nanographite particles. The obtained results open the door for developing a new generation of building paints based on polymeric based economic selective absorber material dispersed with nanographite particles or carbon nanotubes.

3-5: Computational Approaches towards Mechanical Damage, Environmental Degradation

Wednesday Afternoon   Room: Al Wosail 4
January 14, 2015   Location: Ritz-Carlton Doha

Session Chair: Fodil Meraghni, University of Lorraine

13:30 Introductory Comments

13:40 Invited

Predicting Ductile Fracture Toughness: *Alan Needleman*[1]; [1]Texas A&M University

A fundamental question in the mechanics and physics of fracture is: What is the relation between observable (and hopefully controllable) features of a material's microstructure and its resistance to crack growth? I will report on recent calculations of mode I ductile crack growth aimed at addressing this question in that context. An elastic-viscoplastic constitutive relation for a progressively cavitating plastic solid is used to model the material. A characteristic length is needed, if only from dimensional considerations, to predict fracture toughness and in the calculations this is introduced via a discretely modeled microstructural feature such as the mean spacing of inclusions that nucleate voids or the mean grain size. Measures of crack growth resistance such as JIC and the tearing modulus are related to features of the material's microstructure and the nature of the ductile crack growth process. Implications for developing more fracture resistant microstructures will be discussed.

14:20

Investigation of Damage and Fracture in Two Magnesium Alloys: *Amine Benzerga*[1]; B. Kondori[1]; [1]Texas A&M University

Damage accumulation to fracture is investigated in AZ31 and WE43 alloys. Plastic flow anisotropy is characterized using tensile and compression specimens along six orientations. In-situ measurement of diameter contractions enabled the monitoring of relative volume change and strain ratio evolution. Fracture loci are obtained using round notched bars to quantify triaxiality effects. Microstructural characterization included texture, chemical composition, volume fraction, shape and spatial arrangement of second-phase particles. Image analysis was also carried out on specimens deformed to incipient or complete fracture to characterize voids nucleated at particles and twin-initiated micro-cracks. A micromechanics-based continuum damage model is used to rationalize the main experimental trends. The model has two components: (i) a shape-dependent void growth part dealing separately with particle-induced voids and twin-induced micro-cracks; and (ii) a shape-dependent void/crack coalescence part. Void/micro-crack nucleation is assumed to occur in the early stages of deformation, in keeping with experimental observations.

14:40

Micromechanical Fatigue Visco-damage Model for Short Glass Fiber Reinforced Polyamide-66: Nicolas Despringre[1]; Yves Chemisky[1]; Gilles Robert[2]; *Meraghni Fodil*[1]; [1]ENSAM - Arts et Métiers ParisTech; [2]Solvay Engineering Plastics

This work presents a micromechanical fatigue damage model developed for short glass fiber reinforced PA66. It has been developed to predict the high cycle fatigue behavior of PA66/GF30. The model is based on an extended Mori-Tanaka method which includes coated inclusions, matrix viscoelasticity and the evolution of micro-scale damage. The developed model accounts for the nonlinear matrix viscoelasticity and the reinforcement orientation. The description of the damage processes is based on the experimental investigation of damage mechanisms previously performed through in-situ SEM tests and X-ray micro-computed tomography observations. Damage chronologies have been proposed involving three different processes: interface debonding/coating, matrix micro-cracking and fiber breakages. Their occurrence strongly depends on the microstructure and the relative humidity. Each damage mechanism is introduced through an evolution law coupled to local stress fields. The developed model is implemented using a UMAT subroutine. Its experimental validation is achieved under stress or strain controlled fatigue tests.

15:00 Break

15:20

Crystal Plasticity and Fracture Simulations Using a New 2.5D Dislocation Dynamics Method: *Shyam Keralavarma*[1]; William Curtin[2]; [1]Indian Institute of Technology Madras; [2]Ecole polytechnique federale de Lausanne

The widely used two dimensional discrete dislocation plasticity (DD) model of Van der Giessen and Needleman requires additional so called "2.5D" constitutive rules to model strain hardening, since the forest interaction mechanism is inherently three dimensional. We present a new algorithm for 2.5D simulation of crystal plasticity that incorporates the junction strength and the mean free path for dislocation glide as the only parameters, whose values can be obtained from three dimensional DD simulations. The resulting model predicts the combined strengthening effect of pre-existing obstacles such as precipitates and the forest junctions on the effective flow strength, in agreement with analytical estimates of the same. We show that the model reproduces the correct ranges for the strain hardening rates under multiple slip conditions using periodic cell model calculations. Finally, simulation results are also discussed for the effect of strain hardening at the crack-tip on fracture toughness under mode-I loading conditions.

