Vancouver, BC

June 10 - 13, 2019

Final Program

General Information

Nametags: Behind your name tag will be tickets for the student mixer, drink for the poster session

and banquet if ordered

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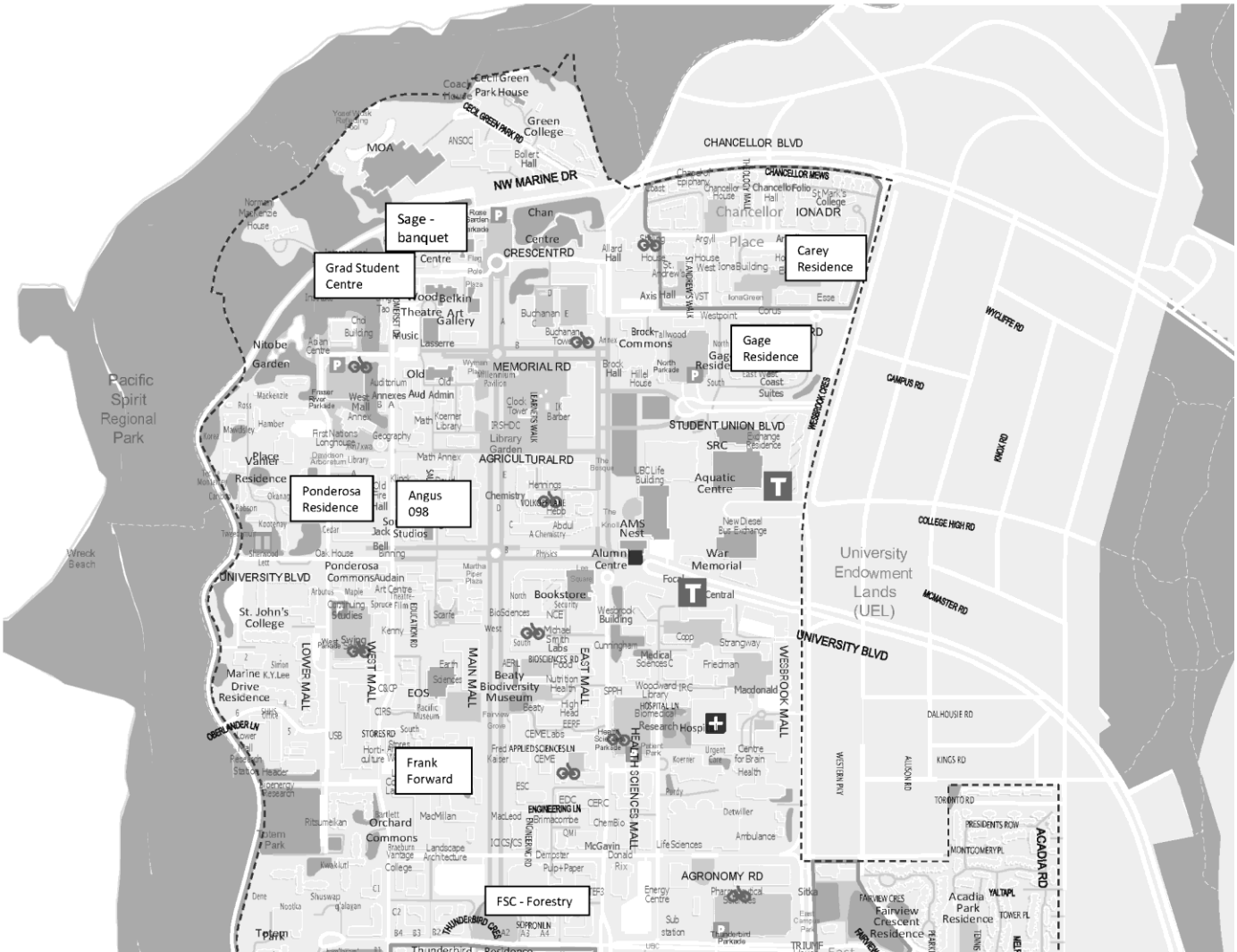
FSC - Forest Sciences Centre 2424 Main Mall (Breakfast, Lunch and Plenary)

FF - Frank Forward Building 6350 Stores Rd (Coffee and Breakout sessions)

Angus - Henry Angus Building 2053 Main Mall (McDonald Lecture)

Sage – PWIAS 6331 Crescent Rd. (Conference Banquet)

Grad Student Centre – Thea Koerner House 6371 Crescent Rd. (Student Mixer)



Monday, June 10

15:00 – 18:00 (FF103) Registration

18:00 – 22:00 (Grad Student Centre) Student Mixer

Tuesday, June 11

8:00 – 9:00 (FSC Lobby) Registration and Breakfast

9:00 – 10:00 (FSC 1005) Materials Chemistry Lecture

The Development of Corrosion-resistant Copper-coated Steel Containers for the Permanent Disposal of High Level Nuclear Waste

David Shoesmith, University of Western Ontario

The proposed long-term management procedure for used nuclear fuel in Canada is disposal in a deep geological repository (DGR) which has multiple barriers to ensure safe isolation and containment. Within this multi-barrier system, the key engineered barrier is a robust container consisting of a carbon steel inner vessel coated with ~ 3mm of copper applied via electrodeposition and cold spray deposition. Once emplaced in the DGR the container will be exposed to conditions which evolve from warm, dry and oxic to cool, wet and anoxic. To justify the use of such a container requires the optimization of the copper coating procedures and a thorough evaluation of the possible corrosion/degradation processes that could occur. This presentation will describe the container design, discuss the key issues involved in achieving a durable coating, and outline some of the key corrosion processes likely to occur on the container.

10:00 – 10:20 (FF 217, 303, 317) Coffee Break

10:20 – 12:00 (FF303) Embury Symposium I

Session Chair: W.J. Poole

10:20 – 10:40

Structural and Chemical Phase Transitions at Grain Boundaries

Chad Sinclair

The University of British Columbia

With the growing range of experimental and simulation tools at our deposal we are expanding our appreciation for the richness of the chemical and structural landscape occupied by grain boundaries. In this talk I will survey our research computational work seeking to unlock some of the kinetic and thermodynamic factors that determine chemical and structural equilibrium at grain boundaries. These results will be linked back to possible effects on plasticity and fracture observed at a macroscopic scale.

10:40 – 11:00

Phase Transitions, Stresses, and the Physical Properties of Solids

(INVITED)

Gary Purdy

McMaster University

David Embury's 80th birthday will be celebrated with a symposium of great breadth as well as depth. This is appropriate: David's interests and contributions have spanned a good portions of the scope of Materials Science. This talk will recount some mutual interests, beginning in the 1960's when David first came to McMaster from US Steel laboratories and continuing to the present day.

A landscape can be defined that includes the origins of different scales of structure, the interactions of applied stress with structure development, and, finally, the resulting physical properties. At one limit, the process of structure development reduces to the study of phase transitions; at the other, to the effects of existing structure on the physical response of the material. The intervening territory, the effects of applied stress on the processes of structure development, is also of interest.

11:00 – 11:20

Precipitation in Aluminium Alloys

(INVITED)

[1]Christopher Hutchinson, [1]Wenwen Sun, [1]Qi Zhang, [1]Yuman Zhu, [2]Ross Marceau, [1]Lingyu Wang, [1]Xiang Gao

[1]Monash University, AUSTRALIA

[2]Deakin University, AUSTRALIA

High strength Al alloys exploit solid state precipitation to tailor their mechanical response. This precipitation requires two ingredients: a thermodynamic driving force and atomic mobility. For a given alloy, the heat treatment temperature is chosen as a compromise between having sufficient driving force for precipitation and sufficient atomic mobility so that the precipitation reaction occurs in a reasonable time frame. It is this compromise that frames the competition between nucleation, growth and coarsening that constrains the possible precipitate distributions and hence mechanical responses.

We demonstrate a new approach to precipitation hardening that does not use thermal treatments. The approach uses small amplitude cyclic plasticity at room temperature as a means of pumping vacancies into the system under conditions of high driving force. The approach can be used as a new processing

route for high strength Al alloys, or as a 'training' routine to improve the high cycle fatigue properties of precipitate strengthened Al alloys. Both examples will be shown in this presentation.

11:20 – 11:40

Opportunities for the Development of Compositionally-Graded Steels

(INVITED)

Bosco Yu, Hamid Azizi, David Embury, Hatem Zurob
McMaster University

Compositionally-graded steels provide an extra degree of freedom for optimizing material properties. Recent efforts to commercially produce graded materials with gradients of substitutional and interstitial elements will be reviewed. The deformation and fracture behaviour of selected compositionally graded materials will be discussed.

11:40 – 12:00 Discussion

10:20-12:00 (FF317) Advanced Characterization of Materials I

Session Chair: G. Miyamoto

10:20 – 10:40

Understanding Materials with Advanced Electron Microscopy

(INVITED)

Gianluigi Botton
Canadian Light Source and McMaster University

Electron microscopes have become very power tools to study the structure of materials at unprecedented resolution. From their invention, these tools have provided essential information on the structure and properties of the broadest range of materials used today in structural and functional applications. However, electron microscopes provide much more than images. In this presentation, the major breakthroughs in the field of electron microscopy of the last few decades will be presented. It will be shown that, in addition to images, electron microscopes provide much more than structural information with techniques such as electron energy loss spectroscopy and scanning transmission electron microscopy. Several examples related to the analysis of nanoscale energy storage and conversion materials, semiconductors and alloys will be presented. This work demonstrates that one can study where atoms are in a solid, or in a defect, with exceptional precision and accuracy so that even the strain field at interfaces, in devices and around defects can be obtained. Examples also show that spectroscopic information on the valence of atoms, even in complex materials such as high-temperature superconductors can be obtained at atomic resolution. The use of complementary characterization tools, such as focused ion beams and 3D-atom probe tomography and various synchrotrons beamlines, highlights the powerful arsenal available to materials scientists and engineers to understand the behavior and properties of materials.

10:40 – 11:00

Material Characterization on VESPERS Beamline at CLS

Renfei Feng
Canadian Light Source

Canadian Light Source is the only synchrotron radiation facility in Canada. VESPERS beamline is a hard X-ray microprobe beamline there dedicated to X-ray micro-diffraction (μXRD), X-ray micro-fluorescence (μXRF), and micro X-ray absorption spectroscopy (μXAS) studies. The beamline offers four widely differing bandwidths, ~0.01%, ~1.6%, ~10%, and fully polychromatic beam, which allows to simplify the Laue diffraction analysis, to optimize XRF excitation, and to enable X-ray absorption spectroscopy measurement. The set of techniques provided by the beamline enables the determination of elements, material phases, and chemical speciations for a local micron-sized area, which is particularly useful for the inhomogeneous sample. The mapping capability is available using both XRF and XRD, especially micro-Laue-diffraction, simultaneously or consequently, to obtain the spatial distribution of elements, phases, and speciations. The beamline has been in operation for more than 10 years. The beamline capabilities, together with some case studies in material characterization, will be presented.

11:00 – 11:20

Materials Research Using Synchrotron: From Good to Better, Impossible to Possible

Feizhou He
Canadian Light Source

Synchrotron light source is a versatile, and often indispensable tool for materials research. Each year, thousands of researchers from Canada and other countries come to the Canadian Light Source, the national synchrotron facility of Canada, to characterize a wide variety of materials, including engineering materials, nano-catalyst, biological materials, and novel electronic materials, etc. This talk will provide an overview of the research activities at a synchrotron facility, with a few research highlights, such as non-destructive micro-CT imaging, in-situ measurements of battery materials in operation, and understanding the properties of materials at fundamental level. These advanced imaging, spectroscopic and diffraction techniques are either impossible or very difficult without a synchrotron source. The researches enabled by synchrotrons are constantly pushing boundaries of materials science and engineering.

11:20 – 11:40

Study of the Formation of Adiabatic Shear Bands in AZ31 Magnesium Alloy During Impact

Francis Tetteh and Solomon Boakye-Yiadom
York University

Materials and structures are being considered for use in increasingly extreme conditions with respect to extremes in applied pressures, strain-rates, strains and temperatures. These mechanical extremes and high rate of deformation events include car frames during collisions, crush tubes under impact, ballistic impacts (a projectile hitting a target) and shock/impulsive loading. During deformation under these extremes, the materials and structures rely on their ability to distribute load as they deform plastically via nucleation and propagation of defects, as well as activation of failure mechanisms such as strain localization, crack nucleation and growth in order to accommodate the excessive deformation. Magnesium (Mg) is the lightest structural metal used for lightweight applications due to its low density. However, mechanism of deformation and damage accumulation in Mg alloys during high strain rate

loading conditions such as impact are not fully understood. In this study, AZ31 Mg alloys were subjected to high strain rate loading using the Direct Impact Hopkinson Pressure Bar (DIHPB) under different impact momentum to understand the mechanism of strain localization and formation of adiabatic shear bands. The pre- and post-impact AZ31 Mg alloys were mounted, ground polished and etched followed by microstructural characterization techniques including electron microscopy and microanalysis to determine where Adiabatic Shear Bands (ASBs) nucleate within the microstructure and the dominant damage mechanisms under dynamic shock loading. Microstructural analysis indicates that at high strain rates, ASBs evolved with fine narrow regions prolonging along regions of propagating cracks. Microhardness measurements indicated that the ASBs regions were hard and brittle compared to regions away from the ASBs. In addition to the evolved ASBs and cracks, it was observed that there was selective grain refinement both within the regions of the shear bands and away from the ASBs. Thus, there were regions with some grains extensively refined surrounding grains that had not undergone any extensive refinement. In addition, high volume fractions of twins and micro twins evolved both within the regions of the ASBs and away from the ASBs. It is inferred that the crystal structure and activation of slip systems in addition to mechanical grain refinement result in the structure of the evolved ASBs.

11:40 – 12:00

Advanced Characterization Techniques for Understanding the Effect of Non-framework Cation Field Strength on the Structure of (Na-Mg) Aluminosilicate Glasses

Harisankar Nellattukuzhi Sreenivasan, Paivo Kinnunen, Elijah Adesanya, Minna Patanen, Anu M. Kantola, Ville-Veikko Telkki, Marko Huttula, Wei Cao, John L. Provis, Mirja Illikainen
Oulu University, Finland and University of Sheffield, United Kingdom

Aluminosilicate glasses are materials with wide technological applications. Due to their desirable properties, they are commercially used as glass-ceramics, container glasses, liquid crystal display (LCD) substrates, optical and laser materials, and so on. They are also considered as potential supplementary cementitious materials with reduced CO_2 emissions when compared to ordinary Portland cement (OPC). Considering significance of aluminosilicate glasses, there is a greater need to understand their structure. One of the key parameters affecting their structure is the cation field strength (defined to be cation charge divided by the square of the cation–oxygen ionic bond distance) of the non-framework cation. Here in this work, we study the effect of cation field strength of non-framework cation (Na and Mg in this case) on the structure of $((Na_2O)^2$-x (MgO)x $(Al_2O_3)^{0.5}$ $(SiO_2)^{2.5})$ glasses using advanced characterization techniques like including Si K-edge EXAFS/XANES, 27Al MAS NMR, 29Si MAS NMR, XPS, XRD, and SEM. Results indicate that due to the high cation field strength of magnesium over sodium, magnesium is preferred for network modification, while sodium is preferred for charge compensation. The aforementioned preference among non-framework cations is found to have a crucial role in determining glass structure.

10:20-12:00 (FF217) Applied Electrochemistry and Degradation of Materials I

Session Chair: E. Asselin

10:20 – 10:40

Multi-Layered Steel as an Alternative to Ferritic Stainless Steel for Automotive Exhaust Systems

(INVITED)

Joey Kish
McMaster University

A feasibility study is being conducted to benchmark the corrosion performance of a multi-layered steel (chromized IF steel) against ferritic stainless steels currently being used to fabricate automotive exhaust systems. Comparative corrosion testing in both simulated "cold-end" and "hot end" environments is being performed for this purpose. The "cold-end" corrosion performance concerns the pitting corrosion susceptibility when exposed in atmospheric near-neutral saline (external) and acidic condensate (internal) environments. The "hot-end" corrosion performance concerns the high temperature wet oxidation susceptibility starting simply with dry versus wet hot air exposures. Relative differences in the corrosion performance observed in both cases are being linked to differences in the starting surface microstructures and how these surfaces evolve during exposure, as revealed by scanning electron microscopy (and associated techniques) coupled with Auger electron spectroscopy. The results are discussed within the context of the suitability of multi-layered steels for this application and pathways for future multi-material development.

10:40 – 11:00

Effects of Stress Intensity Factor and Loading Spectra on Intergranular SCC Crack Growth

Hamid Niazi, Hao Zhang and Weixing Chen
University of Alberta

We studied the effects of different loading waveforms on the first and second stages of High pH Stress Corrosion Cracking in pipeline steel. Obtained results revealed that the correlation between loading spectra and crack growth kinetic is highly depended on the magnitude of the stress intensity factor ahead of the crack tip and the load frequency. When Kmax<KISCC, crack propagation relies on underload (low-R ratio) cycles. These cycles set the stages for new intergranular crack initiation followed by crack coalescence on the exposed surface to concentrated carbonate/bicarbonate environment. Under this condition, crack growth increased three orders of magnitude compared with minor (low-R ratio) cycles. Conversely, the crack growth rate is less sensitive to loading spectra when Kmax>KISCC, and it is in the order of 10^{-7} mm/s. However, underload cycles retard the crack growth due to crack closure effect, decrease in mean stress intensity factor and reduce in strain rate.

11:00 – 11:20

Evaluation of FBE and HPPC Coatings using a Modified Cathodic Disbondment Test

Min (Mina) Xu and Edouard Asselin
The University of British Columbia

To compare the performance of two pipeline coating systems, i.e., fusion bonded epoxy (FBE) and high-performance powder coating (HPPC), in both acidic and alkaline environment, a modified cathodic disbondment test (CDT) was designed and applied. In this modified CDT, the electrolyte pH was controlled at specific values (0, 1, 4, 7, and 12). Via electrochemical impedance spectroscopy as well as monitoring of the coating thickness, it was revealed that the thicker HPPC coatings tend to slow the migration of water and ionic species through the coating and show less disbondment than FBE over the entire pH range studied. For both coating systems, a clear correlation between their disbondment radius and the overpotential (a potential difference between the applied cathodic potential and measured open circuit potential) was observed. The present study suggests that a more negative cathodic potential is needed to reduce coating disbondment at near neutral pH condition.

11:20 – 11:40

Corrosion Behavior of Hot-dip Galvanized Steel in Simulated Soil Solution: A Statistical Analysis

Davood Nakhaie and Edouard Asselin
The University of British Columbia

Hot-dip galvanized steel is often used in the electric power utility industry for power transmission and distribution structures because of its service life performance in many atmospheric and underground conditions. Soil corrosion of galvanized steel lattice towers installed in British Columbia, Canada, is of significant technical and economic importance. In the present study, a full two-level factorial design was employed to assess the relative significance of the possible influencing factors on the soil corrosion of galvanized steel. A series of corrosion experiments were performed in simulated soil solution prepared to represent some aspects of British Columbia's soil and climate conditions. The corrosion current density was the model's response. The influence of chloride, sulfate, bicarbonate, citric acid concentration and temperature was evaluated using statistical analysis of the results. ANOVA was employed to analyze the statistical significance of the results. ANOVA showed that the model is significant, while the curvature is not, suggesting that the model accurately fits the data, hence can reliably be used to interpolate the response. It was found that temperature, citric acid and chloride are individually significant. Temperature/citric acid and temperature/chloride interactions were also found to be significant.

12:00 – 13:00 (FSC Lobby) Lunch

13:00 – 14:20 (FF303) Embury Symposium II

Session Chair: C.W. Sinclair, D. Wilkinson

13:00 – 13:20

Understanding the Fracture Behaviour of Advanced High Strength Steels Through the Application of in situ Methodologies

(INVITED)

David Wilkinson, Javad Samei, Linfeng Zhou, Diyar Salehiyan and Concetta Pelligra
McMaster University

The damage processes that lead to fracture in materials with multi-phase microstructures, such as advanced high strength steels, are complex. A full understanding of the underlying phenomena requires a careful assessment of the strain partitioning amongst the phases and across the material, how the microstructure evolves with strain and how damage, in the form of voids and microcracks, nucleates and grows. This can only be accomplished by applying a range of methodologies, including microscopic digital image correlation (μ-DIC), x-ray computed tomography (XCT) and x-ray diffraction, all of which can be tracked as deformation proceeds. This is supplemented with nanonindentation and electron back scattered diffraction (EBSD). The rich database that results from such studies provide key insights into the underlying mechanisms. When coupled with models for deformation and damage approaches

to developing damage-tolerant microstructures can be developed. I will illustrate this with examples from several dual phase (DP) and Quench and Partitioning (QP) steels.

13:20 – 13:40

Temperature Induced Softening Effects during High Rate (10^3 s^{-1}) Fracture of Ultra High Strength Steel Sheets

(INVITED)

Armin Abedini, Cliff Butcher, Michael Worswick
University of Waterloo

The effect of strain rate (up to 10^3 s^{-1}) on the fracture of hot stamped, ultra-high strength steels (UHSS) used in automotive applications is examined. The fracture behaviour of the materials under quasi-static conditions is relatively well understood, at least under monotonic strain paths, with fracture *loci* often expressed in terms of fracture strain as a function of stress triaxiality and Lode parameter, for example. The effect of deformation rate on fracture strain is not well established, however, and it is not clear whether fracture strain increases or decreases at elevated strain rates for a given stress state. At dynamic rates, the plastic work that is converted to heat does not have sufficient time to fully dissipate from the deforming area, resulting in significant temperature rise and thermal softening. This effect is amplified with increases in strength due to the higher rate of plastic work. Thus, the roles of strain rate and local temperature rise and their complex thermo-mechanical interactions need to be better understood for UHSS.

The current work considers dynamic fracture of hot stamped Usibor® 1500-AS, Ductibor® 1000-AS and Ductibor® 500-AS with nominal tensile strengths of 1,500, 1,000 and 500 MPa, respectively. Coupon-level miniature shear and plane strain notch tension specimens were adopted to study the influence of stress triaxiality and strain rate on hardening behaviour and fracture strain. *In situ* digital image correlation techniques are applied with high speed optical imaging to measure fracture strain, while high speed thermal measurements are used to characterize temperature rise during elevated rate testing. Measured fracture strains are extracted as a function of stress triaxiality for each strength level at quasi static and dynamic rates.

Elevated strain rate can promote increased fracture strain under tensile dominated triaxiality conditions, whereas significant temperature rise and adiabatic shear localization may be operative under high strain rate shear loading, leading to earlier onset of fracture, at least in terms of macroscopic (far-field) strain measurements. The effect of material strength on temperature rise and the resulting high strain rate fracture is examined.

13:40 – 14:00

Thermodynamic Modelling of Stacking Fault Energy in Fe-Mn-C Steels for Alloy Design and Mechanical Property Predictions

(INVITED)

Kevin P. Boyle
CanmetMATERIALS

Many technologically important steels are based on the ternary Fe-Mn-C system, including transformation-induced plasticity (TRIP) steels, twinning-induced plasticity (TWIP) steels, Hadfield steels and some third generation advanced high-strength steels. The utility of these steels largely derives from

the ability to influence their operative deformation mechanisms and work hardening behaviour through alloy modification. Alloying may critically impact stacking fault energy (SFE), which can be related to the dislocation and austenite phase stability and to the resulting work hardening behaviour. In order to develop work hardening models which are informed by alloy chemistry, the current status of thermodynamic modelling of SFE in Fe-Mn-C using the CALPHAD method is critically assessed. Particular attention is given to the influence of magnetic ordering, the thermoelastic constants, grain size and the surface energy of the stacking fault. Experimental results from the literature are also assessed in order to obtain a more consistent data set for comparison with the modelling results. Our assessment leads to an updated mapping of alloy chemistry and temperature to SFE. The significance of the results with respect to the operative deformation mechanisms and work hardening in Fe-Mn-C steels will then be discussed.

14:00 – 14:20 Discussion

13:00-14:20 (FF317) Advanced Characterization of Materials II

Session Chair: G.Botton

13:00 – 13:20

Solute Clustering and its Hardening Effect in Ferrous Alloys

(INVITED)

Goro Miyamoto and Tadashi Furuhara
Tohoku University

In the nitriding of ferrous alloys containing strong nitride forming element (M), it has been recognized that surface hardening occurs by precipitation of fine nitrides. The present authors directly observed that surface hardening in the nitriding of Ti or V-added specimens occurs not by the precipitation of stable alloy nitrides but by meta-stable mono-layer M-nitrogen(N) clusters by means of high resolution transmission electron microscopy. On the other hand, clustering was not observed in Al or Cr-added specimens. Those clustering and precipitation behaviors can be understood by M-N interaction in bcc phase, which induces phase-separation between M-N rich and poor regions in bcc lattice. Furthermore, in nitriding of ternary alloys containing cluster-forming and non-forming elements, such as Fe-Al-(V, Ti) alloys, V-N clustering induces nucleation of AlN particles and refines distribution of them, which results in significant surface hardening. This indicates pre-cursor solute clustering can be used to control precipitation reaction in ferrous alloys.

13:20 – 13:40

Comparative Studies of the Effect of Warm and High Rolling Temperatures on the Microstructure and Texture of API X70 Pipeline Steel

Joseph Omale and Jerzy Szpunar
University of Saskatchewan

The evolution of microstructure and texture of API 5L X70 pipeline steel after warm and high temperature rolling has been studied using X-ray diffraction and electron backscatter diffraction (EBSD). EBSD investigations revealed that the microstructure after the rough rolling stage consist of coarse large-grained ferrites. The warm rolled showed mainly deformed and elongated ferrites in the rolling direction while high temperature rolled specimen showed recrystallized and equiax polygonal shaped ferrite grains. EBSD investigations confirmed that both recovered and deformed grains were mostly

dominant at warm rolled specimen while high temperature rolling produced higher fraction of recrystallized grains with few deformed and recovered grains. X-ray macro-texture measurement showed that the finish rolling temperatures played a key role in the development of the texture.