15:40

Multiparadigm Modeling of Material Safety and Sustainability: Stress Corrosion Cracking: *Tahir Cagin*[1]; Hieu Pham[1]; Amine Benzerga[1]; [1]Texas A&M University

Corrosion is an enormously complex technological problem with major economic impact. The safety and sustainability are the requirements for the operation of structural systems exposed to corroding conditions under mechanical loads. To prevent SCC and to predict the lifetime beyond which SCC may cause failure requires that we understand the mechanisms underlying SCC; i.e. conditions influencing initiation, dynamics, and growth rates of SCC. Hence, the science of SCC provide a rich and challenging set of applications involving simultaneous chemical, physical, and material processes. To optimize the performance of structures and systems in chemically aggressive environments, it is essential to develop multiscale multi-paradigm models based on first-principles for all aspects of SCC including the role of pH, electrochemical potential, material microstructure, temperature, and stress with probabilistic predictions. Here, we will present an approach using DFT, Molecular Dynamics, continuum mechanics and Bayesian statistics as applied to study of SCC in metals.

16:00

Understanding Dusting Corrosion in Iron from Kinetic Monte Carlo Simulations: Oscar Antonio[1]; *Fadwa El-Mellouhi*[2]; Othmane Bouhali[3]; Charlotte Becquart[4]; Normand Mousseau[1]; [1]Universite de Montreal; [2]QEERI; [3]Texas A&M University at Qatar; [4]École Nationale Supérieure de Chimie de Lille

Metal dusting is a severe form of corrosion that occurs when susceptible materials are exposed to environments with very high carbon activities. It results in uniform metal loss and severe pitting observed in many industrial processes, such as steam methane reforming and petrochemical refining. Understanding the mechanism of metal dusting corrosion is primordial to help develop techniques to prevent it, and requires growth models that can simulate it efficiently. Over short time scales, molecular dynamics is an ideal tool for exploring such atomic scale behavior, but due to the very small scale of atomic vibrations and relatively rare transitions between atomic configurations, this method is nearly useless for modeling carbon growth and non-equilibrium behavior. We will propose to use a newly developed Kinetic Monte Carlo (KMC) method called Kinetic-ART (KART) to model the the carbon diffusion in iron over long time scales.

16:20

Analysis of Thermo-Mechanical Rigidity of Continuously Cast Steel Slabs: *Mostafa El-Bealy*[1]; [1]Ain Shams University, (CC)

A new design of air-water mist nozzle "AWM" has been developed to improve the thermal rigidity of continuously cast steel slabs. This is by maximizing of solid shell resistance against thermo-metallurgical and mechanical stresses. The idea behind this design is optimizing the homogeneity degree of cooling pattern between a pair of rolls. The design description of air-water mist nozzle and the effect of nozzle characteristics on its function have been explained. The design description of mist nozzle consists of two main systems where the first one is mixing chamber system and the second is tip and inlet design. The mathematical model of thermal, solidification, solid shell resistance and cooling conditions has been developed. Also, the model can be computed the new concept to examine the micro-quality defined as micro thermo-mechanical rigidity "Mic-TMR".