13:40 – 14:00

In situ Electron Microscopy Study of the Structural Evolution of Nanostructured Palladium during Electrodeposition

Jie Yang, Leyla Soleymani and Gianluigi A. Botton
McMaster University

Palladium nanostructures are widely used in applications related to biosensing and energy conversion. The functionalities of these materials are highly dependent on the morphology and size distribution of the nanostructures. To further understand the mechanism of palladium nanostructure formation under various electrochemical conditions, in situ scanning transmission electron microscopy (STEM) has been applied. In this work, the effect of a supporting electrolyte (HCl) on palladium deposition has been studied. A liquid cell was used inside a TEM and the electrochemical response and structural evolution of palladium particles were simultaneously acquired. In situ cyclic voltammetry and chronoamperometry were performed to study the palladium/hydrogen co-deposition and the effect of chloride ions on palladium structure formation. It was found that during in situ cycling adding HCl enhanced aggregation and detachment of deposited palladium, corresponding to the characteristics of hydrogen adsorption/absorption/evolution and desorption. Furthermore, under the electrodeposition potential at which hydrogen adsorption/absorption occurred, porous and non-spherical structures were formed. Through this work we have shown that the in situ TEM technique provides direct experimental evidence of intermediate products during the early stage of electrochemical processes in their native environment, which gives insights into development of nanostructured materials by tuning electrodeposition conditions.

14:00 – 14:20

Analyzing the Fracture Behaviour of Tool Steels in Various Stress Triaxialities

Alexandra Rose, I. Sari Sarraf, R. Marentette, A.T. Alpas, D.E. Green
University of Windsor

The wear of trimming dies causes scratches, burrs, reduced edge stretchability and slivers in trimmed parts. Thus, predicting the useful life of tool steels such as D2, a high chromium, high carbon steel, through numerical simulation can help to improve part quality. Besides compression tests, a range of mechanical tests with different stress triaxialities are required to fully characterize the dominant damage mechanisms in tool steels. In this study, uniaxial tension, shear and compression tests were conducted using miniature tension, miniature shear, and cylindrical compression specimens. Digital image correlation (DIC) was used to measure strains. Scanning electron microscopy (SEM) was used to characterize the fracture surfaces of test specimens. Although some plastic deformation was observed in compression tests, apparent facets and cleavage steps showed that the dominant fracture mode is brittle with a small amount of ductile fracture in both tension and compression.

13:00-14:20 (FF 217) Applied Electrochemistry and Degradation of Materials II
Session Chair: E. Asselin

13:00 – 13:20

Using In – Situ Surface Enhanced Raman Spectroscopy to Study the Effect of Triazine-Based H_2S Scavenger on the Film Composition and Cracking of Carbon Steel

(INVITED)

Vinicio Ynciarte Leiva and Brendy Rincon Troconis
The University of Texas at San Antonio

The common practice used to reduce the concentration of hydrogen sulfide in the hydrocarbon production fluids is to inject a hydrogen sulfide scavenger into the gas transmission line. However, failures in the form of stress corrosion cracking (SCC) of steel pipes have been reported when using certain triazine based scavengers. One of the most frequently used H_2S scavenger triazine is hexahydro-1,3,5-tris(hydroxyethyl)-triazine, which is a monoethanolamine derived triazine (MEA-triazine). Its reactions with H_2S are well documented. One mole of triazine will generally react with two moles of H_2S from the gas stream and liberate two moles of amine. The MEA by-products that form during the scavenging process, have been hypothesized to cause SCC.

A vast amount of information is available in regards to the corrosion problems associated to MEA-CO_2 and MEA-H_2S sweetening reactions throughout the years. However, the corrosive effects of MEA-triazine byproducts is still unknown. In addition, there is no in-situ study related to this topic. Based on the literature, it is suggested that SCC is governed by corrosion processes and specifically by a possible transition from a passive surface to an active surface. This transition is a complicated function of acid gas concentration (CO_2/H_2S) and amine adsorption. There are several possible mechanisms by which cracking can be induced. First, a reduction in H_2S content could reduce the semi-protective iron-sulfide film, thus changing the nature of the active/passive transition and making cracking more likely. Second, specific adsorption of amines onto the surface of the steel could result in a change in the active/passive transition. Third, the reaction of MEA with CO_2 could form a combination of carbamate, bicarbonate, and carbonate, which could result in alkaline carbonate stress corrosion cracking. Therefore, characterization of the MEA/H_2S/CO_2 reaction process, the adsorption of amines onto steel, and the electrochemical behavior of the steel are important factors that need to be explored.

In this work, we seek to explore the role of MEA-triazine by-products on SCC of carbon steel. In-situ Raman spectroscopy was used to measure H_2S and CO_2 in the liquid phase, as well as identifying the chemical species present in the test solution prior to and following the scavenging process. Surface Enhanced Raman spectroscopy was utilized to measure specific adsorption of amine by-products on the steel, as well as, changes in the surface film composition based on previous electrochemical studies. Finally, slow strain rate testing was performed to evaluate SCC susceptibility.

13:20 – 13:40

Evaluation of Material Susceptibility to Hydrogen Embrittlement (HE) Based on Experimental and Finite Element (FE) Analyses

Tuhin Das, Jun Song, Stephen Yue
McGill University

Hydrogen Embrittlement (HE) has been a serious problem for decades in various industries such as aerospace, automotive, oil and gas, fastener etc. HE causes structural metals, including high-strength steels, superalloys and aluminum alloys to suffer premature and catastrophic failures, threatening their

reliability and durability. A number of factors such as stress gradients, environment during applications etc. are responsible for HE failure of materials, but material susceptibility could be identified as a critical parameter among them. Therefore, in the present study, a combined approach based on finite element analyses (FEA) and experimental investigations has been adopted to evaluate material susceptibility to HE. The stress coupled hydrogen diffusion finite element study further develops a better understanding of HE failure of materials by addressing the fundamental aspects of the problem.

13:40 – 14:00

Electrochemical Behavior of Metallic Bipolar Plates under Fluctuating Potential Conditions

Yuanyuan Hong, Jingli Luo, Cadien Ken
University of Alberta

Degradation of metallic bipolar plates (BPPs) under the aggressive working conditions is a serious issue impeding the commercialization of proton exchange membrane fuel cells (PEMFCs). Fluctuating potentials generated during the dynamic operating stages of PEMFCs could further degrade its stability and durability. In this study, square wave potential pulses are applied to 316L stainless steel (316L SS) to simulate the potential fluctuations on BPPs. Results show that transient potentials would accelerate the degradation of 316L SS. A larger potential fluctuation generates a much higher frequency of passive film breakdown events than that generated by a smaller potential fluctuation during the cyclic pulse tests, besides, negative current is detected at large potential fluctuation conditions. The Mott-Schottky results suggests that the breakdown events are closely related to the disorder degree of passive films formed at different lower potentials; a protective passive film with less localized states is beneficial to mitigate the dissolution induced by the transient potentials. The development of bipolar plates with less defective surface structure and assessment of its performance under transient potentials are necessary for improving PEMFC stability and durability.

14:00 – 14:20

Effect of Deposit Particle Size on the Corrosion Behavior of API-X100 Pipeline Steel

Hongxing Liang, Rebecca Filardo Schaller and Edouard Asselin
The University of British Columbia

Emulsified droplets containing chlorides can be identified in diluted bitumen (referred to as “dilbit”) pipelines [1]. The chloride droplets coupled with solid deposits may accumulate on the inside surface of dilbit pipelines [2]. The corrosion mechanisms of chloride droplets under paraffin oil [3] and simulated dilbit [4] have been investigated in our previous studies. The solid particles deposited on dilbit pipeline have varying sizes (from less than 40 μm to more than 400 μm) [5]. However, to our knowledge, the effect of sand particle size on the droplet corrosion behavior of steel covered by dilbit has not been investigated.

The particle size where the cumulative distribution is 80% is marked as particle diameter ($d_{v,0.8}$) [6]. The droplet corrosion behavior under 40 mesh ($d_{v,0.8}$, 540 μm) and 200 mesh ($d_{v,0.8}$, 43 μm) silica deposits on X100 pipeline steel covered by simulated dilbit for 24 and 240 h was studied in order to understand the effect of sand particle size. Scanning electron microscopy was used to monitor the corrosion development and profilometry was used to characterize the corrosion depth. After 24 h of exposure, localized corrosion coupled with uniform corrosion occurred for both the 40 and 200 mesh silica deposits. After 240 h, the corrosion under both sizes of silica continued to develop. The maximum penetration rate of localized corrosion under the 40 mesh silica was faster than under the 200 mesh

silica. The corrosion products formed under two types of silica consist of lepidocrocite and hematite, as indicated by scanning electron microscopy and transmission electron microscopy.

References
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[2] J. Been, Comparison of the corrosivity of dilbit and conventional crude, Report of Alberta Innovates Technology Futures, 2011.
[3] H. Liang, J. Liu, R. Schaller, E. Asselin, A new corrosion mechanism for X100 pipeline steel under oil-covered chloride droplets, Corrosion, 74 (2018) 947−957.
4] H. Liang, J. Liu, A. Alfantazi, E. Asselin, Corrosion behaviour of X100 pipeline steel under a salty droplet covered by simulated diluted bitumen, Mater. Lett. 222 (2018) 196−199.
[5] T.D. Place, M.R. Holm, C. Cathrea, T. Ignacz, "Understanding and Mitigating Under-Deposit Corrosion in Large Diameter Crude Oil Pipelines–A Progress Report," Proceedings of IPC2008, paper 64562 (2008).
[6] Y. Liu, Y. Yang, S. Mai, D. Wang, C. Song, Investigation into spatter behavior during selective laser melting of AISI 316L stainless steel powder, Materials & Design, 87 (2015) 797-806.

14:20 – 14:40 (FF 217, 303, 317) Coffee Break

14:40 – 17:00 (FF303) Embury Symposium III

Session Chair: C.W. Sinclair, D. Wilkinson

14:40 – 15:00

Measurement of Back Stress Evolution During Deformation of Dual-Phase Steels

(INVITED)

Doug Boyd, Hossein Seyedrezai, Nick Schwenger, Keith Pilkey
Queen's University

In plastically deformed dual-phase (DP) steels, a directional back stress (τ_B) develops with increasing strain. τ_B contributes significantly to the flow stress and produces a Bauschinger effect, which is important in sheet-forming models for DP steels. In the current study, τ_B has been measured in several DP steels by reverse in-plane shear tests. τ_B initially increases with increasing pre-strain in agreement with the Brown and Stobbs model. τ_B depends strongly on the volume fraction of martensite (M), but is less dependent on microstructural parameters such as ferrite grain size, or M size, shape or spatial distribution. At high pre-strain, τ_B becomes constant ('saturates'), owing to damage (decohesion/fracture) of M particles.

15:00 – 15:20

Crystal Plasticity Modelling of Large Strain Behaviour of Metals

(INVITED)

Peidong Wu
McMaster University

We first introduce various polycrystal plasticity models including the Visco-Plastic Self-Consistent (VPSC) model, the Elastic-Plastic Self-Consistent (EPSC) model, and the Elastic Visco-Plastic Self-Consistent (EVPSC) model, as well as twinning models including the Predominant Twin Reorientation (PTR) model and the Twinning and De-Twinning (TDT) model, with emphasizing on characteristic differences between

these models. Then, we demonstrate that the EVPSC-TDT model is able to capture key features of large strain behaviour of metals under various deformation processes.

15:20 – 15:40

In-situ High Resolution TEM on Deformation Twinning Process in BCC Crystals

(INVITED)

Scott X Mao
Dept. of Mechanical Eng. and Materials Science
University of Pittsburgh

Twinning is a fundamental deformation mode that competes against dislocation slip in crystalline solids. In metallic nanostructures, plastic deformation requires higher stresses than those needed in their bulk counterparts, resulting in the phenomenon that the smaller is the stronger. Such high stresses are thought to favour twinning over dislocation slip. Deformation twinning has been well documented in face-centred cubic (FCC) nanoscale crystals. However, it remains unexplored in body centred cubic (BCC) nanoscale crystals. Here, by using in situ high-resolution transmission electron microscopy and atomistic simulations, we show that twinning is the dominant deformation mechanism in nanoscale bi-crystals of BCC tungsten and tantalum. Such deformation twinning is found to be pseudoelastic, manifested through reversible detwinning during unloading. We find that the competition between twinning and dislocation slip can be mediated by loading orientation, which is attributed to the competing nucleation mechanism of defects in nanoscale BCC bi-crystals. Our work provides direct observations of deformation twinning as well as new insights into the deformation mechanism in BCC nanostructures. In-situ observation on atomic scaled twinning nucleation and growth processes and models in the BCC crystals will be presented.

15:40 – 16:00

The Role of Simple Shear in Material Processing

(INVITED)

Tayfur Ozturk
Middle East Technical University, Ankara 06800, Turkey

Simple shear differs from other forms of deformation with regard to rigid body rotation with which it is associated. This is with the result that while grains in polycrystals normally follow a steady lattice rotation paths, finally reaching the stable end orientations, this is not the case with simple shear. With large associated macroscopic rotations, grains in simple shear are subject to faster lattice rotations, but then reach orientations that are, at best, metastable. Often lattice rotations overshoots these orientations, and thus with continued deformation, the texture is renewed without much further intensification. The absence of truly stable end orientations in simple shear has microstructural implications. With steady lattice rotations in conventional processing, upon reaching the stable end orientations, the alterations soon decelerate, forming a deformed microstructure having cells or subrains of small misorientations. Initially rapid accumulation of dislocations soon slows down reaching often a saturation point. With simple shear, as the texture is renewed, so is the deformed microstructure. As a result, under comparable conditions, cells or subgrains in deformed structure are often smaller and have higher misorientations across them. Clearly with these features, the simple shear processed materials are capable of accommodating more dislocations in their structure. In this work, first we will compare simple shear with pure shear in copper and alpha brass in specially designed experiments. We show that the texture in simple shear is indeed less severe than the pure shear. This

difference while quite noticeable in deformation shows up extremely well in the subsequent annealing. Here the pure shear produces an extremely sharp textures, especially in copper, while the texture in simple shear is rather diffuse. We then make reference to equal channel angular pressing where there is a voluminous data in literature with regard to advantages of simple shear in obtaining high strength in a variety of materials. We then look at cases where the simple shear is brought into operation in conventional processing as an additional process, i.e. strain localization. First example we will dealt with will be heavily rolled brass where the simple shear is operative in the form of shear bands. We will then examine shear band formation in hexagonal metals where the relative hardness of grains is substantially different from each other, often, a cause of strain instability leading to shear band formation. The simple shear is also an aiding process in deformation of multilayer metallic composites especially when the relative hardness of the constituent layers differs from each other by a factor of more than three. The last example we will deal with will be ball milling of elemental powders where the process makes use of simple shear as a way of forming structure with dense dislocations leading to amorphization.

16:00 – 16:20 Discussion

16:20 – 16:40

On the 'Assemblage Mechanics' Associated with Materials Optimization

(INVITED)

Glenn Hibbard

University of Toronto

Our ability to make the best use out of a material system is based on our ability to solve inverse materials design questions and to overcome the associated 'information barriers'. Properties are based on internal dynamics unfolding over a range of different length and time scales, with different material 'things' taken to exist at each different organizational scale [e.g. 1], while an inverse problem is one in which the output (maximizing a specific material performance) is specified and one tries to find the input (an internal material structure) that best meets the optimization criterion [2].

There are several layers to an optimization question. For example, it is not simply enough to know how to build a particular material-structure (the process-structure relationship), one also needs to predict the behavior (the structure-property relationship) and to know precisely which configurations to fabricate from the accessible state space (the optimization step). These are questions involving large parameter spaces with no general solution. In all cases however, the key issue is specifying the internal structure.

In 1976 the MIT Materials Scientist Morris Cohen wrote that 'the structural ladder embodies machinery within machinery within machinery until the mind runs out of comprehension' [3]. Formalizing our understanding of this domain would be a helpful step towards the realizing the potential of materials optimization. Accordingly, this talk will begin from the 1964 book 'Mathematical Foundations of Thermodynamics' by Robin Giles [4]. Giles believed that there were three essential elements to the ideal theoretical framework of thermodynamics: states, the union of states, and the transition between states. We will use a case study approach to examine Giles's idea in the context of multi-scale material dynamics.

[1] G.B. Olson, Science 277 (1997) 1237

[2] M.F. Ashby, Materials Science and Technology February 8 (1992) 102

[3] M. Cohen, Materials Science and Engineering 25 (1976) 3

[4] R. Giles, Mathematical Foundations of Thermodynamics, Pergamon Press (1964)

16:40 – 17:00

Materials Science and Materials Systems

(INVITED)

Mike Ashby (1) and Marc Fry (2)

1) **University of Cambridge, UK**
2) **ANSYS GRANTA Education Division, Cambridge, UK**

Materials science has a long pedigree with roots in the ability to manipulate ceramics (10,000 BC), to alloy metals (2,500 BC) and polymer synthesis (1839). The great development of the second half or the 20th century was the blending of these into a science of materials that enabled links with the pure sciences (physics, chemistry) and the applied (design).

When I joined the Engineering Department in Cambridge some years ago, my remit was to upgrade the teaching of Materials to Engineering students. The students did not respond well to the traditional physics-oriented bottom-up ("atoms-to-artefacts") approach that was then current and had no mental map of the materials universe or tools for selecting them to meet design specifications. Our approach was to reverse the sequence, taking a top-down approach and to provide students with maps of material properties, software to make them and techniques for selection. From a teaching perspective, this succeeded pretty well. What we had not anticipated was the subsequent commercialisation through a University spin-off, Granta Design, now ANSYS GRANTA.

Understanding materials, improving them and developing new ones remain principal concerns of Materials Scientists. But the Granta experience highlighted that the role of the materials expert in the commercial world can be rather different. Materials are traded globally, but the trade is not "free". Material price stability, supply chain security, restrictions and reporting requirements, the environment, circularity and social responsibility can be greater concerns – and it is the job of the materials expert to advise and guide decision-making in the materials-aspects of all of these. A proper scientific understanding of material families and of single materials remain essential core skills, but the ability also to think in terms of materials systems – the context in which materials are sourced, used and re-circulated, and the influence of geopolitical and trade constraints on these, become important too.

Do we teach our students about these broader aspects of materials? Materials courses are already overloaded – adding more layers seems impractical. But at least students should be made aware that these issues exist. A short, well-designed presentation can at introduce them, at the simplest level, in less than 30 minutes. The present talk is a (truncated) version of an attempt to do so.

15:00-16:40 (FF317) Advanced Characterization of Materials III

Session Chair: G. Botton

15:00 – 15:20

Plasmonic Behavior of Wrinkled-gold Surfaces

S. Shayan Mousavi Masouleh, Isobel C. Bicket, Edson P. Bellido Sosa, L. Soleymani, Gianluigi A. Botton

McMaster University

Wrinkled gold surfaces (WGSs) are known for their excellent performance in fields such as electrocatalysis [1]. Recently, WGSs have attracted much attention as they show high surface plasmon (SP) activity. Different experiments have probed the optical and plasmonic properties of WGSs and their potential application in fields such as photoelectrocatalysis [2]. Here we have utilized electron energy loss spectroscopy (EELS) to provide high spatial and energy resolution information on the SP activity. The 2D EELS maps of the SP activity are used to investigate the plasmon behavior and resonance localization.

Based on our observations, these structures provide promising conditions for SPs propagation. WGSs show multiple surface plasmon excitations, making these materials strong candidates for plasmon tuning applications, such as multi-wavelength photocatalysis and broadband absorption devices.
[1] Gabardo, et al. Sci. Rep. 7 (2017): 42543.
[2] Zhang, et al. ACS Nano 5.6 (2011): 4407-4413.

15:20 – 15:40

Atomic and Electronic Structures of Nanoscale Constituents within Solids

Guozhen Zhu
University of Manitoba

The discovery of defects within solids and corresponding properties has been largely accelerated using the state-of-the-art technology in directly resolving their atomic and electronic structures. Herein, I will discuss a few unique nanoscale constituents at dislocations and boundaries. These structures have distinct compositions and atomic arrangements, and cannot be isolated from abutting solids. Within Mg-Gd alloys, a hexagonal pattern of Gd nano-fibers, templated by dislocations, was self-assembled after thermal-mechanical processing. Such patterns are able to regulate the relative activities of basal and non-basal slips, and in turn, improve the strength and ductility of Mg alloys. In addition, interface reconstructions, with a significant atomic rearrangement, was discovered between gold and oxides, which can provide a way to tune the mass transport of oxides and further the synthesis of oxide nanostructures. The deep understanding of such structures will be useful to discover, predict, and design advanced nanostructured materials.

15:40 – 16:00

The Effects of Microstructure and Microtexture Generated During Solidification on Deformation Micromechanism in IN713C Nickel-based Superalloy

Gang Liu and Soran Birosca
The University of British Columbia

Nickel-based superalloy IN713C produced by investment casting method are used for turbine blade of turbocharger in modern vehicles. IN713C alloy possesses good strength, fatigue, creep and high temperature oxidation resistance that make the alloy suitable to be used in harsh service environment such as in the heating part of turbocharger. However, this material suffers from microstructure and microtexture heterogeneity produced during solidification. This microstructure heterogeneity across the component will inevitably give rise to local stress and strain accumulation which may facilitate crack initiation and affect crack propagation. Fatigue, both LCF (Low Cycle Fatigue) and HCF (High Cycle fatigue) are the common failure modes of turbine blade component in turbocharger. The necessity of optimisation of fatigue property for the newly developed turbocharger component parts is becoming critical and a fundamental research for understanding fatigue deformation micromechanism and the influence of microstructure (dendrite structure, carbides / oxidised carbides, grain size, etc.) and microtexture (individual crystallographic orientation, cluster of grains, etc.) is required.
In the current investigation, LCF and HCF fatigue tests are conducted on real turbine blades as well as on bars produced via investment casting. Various microstructure characterisation tools were used to identify the deformation micromechanics during LCF and HCF fatigue conditions. The results showed that in real turbine blades where there are much less casting defects than in the testing bar, the fatigue crack initiated from blade surface and crack propagation process was mainly dominated by oxidation-assisted process with oxidised carbides during LCF test. During the late stage of crack propagation, the

interdendritic area was found to deform differently from the surrounding area to accommodate accumulated strain heterogeneity. Whilst for HCF, facet was initiated from slip planes with the highest Schmid factor and assisted by small porosity in most cases.
As for the fatigue tests conducted on test bars produced via investment casting, the dendrite structure played a vital role in crack propagation mechanism. Based on the observations throughout this study, a concept of 'crack propagation unit (CPU)' was proposed. From this proposed micro deformation mechanism, a new perspective of Hall-Patch effect of small grain size in casting alloys (containing dendrite structure) was further elucidated during both LCF and HCF.

16:00 – 16:20

Effect of Nitrogen Ion Implantation on the Fatigue Life of AISI 1018 and AISI 1045 Carbon Steels

Emmanuel Awoyele, Oguocha, I.N.A., Odeshi, A.G, Bradley, M P
University of Saskatchewan

Plasma ion immersion implantation (PIII) is a surface modification technique, which has proven to improve the hardness, corrosion and wear properties of steel. In this research, the effect of nitrogen ion implantation on the fatigue life and surface properties of AISI 1018 and AISI 1045 carbon steels was studied. All test specimens were implanted using 5 kV bias voltage at a pressure of 15 mTorr for two hours. After that, surface roughness measurement, micro and nanohardness test, X-ray diffraction and X-ray photoelectron spectroscopy were performed to investigate the effect of nitrogen implantation on surface properties of the alloy. Rotating bending fatigue test at 50 Hz was performed on both treated and as-received specimens. Fatigue life of both steels improved at low stress amplitudes but decreased at high stress amplitudes. This effect was more pronounced in AISI 1045 steel compared to AISI 1018 steel. This and other findings from this work would be presented.

16:20 – 16:40

Boiling Heat Transfer During Run-out Table Jet Impingement Cooling of a Stationary Steel Plate

Debanga Kashyap, Vladan Prodanovic, Matthias Militzer
The University of British Columbia

Controlled accelerated cooling on the run-out table of a hot mill regulates the tailored microstructure and mechanical properties of thermo-mechanically controlled processed (TMCP) steels. Hence, a study was conducted to quantify the heat transfer during bottom jet impingement cooling of a stationary steel plate by a planar nozzle. Transient experiments were conducted in a unique pilot-scale run-out table facility under controlled conditions to study the effect of different process parameters (water flow rate, water temperature, jet inclination). From the experimental data, empirical correlations were developed for the heat fluxes as a function of plate surface temperature for two distinct cooling regions viz. impingement zone and parallel flow zone.

14:40-17:00 (FF217) Additive Manufacturing

Session Chair: H. Lebbad

14:40 – 15:00

Fatigue Behaviour of Shot-peened Additive Manufactured Ti-TiB

Liza-Anastasia DiCecco and Afsaneh Edrisy
University of Windsor

The fatigue behaviour of an alpha titanium featuring low amounts of TiB (<1wt% boron) made through an additive manufacturing process termed plasma transferred arc solid free form fabrication (PTA-SFFF), was investigated. The study focuses on the influence of shot peening samples for fatigue improvement, which through microhardness profiling has shown increases in hardness up to 1mm deep in samples. An RBF-200 HT rotating beam fatigue machine was used to conduct rotating-bending fatigue tests. Prior to testing, tensile testing was performed and used as a basis to begin the fatigue tests, which began at 1/3 the ultimate tensile strength. Based on changes in cycles-to-failure with increasing load, S-N curves were constructed. Fracture surfaces were observed and characterized by scanning electron microscopy (SEM) equipped with elemental diffractive spectroscopy (EDS). Modes of failure will be presented, and fatigue behaviour patterns will be summarised.

15:00 – 15:20

Effect of Printing Parameters on Porosity and Micro-Hardness of AISI 316L Fabricated by DMLS

Ali Eliasu, Solomon Boakye-Yiadom, Alex Czenkanski
York University

Metal 3D printing has seen lots of attention in the past few years but has not gotten to the same level as other forms of 3D printing since the mechanical properties of part fabricated by such a process cannot be predicted due to several defects. The major defect that influence the load bearing capability of structural materials is level and nature of porosity present. The porosity is analyzed qualitatively using area fraction of the entire surface of the samples. The porosity levels reduce as the laser energy input increases to a point with the lowest porosity and then starts rising again as the energy density exceeds a certain threshold. Due to the characteristic rapid heating and cooling cycles of Powder bed fusion technologies, fine-substructures are present in the microstructure that increases the hardness within 209HV-241HV which is higher than the hardness of the conventionally manufactured AISI 316L.