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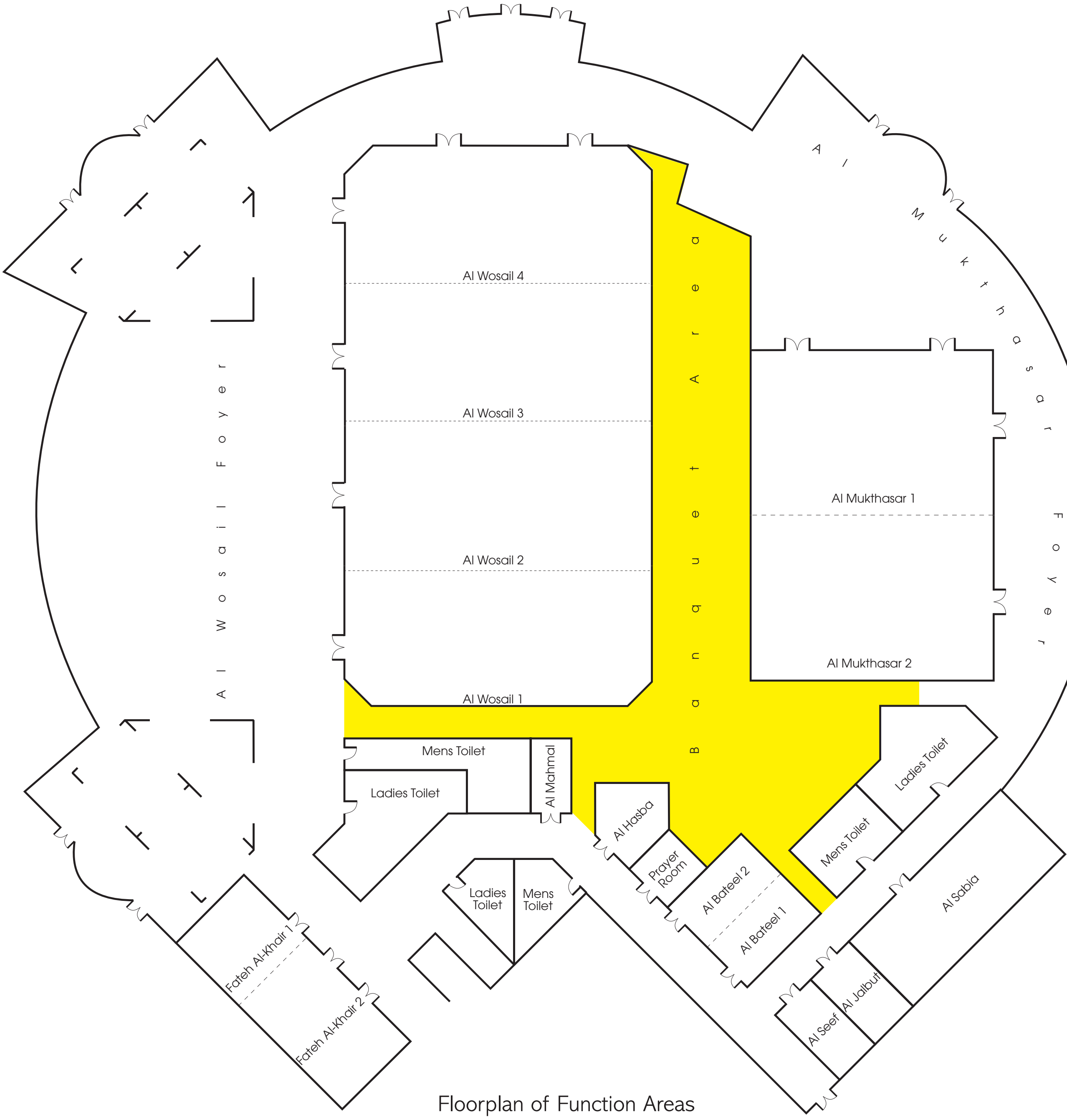
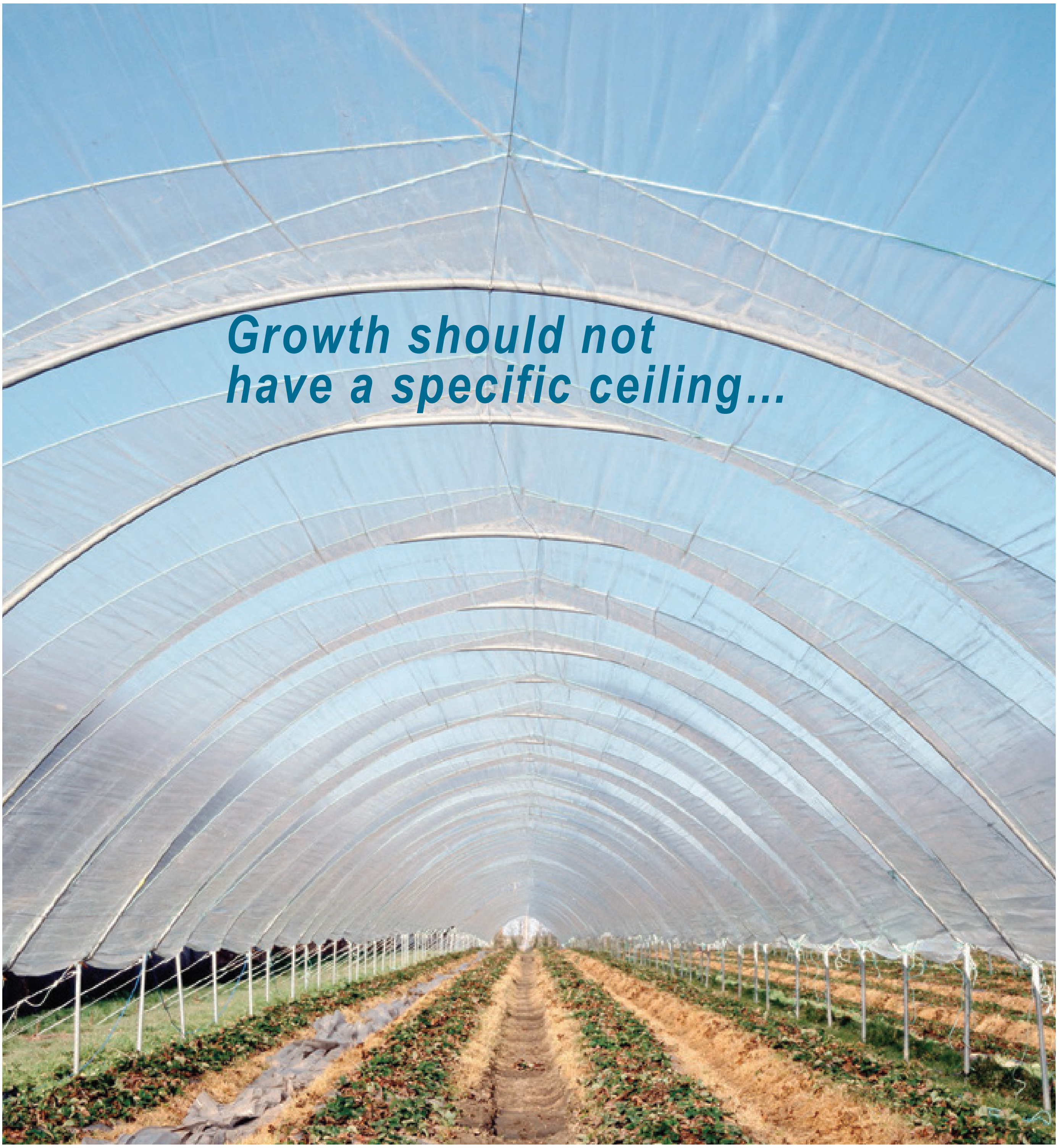
FLOOR PLAN