15:20 – 15:40

Effect of Heat Treatment on the Microstructural Evolution of 3D-printed WC-Co Cemented Carbides

Joseph Agyapong, Czekanski Alex, Boakye-Yiadom Solomon
York University

Tungsten Carbide-Cobalt (WC-Co) cemented carbides are well known for their high hardness and wear resistance with extensive applications in manufacturing and mining industries. However, this material is very difficult to process using metal-based Additive Manufacturing processes due to high temperature gradients resulting in high residual stresses, cracks, non-equilibrium microstructures and unpredictable mechanical properties. In this study, optimized processing parameters were used to produce WC-Co (87wt%-17wt%) using Selective Laser Sintering. The specimens were heat treated to understand the effect of heat treatment on the microstructural integrity of the specimens by characterizing the microstructural evolution of the specimens during heat treatment using Scanning Electron Microscopy and X-Ray diffraction. Results showed decomposition of W2C and formation of W-C-Co phases in heat treated samples which contributed significantly to the mechanical properties. In short, careful selection

for post treatment of additively manufactured WC-Co needs to be done in order to achieve better and desirable properties.

15:40 -16:00

Characterization of Mechanical Behavior of 3D Printed Composite Parts

Madhukar Somireddy and Alex Czekanski
York University

The present study investigated the mechanical behavior of the additively manufactured (AM) composite parts. Final properties of the printed parts were different from their initial material used for printing, the final properties were influenced by printing process. Reasons for this anisotropy were unveiled during characterization of microstructure of the parts using μ-CT scanner. Printing process parameters such as printing direction, layer thickness affected the orientation of reinforcements, bonding between the extruded fibers, and additionally density of voids in the mesostructure of the parts. Further, mechanics of the printed parts for characterizing their mechanical behavior under mechanical loads were explored. For this, 3D printed composite parts subjecting to tensile and flexural loads were tested, and then the laminate mechanics were employed for characterizing their mechanical behavior. Results confirmed that the mechanics of laminates can be employed for characterizing the mechanical behavior of the printed parts.

16:00 – 16:20

Using Additive Manufacturing to Tailor the Design of Heterogeneous/Graded Architected Cellular Metamaterials

Bosco Yu, Derek Aranguren van Egmond, Dalia Mahmoud, Glenn Hibbard, Ben Hatton, Mo Elbestawi, David Wilkinson, David Embury, Hatem Zurob
McMaster University, University of Toronto

Cellular materials are a class of structural metamaterials that can fill the unattained regions in the "Ashby" material-property-space. Currently, cellular materials used for industrial applications are generally fabricated via traditional manufacturing processes such as casting, forming, and machining. To minimize the processing timing, these cellular structures are normally fabricated to have periodic unit cells (i.e. lattices). While lattices have been able to achieve impressive stiffness-to-weight ratios, their periodicity (or homogeneity) imposes a limitation on their architectural design – which hinders the development of properties such fracture toughness, impact energy absorption, etc. We have recently demonstrated that additive manufacturing can be utilized to produce highly complex heterogeneous or graded architected materials without paying the penalty of higher manufacturing costs. Through experiments and simulation, we have demonstrated that these heterogeneous cellular materials offer superior performance in structural/bio-implant applications that require high fracture toughness, impact resistance/energy absorption, and fatigue strength. Future research opportunities will also be discussed.

16:20 – 16:40

Tantalum Coatings by High-pressure Cold Spray for Wear and High-temperature Corrosion Protection Applications

Jagannadh Sripada and Gobinda Saha
University of New Brunswick

Cold spray is a relatively novel solid-state material additive manufacturing process which works on the principle of transforming kinetic energy into high-impact particle velocity in a supersonic environment. Thin layers of materials are deposited in the form of protective coatings on substrates or standalone 3D freeform object creation. The resulting material structure is dense, and with very limited porosity presence, making the technology attractive for design, develop and test many material systems, including metals, ceramics, cermets, polymers, thermally-dissimilar materials, etc. for corrosion resistance, wear, high-temperature oxidation protection applications. In this research, Tantalum is chosen to work with high-pressure cold spray process and develop thin coatings on AISI 1018 carbon steel substrates to achieve a combined wear and corrosion resistance to substrate. Tantalum is a refractory metal with melting point 2,996oC, and is known for its superior corrosion resistance under extreme conditions, as well as good machinability. In this work, the feedstock particle (Ta) of spherical morphology with size distribution 5-60 micron is used to develop three different coating thicknesses: 100 µm, 200 µm, and 300 µm. HPCS spray process parameters are studied to achieve a desired coating microstructure and deposition efficiency (DE). Results show that the porosity percentage can be suppressed to below 0.1 with the developed parameters, and there appear to be an excellent interfacial bonding between substrate and coatings. From XRD results, it is further confirmed that the coatings are devoid of any noticeable phase formation.

16:40 – 17:00

The Influence of Post-Deposition Heat Treatments on the Microstructure and Mechanical Properties of Wire-Arc Additive Manufactured (WAAM) ATI 718Plus Superalloy

Oluwasanmi Oguntuase and Jonathan Beddoes
University of Manitoba

The influence of post-deposition heat treatments on the microstructure and mechanical properties of wire-arc additive manufactured (WAAM) ATI 718Plus is presented. The application of the standard heat treatment recommended for the wrought ATI 718Plus results in the formation of excessive eta (η) phase particles along the interdendritic spaces. This microstructure degrades the tensile properties of the WAAM alloy and causes a profound anisotropic effect. The use of experimental and thermodynamic simulation tools enable the development of Time-Temperature-Transformation (TTT) diagrams that elucidate the stability and growth kinetics of η phase in the WAAM ATI 718Plus and allow the design of new heat treatments capable of precipitating a moderate amount of η phase. The newly developed heat treatments significantly improve the mechanical properties of the WAAM alloy and also reduce the anisotropic effect.

17:15-19:00 (FSC Lobby) Poster Session

Poster 1:

Quantitative Metallography of Al-Zn-Mg Structural Alloys Manufactured by High Pressure Die Casting process: As-Cast and Solution Heat Treatment Tempers

Chufan Wu and Sumanth Shankar
McMaster University

Al-Zn-Mg alloys are a strong candidate in the structural automotive industry for lightweighting opportunities due to their high strength-to-weight ratio. The poor castability of these alloys have been significantly improved with the development of new series of these alloys to enable sound net shaped castings using the high pressure die casting (HPDC) process. Using samples from structural components

cast by HPDC, extensive quantitative metallography was carried out, both in the as-cast (F) and solution treated (T4) temper conditions. Light optical microscopy, SEM (with EDS) and TEM were used in the quantify primary grains, secondary phase and precipitation phases during natural ageing and heat treatment. Based on the results, a discussion on the ability to cast these alloys in to net shaped components is also presented.

Poster 2:
Hot tearing in Net-Shaped Castings of Structural Aluminium Alloys

Amanda Maia Aguiar, Kumar Sadayappan, Xiaochun Zeng and Sumanth Shankar
McMaster University
CanmetMATERIALS

Hot tearing is a defect that occurs during solidification of a casting. Several experimental models have been proposed for hot tearing in DC castings, however, experiment models in net-shaped castings are still a subject in the study. A quantitative hot tearing and a unidirectional solidification experiment were performed on structural aluminum alloys, such as B206 and Al-Zn-Mg family (with various levels of Zn and Mg) in order to develop experimental models that support net-shaped casting. Experiments on hot tearing mould and on unidirectional solidification were done. The three datasets obtained, a transient temperature, loading and displacement curves were used to derive quantitatively stress and strain and also, related with the cooling curve obtained from the unidirectional solidification and microstructural analysis from both experiments to measure hot tearing susceptibility as a function of alloy composition.

Poster 3:
Directionality of Strain Aging Effect in Ultra Low Carbon Steels

Wendel Melo
The University of British Columbia

The strain aging effect in ultra low carbon steels is well-understood when the material is deformed in the same direction before and after aging. When the direction after aging is different to that before aging, significant differences are observed. These differences are poorly understood. In the present work the effect of strain aging in ULC steels was analysed through experimental work. The strain aging effect of ULC steels was studied for two different deformation histories: Pre-deformation (tension) + final deformation (tension) and pre-deformation (cold rolling-plane strain) + final deformation (tension). A finite element model has also been developed so as to predict the Lüders band formation.

Poster 4:
Contribution of Intragranular Misorientations to the Rolling Textures of Ferritic Stainless Steels

Arthur Despres, M. Zecevic, Ricardo Lebenshon, Chad Sinclair
The University of British Columbia
Los Alamos National Laboratory

Deformation textures of polycrystalline materials are to a first order resulting from the average rotations of grain orientations, but there is increasing evidence that intragranular misorientations play a

role. To investigate this phenomenon, samples of ferritic stainless steels having different grain shapes were cold rolled and their macro- and micro-texture measured as a function of the processing and microstructural parameters. The experimental results were compared with the Grain-Fragmentation Visco-Plastic Self-Consistent model. It is shown that intragranular misorientations exert a significant influence on the texture strength, but also on the relative development of - industrially important - texture components. We show that this second aspect comes from the anisotropy of intragranular misorientations, which helps to distinguish between stable and metastable orientations.

Poster 5:

Sealing Design and Sealing Performance Analysis of One-way Valve Oil Docking Device

Haixia Gong, Tang Wei, Cheng Yanyan
University of Alberta
Harbin Engineering University

One-way valve oil circuit docking device is one of the various forms of hydraulic oil circuit docking in underwater switching system. Spring and sealing ring are the key parts to determine its sealing performance. The forces acting on the two sides of the spring designed with 1Cr18Ni9Ti as spring wire material during the butting process are analyzed. The analysis results show that the spring can realize the oil-line docking of the one-way valve. The Mooney-Rivlin model of NBR is established. The deformation and contact stress of the sealing ring with NBR as sealing material under different working conditions are analyzed. The sealing ring with NBR as sealing material can meet the sealing requirements. The material design of spring and sealing ring is of great significance to the study of one-way valve oil circuit docking device, which can improve the success rate of docking and lay a foundation for future design.

Poster 6:

Effect of Mg and Si Content on the Microstructure and Hemming Performance of Al-Mg-Si Alloys

Zhenguo Li
The University of British Columbia

Al-Mg-Si alloys used for automobile are delivered to manufacturer as semi-finished products. The products are usually shaped in the T4 or T4P temper prior to the final bake-paint process to gain high strength. In the forming route, hemming operation is the primary practice used to joining of outer skins to inner sheet panels because it is performable easily and environmental friendly. However, the outer skin undergo severe 180º edges bending during hemming process which quite often results in cracking or complete tearing of the bend surface, which restricts the further application of the hemmed products. The microstructures and hemming performance of AA6014 alloy sheets in T4P temper were studied in this work by means of atom probe tomography, scanning electron microscopy and three-point bend test. It was found that the Mg and Si content is the main parameter controlling the hemming performance through the amount of the precipitated co-clusters in T4P temper. The hemming performance significantly decreased with increasing the Mg and Si content. Cracking was initiated by formation of strain localization in the form of shear bands during hemming process.

Poster 7:

Microstructure and Fracture Behaviour of the Heat Affected Zone in Line Pipe Steels

Madhumanti Mandal[1], Warren J. Poole[1], Matthias Militzer[1], Laurie Collins[2]

[1] The University of British Columbia

[2] Evraz Inc NA, Regina

Low carbon micro-alloyed steels are used for line pipe applications as they combine high strength and acceptable fracture toughness with good weldability. During welding, the strength and fracture toughness of the material in the heat affected zone (HAZ) is potentially degraded. Using a Gleeble thermomechanical simulator, bulk microstructures were produced that are representative for the HAZ in gas metal arc welding. Here, the first weld pass produces a bainitic microstructure that is characteristic of the coarse-grain heat affected zone (CGHAZ) and the second weld pass involves intercritical annealing of this region (ICCGHAZ), producing martensite films along the prior austenite grain boundaries. The effect of the intercritical austenite fraction and the resulting martensite-austenite constituents on the ductile-brittle transition temperature has been quantified. EBSD and fractography studies have been conducted to correlate the fracture behaviour with the microstructural features. Finally, the role of carbon content on crack propagation has been considered for ICCGHAZ microstructures.

Poster 8:

Fatigue of Dissimilar Aluminum Alloy Friction Stir Spot Welds

Brad Diak, Jessica Generoso, Adrian Gerlich

Queen's University

University of Waterloo

Future light-weight automobile manufacturing will utilize a variety of light-weight materials that need to be joined in the final structure. Current aluminum intensive vehicles join different alloys by riveting since traditional welding of aluminum is difficult. The current work investigates dissimilar aluminum alloy lap joints made by refill friction stir spot welding of 6XXX and 7XXX aluminum alloys. The high cycle fatigue behaviour of the spot weld was characterized at loads, Lmax, less than the yield load, a load ratio, R=0.1 and frequency of 5 Hz using a servohydraulic Instron test frame. The results followed a power law relationship, Lmax=A (logN)^b, where the Basquin-like slope, b ranged from -0.20±0.02 to -0.30±0.03 depending on the alloy stack-up order. Select samples were analyzed by optical microscopy to investigate the origin, growth and propagation of the crack leading to failure. A comparison of relative crack growth will be presented.