Floorplan of Function Areas

SCHEDULE AT-A-GLANCE

Sunday, January 11		
16:00 to 19:30	Registration	Fateh Al Khair
18:00 to 19:30	Welcome Reception	Fountain Courtyard
Monday, January 12		
07:00 to 17:00	Registration	Fateh Al Khair
08:00 to 08:20	Opening Remarks	Mukhtassar
08:20 to 09:05	Keynote: Bill Curtin	Mukhtassar
09:05 to 09:20	Break	Al Wosail Foyer
09:20 to 11:20	Session 1-1: Cemenetitious Materials, Composites	Mukhtassar
09:20 to 11:40	Session 2-1: Ferrocaloric Materials	Al Wosail 1
09:20 to 11:20	Session 3-1: Ab-Initio Approaches	Al Wosail 4
11:40 to 13:30	Lunch	Al Wosail 2&3
13:30 to 17:00	Session 1-2: Cementitious Materials Sustainability	Mukhtassar
13:30 to 17:00	Session 2-2: Energy Storage Materials	Al Wosail 1
13:30 to 17:00	Session 3-2: Energy Materials Simulation	Al Wosail 4
15:00 to 15:20	Break	Al Wosail Foyer
15:20 to 17:00	Session 2-8: Lightweight and High Performance Materials I	Mukhtassar
19:00 to 21:00	A Fun Evening Out in Doha (Sponsored by Texas A&M University of Qatar)	Bus departs at 18:30
Tuesday, January 13		
07:30 to 17:00	Registration	Fateh Al Khair
08:00 to 08:55	Keynote: Rustom Hughes	Mukhtassar
08:55 to 09:10	Break	Al Wosail Foyer
09:10 to 11:30	Session 1-3: Multi-scale Characterization and Simulations of Infrastructure Materials	Mukhtassar
09:10 to 11:30	Session 2-3: Nano-Engineered Materials for Energy Conversion	Al Wosail 1
09:10 to 11:30	Session 3-3: Modeling Materials Across the Scales	Al Wosail 4
11:30 to 13:30	Lunch	Al Wosail 2&3
13:30 to 15:20	Session 1-4: Environmental Degradation	Mukhtassar
13:30 to 15:20	Session 2-4: Ferroelectric Materials in Energy Conversion	Al Wosail 1
13:30 to 15:20	Session 3-4: Alloy and Microstructure Design	Al Wosail 4
15:20 to 16:30	Session: Poster Session	Al Wosail Foyer
18:00 to 20:00	Congress Banquet	Fountain Courtyard
Wednesday, January 14		
07:30 to 17:00	Registration	Fateh Al Khair
08:00 to 08:55	Keynote: Dallas Little	Mukhtassar
08:55 to 09:10	Break	Al Wosail Foyer
09:10 to 11:30	Session 1-5: Asphaltic Materials	Mukhtassar
09:10 to 11:30	Session 2-5: Shape Memory Alloys in Energy Conversion	Al Wosail 1
09:10 to 11:30	Session 2-7: Materials Issues in Energy Conversion	Al Wosail 4
11:30 to 13:30	Lunch	Al Wosail 2&3
13:30 to 16:40	Session 2-9: Lightweight and High Performance Materials II	Mukhtassar
13:30 to 16:40	Session 2-6: Photovoltaics and Solar-Thermal Energy Conversion	Al Wosail 1
13:30 to 16:40	Session 3-5: Computational Approaches towards Mechanical Damage, Environmental Degradation	Al Wosail 4
15:00 to 15:20	Break	Al Wosail Foyer


Growth should not
have a specific ceiling...