Poster 9:

3D Phase Field Simulation Study to Predict the Recrystallized Texture after High-temperature Axisymmetric Extrusion

Khajezade A.[1], Poole W.J.[1], Militzer M.[1], Greenwood M.[2]

[1]The University of British Columbia

[2]CanmetMATERIALS

As the use of aluminum extrusions has increased in automotive applications, the role of crystallographic texture after extrusion has increased in importance. In many cases, recrystallization occurs immediately after the large deformation of extrusion and the prediction of the recrystallization texture is of interest. In this study, recrystallization from a deformed state is studied by utilizing phase field simulations. A 3D statistically representative deformed microstructure is produced using two orthogonal sections from EBSD analysis of an non-recrystallized alloy. This microstructure is used as an input for a multiphase field

model to simulate sub-grain growth. Here, the anisotropy of sub-grain boundary energy and mobility are incorporated by the Read-Shockley and Huang-Humphrey's relationships, respectively. The recrystallization texture obtained from the phase field simulation is compared with the experimentally measured texture by comparing the corresponding orientation distribution functions.

Poster 10:
Microstructure Evolution in Al-Mg-Si alloys During Porthole Die Extrusion

Andrew Zang[1], Warren J. Poole[1], Nick Parson[2], Mei Li[3]
[1] The University of British Columbia
[2] Rio Tinto Aluminum, Jonquière QC
[3] Ford Motor Company, Dearborn, Michigan, USA

There is currently interest in using extruded hollow aluminum profiles in automotive applications such as crush tubes and side rails. Hollow profiles can be produced using porthole dies where the material is separated into several flow channels (ports) prior to coming back together in the weld chamber. In this study, the microstructure evolution during extrusion was examined. Specifically, the material flow through the porthole creates inhomogeneity in the microstructure of the final extruded product. The resulting variation in microstructure and crystallographic texture was studied using electron backscatter diffraction (EBSD) and the local stress-strain response was calculated using the visco-plastic self-consistent (VPSC) polycrstal plasticity code. For alloys where recrystallized is suppressed during extrusion, it was found that the material near the weld line can have a lower flow stress than the surrounding material due to differences in crystallographic texture. This can result in localization of deformation near the weld line.

Poster 11:
Chemistry Sensitive Modelling of Austenite Grain Growth and Decomposition in the CGHAZ of Line Pipe Steels

N. Romualdi[1], M. Militzer[1], W.J. Poole[1], L. Collins[2], R. Lazor[3]
[1]The University of British Columbia
[2]Evraz, Inc. NA, Regina, SK
[3]Transcanada Energy, Calgary, AB

The mechanical properties of line pipe steels are obtained by combining chemistry design with thermomechanically controlled rolling (TMCP). In construction, pipe segments are joined by welding which may compromise the fracture toughness properties of the coarse grain heat affected zone (CGHAZ). This study aims to predict the mean characteristics of the CGHAZ microstructure. Austenite grain growth is measured in-situ by a laser ultrasonics for metallurgy (LUMet) system attached to a Gleeble thermos-mechanical simulator. Austenite decomposition is measured by dilatometry during continues cooling at rates relevant for the CGHAZ. Austenite grain growth kinetics are modeled incorporating the effect of alloying elements (e.g. C, Nb, Mo, Cr) in the grain boundary mobility and of TiN particles in the limiting grain size. Austenite decomposition is modeled using a modified JMAK equation that incorporates the effect of Nb in solution on the decomposition kinetics.

Poster 12:
The Effect of Quench Rate and Grain Boundary Misorientation on Grain Boundary Precipitation in an Extruded Al-Mg-Si Alloy

Zhijun Zhang[1], Nick Parson[2], Mei Li[3], Warren J. Poole[1]
[1] The University of British Columbia

[2] **Rio Tinto Aluminium, Jonquière QC**
[3] **Ford Motor Company, Dearborn, Michigan, USA.**
The increasing use of extruded Al-Mg-Si (AA6xxx) alloys in automotive applications has renewed interest in grain boundary precipitation of Mg-Si phases during the quench after extrusion as this is the key factor affecting intergranular fracture. In this study, cooling rates of 1000 ^{o}C/s (water quench), 45 ^{o}C /s and 2 ^{o}C/s (air quench) were examined to study the influence of quench rate on the grain boundary precipitation in a Mn free extruded Al-Mg-Si (AA6082) alloy. The size and number density (number of precipitates per length) of precipitates on the grain boundary was quantified for different quench rates using Field Emission Gun Scanning Electron Microscopy (FEG-SEM), while the orientation of grain boundaries was determined by Electron Backscatter Diffraction (EBSD). The results indicate that the size and number density of grain boundary precipitates depend not only the quench rates but also the misorientation of the grain boundaries.

Poster 13:
A Microstructure-Based Model to Predict the Work Hardening Rate of AA7075 under Various Aging Treatments

Kaab Omer, Atekeh Abolhasani, Shahrzad Esmaeili and Michael Worswick
University of Waterloo

A microstructure-based model is developed, which is capable of predicting the work hardening rate (WHR) and stress-strain properties of AA7075 subjected to various age hardening treatments. The model uses kinetic parameters established in the literature to determine the relative volume fraction of precipitates in the material, its average precipitate radius and yield strength. The kinetic parameters are then used to predict the WHR, and therefore, the stress-strain curves of the alloy using its microstructural and mechanical properties. Experimentally obtained stress-strain curves for series of aging conditions were initially used to calibrate the model. The calibrated model was then used to predict the WHR and stress-strain curves of AA7075 subjected to other heat treatments not included in the calibration. The predicted curves were compared against experimentally obtained stress-strain curves and were found to match well. The model developed in this work has applicability in hot stamping applications, after the formed part has been subjected to an aging cycle.

Poster 14:
Characterisation of the Austenite-ferrite Interfaces at Nanoscale in Medium Carbon Fe-C-Mn Steels

Olha Nakonechna[1], Mohamed Goune[2], Didier Huin[3], Elena Zapolsly[1] and Frederic Danoix[1]
[1]**GPM, University of Rouen Normandie, France**
[2] **ICMCB, University of Bordeaux, France**
[3] **ArcelorMittal research SA, Maizières Les Metz, France**

The austenite to ferrite phase transformation is one of a key factor in the processing of advanced high-strength steels (AHSS), for example dual-phase (DP) steels. During this phase transformation the interaction and segregation of alloying elements with migrating interface directly affects interface mobility. Knowledge about its interaction can be a critical for a better understanding of the mechanism of this phase transformation. In this work the atomic scale redistribution of interstitial (C) and substitutional (Mn) elements across the austenite-ferrite interface in a medium carbon Fe-C-Mn steels is investigated. Combination of the EBSD, FIB, TKD and Atom probe tomography (APT) techniques were used to provide full chemical and orientation characterization of samples. Experimental results are compared with the existing interfacial models for phase transformation in steels.

Poster 15:

The Dependence of Ductility on Quench Rate for Al-Mg-Si-Mn Alloys

Mojtaba Mansouri Arani[1], Nick Parson[2], Mei Li[3], Warren J. Poole[1]
[1] The University of British Columbia
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[3] Ford Motor Company, Dearborn, Michigan, USA

The ductility of Al-Mg-Si-Mn extrusion alloys is an important property which affects the forming of automotive parts and their in-service behaviour, e.g. crash performance. Two major factors influencing strain to fracture in these alloys are: i) the quench rate after extrusion and ii) the dispersoid density. In this study the influence of these factors on the extent of strain concentration at grain boundary and consequently fracture strain is studied using high resolution digital image correlation (HRDIC). It was found that reducing quench rate results in very high strain concentration at the grain boundaries (30 times more than the average applied strain). This correlates with the soft PFZ formed near grain boundary as the cooling rate decreases. It was also found that increasing the dispersoid density reduces the extent of strain concentration by reducing the planarity of slip within the grains.

Poster 16:

Quantifying Sintering Kinetics and Heat Transfer in EBAM Powder Beds

William Sparling, Chad Sinclair & Steven Cockcroft
The University of British Columbia

The sintered state of the powder bed in Electron Beam Additive Manufacturing (EBAM) impacts heat transfer to and from the build as well as powder recyclability. Most models which accounts for heat transfer within the powder bed assumes a constant degree of sintering. However, sintering varies as a function of time and temperature, and as such, should be expected to vary as a function of time and position within the EBAM powder bed. This work seeks to identify sintering kinetics and their impact on heat transfer within EBAM powder beds. An automated method for identifying sintering from optical metallography is presented and results of a finite element model for heat transfer in sintered powders are discussed.

Poster 17:

Carbon Deprivation in CO_2 Saturated SRB Culture Intensifies Pipeline Steel Corrosion

Ubong Eduok and Jerzy Szpunar
University of Saskatchewan

In this work, the survival of sulphate reducing bacteria (SRB) cells and their impact on corrosion within simulated CO2-saturated oilfield-produced water with different concentrations of organic carbon have been investigated for pipeline steel. Cell counts reduced with the level of carbon source reduction after incubation, but more cells survived at moderate compared to extreme starvation conditions. The energy needed for cellular survival as well as support towards microbiologically induced corrosion could have been harnessed by a combination of extracellular Fe oxidation and intracellular sulphate reduction even after carbon source starvation. Severe anodic steel dissolution was observed at the end of the culture period within the simulated produced water, and this was attributed to biocorrosion. Pipeline steel corroded more when cultured at moderate starvation conditions compared to the medium with lactate and citrate. Steel substrate corroded less at extreme carbon reduction due to severely weakened SRB biofilms from nutrient deprivation.

Poster 18:
Computational Study of Effect of Substrate Nature of the Growth of Hydrocarbon Film from Acetylene Monomers and Radicals

Mohammad Zarshenas
Universite Catholique de Louvain

Molecular dynamics computer simulations investigating the deposition and reaction of a mixed gas of acetylene molecules and radicals on the non-reactive gold and reactive diamond substrates. Our study on hydrocarbon coatings shows that the morphology of the films in the initial stages of growth is affected by the underlying substrate. On the non-reactive gold substrate, polymeric chains start to grow horizontally (2D films) and then vertical growth (3D films) occurs, while on the reactive surface of diamond the hydrocarbon chains grow vertically once the precursors reach the substrate. Undercoordinated carbon atoms on the surface of diamond results in fluctuations of the number of carbon atoms with sp, sp2 and sp3 hybridization over time in the early stages of deposition. However, our results show that types of hybridization of carbon atoms in the films become substrate independent as the film continues to grow in 3d regime. The polymerization-connectivity formalism shows that the films grown in the vicinity of the gold are more cross-linked and have longer chains as compared to the films grown in the vicinity of the diamond. Finally, this formalism reveals that the structure of the films from cross-linking and polymerization points of is independent of the nature of the substrates while growing the films far from the substrate.

Poster 19:
Structural, Electronic, Optical and Thermodynamic Properties of BaSrTe

Brahim Bahloul, **Khatir Babesse, Azzedine Dekhira, Dalila Hammoutène**
Ecole Normale Supérieure de Bou Saada
Université des sciences et de la technologie Houari-Boumédiène

Structural, electronic and thermodynamic properties of SrTe and BaTe compounds and their ternary mixed crystals BaSrTe in the rock-salt structure have been studied with density functional theory (DFT), whereas the optical properties have been obtained by using empirical methods such as the modified Moss relation. The exchange-correlation potential was calculated using the generalized gradient approximation (GGA) of Perdew–Burke–Ernzerhof (PBE) and the local density approximation (LDA) of Teter–Pade (TP). In the present work, we used the virtual-crystal approximation (VCA) to study the effect of composition (Ba). The calculated lattice parameters at equilibrium volume and the bulk modulus for x=0 and x=1 are in good agreement with the literature data. Furthermore, the BaSrTe alloys are found to be an indirect band gap semiconductor. In addition, we have also predicted the heat capacities (CV), the entropy(S), the internal energy (U) and the Helmholtz free energy (F) of the parent compounds SrTe and BaTe.

Poster 20:
Diffusion of Carbon in Fe-C Glass- A Molecular Dynamics Study

Siavash Soltani, Chad W. Sinclair, Joerg Rottler
The University of British Columbia

We investigate the carbon diffusion in Fe-C glasses with different carbon concentrations using atomistic simulations. We use molecular dynamics and a hop detection algorithm to identify all diffusive jumps of

C atoms in Fe-C glass matrix during iso-thermal annealing. Using mean squared displacement of C atoms during MD runs, we show that the carbon diffusivity drops as its concentration increases. The hop detection algorithm measures jump length, residence time and correlation factor of jumps and indicates that the decrease in diffusivity is mainly due to longer residence times (=higher energy barrier) of jumps in higher carbon concentration samples.
We also found that the glass is less stable in low carbon glasses and the first phase to form from the glass during annealing is nearly carbon free ferrite. However upon formation of ferrite and rejection of C atoms into the matrix, the growth of ferrite slows down and eventually stops.

Poster 21:
Coupling Atomistic Simulations with Solute Segregation Kinetics
Ayush Suhane and Matthias Militzer
The University of British Columbia

Small additions of alloying elements significantly alter the microstructure evolution of industrially relevant alloys including steels. This effect is primarily attributed to the interaction between alloying elements and moving interfaces and often interpreted as 'solute drag'. Here, a methodology is proposed to implement ab initio simulation results of solute binding energies to grain boundaries into phenomenological solute drag models.

Poster 22:
Computational Study of Solute-binding at hcp-Ti near-∑7 Grain Boundary
Hariharan Umashankar, Ilya Elfimov, Matthias Militzer
The University of British Columbia

Grain boundaries are an important class of defects in polycrystalline materials, especially in nanocrystalline materials. However, nanocrystalline grains tend to be unstable and alloying elements can play a crucial role in stabilizing the nanocrystalline state of a metal. Here, we study the effect of technologically relevant solutes on the grain boundary (GB) site binding energies in hcp Titanium. We perform a series of Density functional theory (DFT) calculations on Ti-X systems, where X=Mo, V, Al, Cr. The solutes are added onto different grain boundary sites of a near-∑7 grain boundary to compute solute binding energies at each of these sites. The computed binding energies are later linearly fitted to local GB site volume and solute size to obtain physically relevant quantities such as the solute-induced pressure. The binding energy data calculated here can be useful to mesoscale simulations such as the phase field method to bridge the atomic scale and the mesoscale information.

Poster 23:
Adhesion of Dry Microstructured Surfaces to Human Skin
Aly Hassan, Tobin Filleter, Benjamin Hatton
University of Toronto

As the use of wearable sensors in a more personalized healthcare system increases, the need for a reliable, reusable, and clean adhesive mechanism to skin becomes critical. The current practice of using medical tape to attach sensors to skin is not reusable and can leave patients with skin damage and serious discomfort. Dry adhesives offer a promising alternative but still suffer from serious challenges when adhering to skin, including skin roughness, bodily fluids, and complex strain behavior. This work evaluates existing dry adhesives and their size-scale effects when adhering to both flat and rough skin-

replica substrates. The dual-roughness in human skin's topography alone shows a significant decrease in the adhesion of these microstructured surfaces. A fundamental understanding of dry adhesion to human skin can help guide sensor design and enable long-term patient monitoring devices.

Poster 24:

Facile Synthesis of Silver Nanoparticles on ITO Surfaces: Effect of Size and Density Dispersion on Optical and Electrochemical Measurements

Khalid Nouneh, Sarah Derbali, Abdellah Laazizi, Mouhsin Zekriti, Khalil Elmabrouk, Sebastien Vaudreuil and Munetaka Oyama

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The dense attachment of silver nanoparticles (AgNPs) on indium tin oxide (ITO) surfaces wassuccessfully performed using a refined seed-mediated growth approach. The influence of preparation parameters and cysteamine as linker molecule to attach AgNPs on ITO surfaces on the particle size and density attachment on ITO surface were discussed. Consequently, the results showed a narrower size distribution and much denser attachment compared with those prepared by the normal seed-mediated growth method [1-2]. The grown size was possibly controllable for Ag nanosphere particles smaller than 45 nm by adjusting the growth time less than 2 hours, while larger different shaped AgNPs were formed over 3 hours' growth. The bridging with cysteamine was also found to be effective for denser and homogenous attachment of AgNPs on ITO surface with keeping the dispersion.

Poster 25:

An Insight into the Effect of Buffer Layer on the Electrochemical Performance of MgF_2 Coated Magnesium Alloy ZK60

Usman Riaz and Waseem Haider
Rensselaer Polytechnic Institute
Central Michigan University

Magnesium (Mg) has emerged as potential implant material owing to its property of biodegradation. The roadblock to the commercial use of Mg as implant material is its fast degradation in body fluids. The degradation of the Mg and its alloys can be retarded by surface coatings. In this work, the potential of MgF_2 coating on the surface of Mg alloy ZK60 (Mg-6.9Zn-0.8Zr) was evaluated for its corrosion properties. Two-step chemical conversion process was used to coat MgF_2 on the surface of ZK60 alloy. In the first step, a secondary layer of $Mg(OH)_2$ was introduced by boiling the samples in NaOH solution. In the second step, these samples were immersed in hydrofluoric acid to obtain MgF2 coating. SEM, IR Spectroscopy, and XRD were employed to confirm the formation of Mg(OH)2 and MgF2. The wettability tests showed an increase in surface hydrophobicity as a result of conversion treatment. The potentiodynamic polarization tests exhibited an improvement in the corrosion potential from −1.52 V vs. SCE to −1.49 V vs. SCE after two-step conversion treatment. Moreover, coated sample witnessed a noticeable drop in hydrogen evolution compared to untreated ZK60. For a better insight, the results were compared to the MgF_2 coatings achieved on the surface of ZK60 without any buffer layer. The coating of MgF_2 with a buffer layer of $Mg(OH)_2$ on the surface of ZK60 exhibited a noble corrosion potential, controlled degradation, and nominal hydrogen evolution compared to the untreated ZK60.

Poster 26:

Functionalized Graphene Oxide Coating on Ti6Al4V Alloy for Improved Biocompatibility and Corrosion Resistance

Hassnain Asgar and Waseem Haider
University of Wisconsin
Central Michigan University

The present study focused on the development of magnesium-functionalized graphene oxide (FGO) coating on titanium alloy (Ti6Al4V) by electrophoretic deposition. Graphene oxide (GO) was synthesized by modified Hummers' method and functionalized with magnesium ions. X-ray diffraction, infrared spectroscopy (IR) and Raman spectroscopy were employed to confirm the synthesis of GO and GO-coatings on Ti6Al4V. Functionalization of GO with Mg ions was confirmed by energy dispersive X-ray spectroscopy. The surface morphology of coated samples was examined through scanning electron microscopy. Reduction of FGO coating (labelled as rFGO) by heating at 200 °C was confirmed by IR. The rFGO coated Ti6Al4V was found to be hydrophilic in nature as determined by contact angle measurement which showed reduction in the contact angle of Ti6Al4V from 95.4° to 42.1°. The percent cell viability over the coated sample was appreciably improved compared to as-received Ti6Al4V sample owing to hydrophilicity of the former. The positive shift in open circuit potential and increase in polarization resistance was observed after coating Ti6Al4V samples with FGO. The significant decrease in the corrosion current density and negative polarization loop in the reverse scan of samples also confirmed the improved corrosion resistance of rFGO-coated Ti6Al4V over uncoated Ti6Al4V in the PBS solution. Furthermore, the impedance spectroscopy revealed that the preferential adsorption of ionic species (indicated by large Rads) at the surface improved the barrier characteristics of rFGO coated samples and exhibited an order of magnitude higher Rct compared to as-received samples.

Poster 27:
Mechanical Properties of Bio-cleaned Electrospun Lignin Fibers

Jiawei Chen, Tanushree Ghosh, Cagri Ayranci, Tian Tang
University of Alberta

Lignin is the most abundant aromatic biopolymer in nature. It has been considered as a sustainable alternative for the conventional petroleum-based carbon fiber precursor because of its renewability andcost-effectiveness. Purification of lignin biomass to remove impurities, such as hemicellulose, cellulose, and ash, is vital for carbon fiber production and improving mechanical properties. A novel method is developed by using Pseudomonas fluorescens bacterium to biodegrade the impurities inlignin. The bio-cleaned lignin is electrospun into nanofibers. The electrospinning process is optimized to produce bead-free, uniform and ultrafine lignin fiber mats. Characterization of the electrospun lignin fibers before and after the bio-cleaning is performed by SEM measurements of fiber diameter and fiber orientation. Mechanical properties including elastic modulus and ultimate tensile strength are determined to evaluate the effect of bio-cleaning and electrospinning parameters.

Poster 28:
Direct Growth of Vertical Nanographene Array on Rough Germanium Surface by Plasma Enhanced Chemical Vapor Deposition

Abdulrahman Al-hagri, Ru Li , Shan Cong
Khalifa University of Science and Technology
Suzhou Institute of Nano-Tech and Nano-Bionics

Ascribing to the combined superior inherent properties of graphene and the special structure configuration, vertically aligned graphene nanosheet arrays (VAGNAs) exhibit large surface area, excellent electron transfer capability, and enhanced electrochemical activity, which make them promising in supercapacitors, batteries, and fuel cell catalysts. Here we show that high-quality ultra-clean single layer VAGNAs can be direct grown on rough germanium surface by plasma enhanced chemical vapor deposition. The uniform, large area of centimeter-scale VAGNAs can act as an efficient surface-enhanced Raman spectroscopy substrate with sensitivity down to 1×10-3 mol L-1 rhodamine due to the existed abundant edges.

Poster 29:

Structural and Compositional Analysis of Bulk $CH_3NH_3PbI_3$ and Nanoparticle $CsPbBr_3$ perovskite materials by electron microscopy

Natalia Fernandez-Delgado[1], M. Herrera[1], F. J. Delgado[1], A. H. Tavabi[2], M. Luysberg[2], R. E. Dunin-Borkowski[2], E. J. Juárez-Pérez[3], I. Mora-Sero[3], I. Suárez[4], J. P. Martínez-Pastor[4], G. Botton[5], S. I. Molina[1]

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$CH_3NH_3PbI_3$ and $CsPbBr_3$ perovskite materials are of current interest because of their high efficiencies in solar cell devices and economical fabrication processes [1]. We have investigated different synthesis-deposition methodologies using (scanning) transmission electron microscopy techniques. Bulk $CH_3NH_3PbI_3$ was synthesized using a one-step deposition method, with crystallization of the perovskite occurring directly on the substrate. Although the layer fully covered the substrate, its thickness was irregular because it formed from independent crystals of different size and orientation. Nanoparticles of $CsPbBr_3$ were fabricated using a two-step deposition method, with the nanoparticles first synthesized and then deposited onto the substrate. No agglomeration of the nanoparticles was observed. However, the perovskite film did not produce full coverage of the substrate, as some gaps were observed between the nanoparticles. Our work provides insight for obtaining optimal films for solar cells.

[1] C.R. Kalaiselvi et al., Mater. Lett. 219 (2018)

Poster 30:

Computational Annealing of Superconducting Radio-frequency Accelerating Cavities

Norman Muller and Mauricio Ponga

The University of British Columbia

Superconducting radio-frequency (SRF) accelerating cavities made of Niobium (Nb) are widely used in particle accelerators to increase speed and energy of electron beams. However, SRF cavities suffer from heat losses originated by spurious current generated during the acceleration process. This current is generated due to the magnetic flux pinning that occurs in near the surface of such cavities due to the presence of dislocations and other defects. Thus, several experimental works have shown that the cavities are highly dependent on the annealing process used, which is currently done using trial and error. In this work, we developed a computational annealing model using a 2.5-dimensional dislocation dynamics approach. The model approaches the glide/climb problem using constitutive kinetic laws to

simulate thermally activated kink-pair formation and diffusion of vacancies from the dislocation core. Initial conditions are estimated from the expected residual stresses obtained after a typical sheet metal deep-drawing process simulated using finite element methods. The model presented is relevant to the production and treatment of SRF accelerating cavities in order to optimize the annealing steps used to minimize performance limiting phenomena such as magnetic flux pinning. The model will be validated through experiment using cold-rolled high-purity niobium samples, subsequently vacuum annealed and studied using SEM techniques.

Poster 31:

On the Progress in Additive Manufacturing: Microstructural and Bulk Properties Evolution of Cold-Sprayed Copper Coatings after Low Temperature Annealing

Bosco Yu, Weiwei Li, Jason Tam, Jean-Gabriel Legoux, Dominique Poirier, Jason Giallonardo, U. Erb
McMaster University, University of Toronto, The Nuclear Waste Management Organization (NWMO), National Research Council (NRC)

Cold spraying is an industrial scale additive manufacturing process, its applications include 3D printing, tool repair, and corrosion protective coatings for nuclear waste storage. For these applications, a major concern is whether cold spraying can create deposits with sufficient ductility and mechanical integrity. The electron microscopy analysis in the current study revealed that the brittleness of the as-sprayed metals cannot be explained solely by their porosity or microstructure; their fracture mechanics is most likely governed by the coupling interaction between porosity and the nanocrystalline dynamically recrystallized (DRX) grains adjacent to the pores. Under loading, pores in the as-sprayed copper can act as crack tips which then propagate along the adjacent DRX grains, resulting in a brittle cleavage fracture. Low-temperature annealing did not remove the porosity but promoted recovery and grain growth in these DRX grains. From originally cleavage to eventually dimpling, the tensile ductility increased by ~120 folds.

Poster 32:

Using Titanium Nitride in Solid Oxide Fuel Cells

Taghi Amiri
University of Alberta

Solid oxide fuel cells (SOFCs), which typically operate at higher temperature (above 500°C) compared to other types of fuel cells, have received particular attention in recent years not only for power generation but also for the potential of performing simultaneous dry reforming of methane (DRM) reaction in its anode compartment. The high operating temperature is favored by DRM and, at the same time, the heat released during the electro-oxidation process can partially compensate the energy required for DRM. Nonetheless, the conventional Ni-Y_2O3-stabilized ZrO_2 (YSZ) anode electro-catalyst does not show good in-situ dry reforming activity, nor does it exhibit acceptable electrochemical performance in CH_4-CO_2 mixtures, not to mention that sulfur impurities always significantly deactivate its reforming capability. On the one hand, the coke-sulfur resistant DRM catalyst resulting from recent advancement in this field has not been fully utilized in SOFC research due to many practical barriers, e.g., a sintering temperature as high as >1300^{o}C in SOFC fabrication. On the other hand, a typical Ni-YSZ supported cell

usually shows serious performance degradation when being directly fed with equal amounts of CH_4 and CO_2, although performance could be improved by introducing noble metal catalysts or using novel fabrication methods. In this research, we opt to use titanium nitride (TN) to act as as both current collector and anode. . It has excellent thermal and electrical conductivity comparable to metals. It can also tolerate the oxidation up to 700 °C which makes it a suitable non-metal candidate to be used in oxygen-conductor SOFCs and hydrocarbon feed. Its perfect thermal expansion coefficient with YSZ guaranties its long-term mechanical stability. Our initial results show it has a true potential to be used in SOFCs with perfect overall performance.

Wednesday, June 12

8:00 – 9:00 (FSC Lobby) Breakfast

9:00 – 10:00 (FSC 1005) Materials Physics Lecture

Deformation and Fatigue of Magnesium Alloys: Twinning and Detwinning
Daolun Chen, Ryerson University

Lightweighting is one of the most effective strategies to reduce fuel consumption and anthropogenic CO_2 emissions, since a 10% weight reduction brings about a 6~8% fuel-efficiency gain. It has recently been depicted as the "storm of lightweighting" – a revolution in materials, processes, and business models – which is brewing on the horizon of the automotive industry. Magnesium alloy, as an ultra-lightweight metallic material, has recently received significant attention due to its superior strength-to-weight ratio. However, the hexagonal close-packed crystal structure of magnesium alloys limits the availability of slip systems and leads to strong mechanical anisotropy and tension-compression yield asymmetry owing to the presence of crystallographic texture and the related deformation twinning. For the components subjected to dynamic loading, such asymmetry could exert an adverse effect on the material performance and compromise the structural integrity, safety, and durability of highly-loaded structural components. This issue could be conquered through weakening the basal texture via the addition of rare-earth (RE) elements and other alloying elements to refine grains and generate nano-sized precipitates. To safeguard the structural integrity, durability, and safety of load-bearing structural components, understanding the characteristics and mechanisms of deformation and fatigue of magnesium alloys is of vital importance. In this presentation, several examples on the cyclic deformation behavior of extruded magnesium alloys with and without RE elements will be presented. Moreover, twinning, twin growth, and twin-twin interactions during uniaxial compression in the extrusion direction and de-twinning in the transverse direction will also be discussed.

10:00 – 10:20 (FF 217, 303, 317) Coffee Break

10:20 – 12:00 (FF303) Embury Symposium IV
Session Chair: C. Hutchinson

10:20 – 10:40

Nanoscaled Structure and Properties of Ultrafine Grained Aluminum Stabilized by Ca Grain Boundary Segregations and Intermetallic Particles
(INVITED)
Xavier Sauvage
Normandie Université, UNIROUEN, INSA Rouen, CNRS

The solubility of Ca in Al is extremely low, which makes this alloying element attractive to stabilize a nanoscaled grain structure thanks to GB segregations and to achieve a unique combination of high strength, low electrical resistivity, good thermal stability and low density material. To achieve this goal, an Al-Ca metal matrix composite was processed by severe plastic deformation (SPD), and the resulting nanoscaled structures were characterized with a combination of TEM and APT analyses. We show that

the SPD led to a progressive dissolution of Ca grains and a mean Al grain size of only 25nm, which is stabilized by Ca segregation at GBs and a low supersaturated solid solution of Ca in Al. This gives rise to a hardness up to 300HV but an electrical conductivity lower than 10% IACS. Upon aging, the grain growth is relatively limited, nanoscaled Al4Ca particles nucleate at GBs, and the electrical conductivity is significantly recovered.

10:40 – 11:00

Precipitation Hardening Associated with High Temperature Forming of Heat Treatable Al Alloys

(INVITED)

Atekeh Abolhasani, Massimo DiCiano, Kaab Omer, Michael Worswick, Mary A. Wells and Shahrzad Esmaeili

University of Waterloo

Although conventional manufacturing routes for Al parts are based on room temperature forming practices, the desire to further optimize processing and properties of these alloys for automotive applications is creating considerable interest in their high temperature forming. High temperature forming of precipitation hardening Al alloys, however, interfere with and/or modify precipitate dissolution and formation phenomena. Depending on the choice of the process variables, such interferences and/or modifications may result in enhancement or decline in the precipitation hardening capacity of the alloys and thus the final part strength. For high temperature forming processes to be fully adopted by the automotive industry for manufacturing AA6xxx and AA7xxx aluminum alloy parts, interactive phenomena related to their precipitation hardening behaviours should be comprehensively investigated. This presentation focuses on the evolutions that occur in the microstructure and strength of warm formed AA6013 and die-quenched AA7075 alloys during various thermal processing steps. The applicability of previously-developed modelling approaches to analyze and predict the alloys' behaviours during processing is also presented.

11:00 – 11:20

TEM Studies of the Essential Microstructural Features of Second Phase Particles in Aluminum Alloys

(INVITED)

Xiang Wang

McMaster University

This talk will summarise a number of projects undertaken at UBC to define the nature and essential properties of a variety of second phase particles produced by thermal treatments of a variety of Al alloys, The majority of the characterisation was performed by Electron Microscopy (TEM). Various microstructures will been presented, and analysed including 1) very local information, such as the precipitate structure, composition and morphology, relationship between precipitate with matrix and matrix deformation around precipitate etc. and 2) more global information, such as the precipitate number density, volume fraction, spacing between precipitate and average size etc. The relationship of the detailed microstructures and the corresponding mechanical properties will be correlated.

11:00 – 11:20
A Tribute to David Embury
Muriel Veron
INP Grenoble

11:40 – 12:00 Discussion

10:20 – 12:00 (FF317) Computational Materials Science I

Session Chair: V. Razumovskiy

10:20 – 10:40
Molecular Dynamics Simulation of Structure Evolution of Hydrotalcite and CO_2 Adsorption Behavior in Hydrotalcite and its Derived Oxides
(INVITED)
Hao Zhang
University of Alberta

Hydrotalcite (or LDHs) derived materials are considered to be promising candidates for solid sorbents for CO_2 capture at intermediate temperatures. Using molecular dynamics (MD) simulation, we investigated the atomistic structures of monocarboxylic acid intercalated LDHs. The replacement of carbonate anions by stearate anions and the presence of water molecules could greatly increase the basal spacing. Further, we studied the role of water in the intercalation of CO_2 with hydrotalcite. The contradicting results reported in the literature of CO_2 diffusion and adsorption is partly due to the dipole interaction between H_2O and CO_2 molecules and the reduced interaction between CO_2 and the hydroxyl groups on hydrotalcite. Moreover, we investigated CO2 adsorption behavior on amorphous layered double oxides (LDOs) derived from LDHs at elevated temperatures. The MD simulation of structure evolution upon heating agreed well with experimental results. The simulation results also showed that CO_2 dynamic residence time on LDOs was sensitive to the Mg/Al ratio and the average amount of residence time of CO_2 on surface of LDOs reached maximum when the Mg/Al ratio was 3. Examination of the binding between CO_2 and mixed oxides revealed that both magnesium and oxygen in amorphous LDOs contributed to CO_2 adsorption.

10:40 – 11:00
Impact of Chemical Composition on Core Structure and Glide Behavior of Dislocations in bcc Metals
(INVITED)
Lorenz Romaner
Materials Center Leoben Forschung GmbH

Dislocations are the carriers of plastic deformation and their fundamental atomistic structure is of great importance for the mechanical properties of materials. Owing to its nonplanar core, the screw dislocation has received most attention in bcc metals. Recently, however, also the role of mixed dislocations has been highlighted. We present results on the core structures and mobilities of dislocations in bcc transition elements using atomistic simulations ranging from classical potentials via tight-binding-based bond order potentials to density functional theory. We find pronounced differences for the structure of the dislocation core in terms of dissociation and Peierls barriers. By comparing screw dislocation and mixed dislocations, we provide hints to what extent dislocation characters matter in the

different metals and discuss the implications of our findings for thermal activation of dislocation glide and shape of dislocation loops.

11:00 – 11:20
Large Scale ab-initio Simulations of Dislocations in Mg
Mauricio Ponga
The University of British Columbia

We present a novel methodology to compute dislocations core energies in crystalline metallic materials using large-scale \emph{ab-intio} simulations. The approach is based on a coarse-grained density functional theory (DFT) implementation that tremendously reduces the complexity of the calculations. We first start by providing developing a linear scaling DFT method based on the density matrix approximation. The linear method allows to compute the DFT equations using local information and in real space, making the approach amenable for coarse-grained description and for massively parallel implementation. This leads to a highly efficient computational method that allows to study dislocation cores in metals explicitly including the dislocation long range deformation field. Using this novel methodology, we computed dislocation cores involving prismatic dislocation loops and shear dislocations in Magnesium, and study the interaction energy with Aluminum solutes. The ability of the methodology to describe samples with exceedingly large number of atoms allows us to validate and compare with well known classical elasticity solutions which validates the accuracy of the new approach.

11:20 – 11:40
The Effect of Grain Boundaries on Mechanisms of Small Scale Plasticity
Mahdi Bagheripoor and Robert Klassen
Western University

The effect of grain boundaries on the mechanisms of incipient plasticity during nano-indentation of Au thin films is studied using large scale atomistic simulation. Various symmetric and asymmetric tilt boundaries are analyze to determine the effect of boundary geometry on the operative nano-scale plasticity mechanisms. We present data that illustrate the complex role of a grain boundary in providing both sites for dislocation nucleation and absorption depending upon the configuration and location of the boundary relative to the indentation. We observe that grain boundaries block the glide of existing dislocations, and contribute to forest hardening, at higher indentation depths but not at lower indentation depths.

11:40 – 12:00
Generation of Gradient Nano-grained Heterostructures from High Velocity Impacts
David Funes and Mauricio Ponga
The University of British Columbia

Mechanical properties of crystalline materials, specifically metal and its alloys, are heavily influenced by their microstructure. Recent studies have shown that simultaneous enhancement of strength-ductility can be achieved through a gradient nano-grained (GNG) microstructure. In this work, we study the generation of gradient nano-grained microstructure from high velocity impact of silver microcubes using molecular dynamics simulations. The results reveal that, for certain cases, the single crystal microcubes recrystallize and generate a rich microstructure with grains varying from the impacted area to the top of the microcube. These results are qualitatively compared with experimental observations carried out by our collaborators. We found that the formation of the gradient nano-grained microstructure depends on

the velocity of the impact, the orientation of the lattice and the orientation of the microcube. Finally, our results suggest that the GNG transformation happens if three factors are present in during the impact, i) a large hydrostatic stress, ii) at least eight slip systems are available to accommodate plastic deformation and iii) the kinetic energy is large enough to produce severe plastic deformation.

10:20 – 12:00 (FF217) Emerging Materials and Processes I

Session Chair: J. Kish

10:20 – 10:40

Formability and Windability of Aluminum and Copper Magnet Wire

Lucas Chauvin, A. R. Riahi, N. C. Kar, A. Edrisy
University of Windsor

The demand for lighter and more cost-effective electric vehicles has established the need to investigate replacing conventional copper windings with aluminum. A formability and windability study between electrolytic tough pitch copper and electrical conductor aluminum was performed. Rectangular profile wires were studied since their enamel coating is more prone to damage than round conductors. Standardized mechanical testing was used to characterize the windability and formability of each material. Forming behaviour of both wires was further investigated and compared using a custom-built wire bending machine designed to simulate the wire winding process. Contact pressure, relative speed and wire tension were controlled to analyze their effect on coefficient of friction between wire and counterface. The contact surface of both wire and counterface was analyzed using optical and scanning electron microscopy to study the possible damage induced during winding. Understanding aluminum formability and windability is essential for successful implementation into electric motors.

10:40 – 11:00

Using Microwave to Sinter Leak-Free Proton Conductor Electrolyte to be Used in Solid Oxide Fuel Cells

Taghi Amiri, Jingli Luo, Partha Sarkar, Thomas Etsell
University of Alberta

Most oxides are transparent to regular microwave generators (900 MHz and 2.45 GHz) since these waves are not in the range of their phonons. Increasing the temperature rapidly changes this and causes the specimen to absorb the waves. That is why it is convenient to use a material called a susceptor that can absorb the microwaves at low temperatures and heat the specimen. Above a certain temperature, the specimen itself starts to absorb the waves. We developed a unique method which consists of using the nickel metal-YSZ as a support due to the fact that it can absorb the microwaves and act as a susceptor to heat the BZY ($BaZr_{0.8}Y_{0.2}O_{3-\delta}$) electrolyte until it can absorb the waves itself. Then due to fast sintering process, inhibited grain growth is expected. Also, NiO–GDC ($Ce_{0.8}Gd_{0.2}O_{1.90}$) can absorb the waves at room temperature which opens up another possible candidate. We successfully managed to make leak-free electrolyte using this technique which would need 1700 °C sintering temperature otherwise.

11:00 – 11:20

Thermophysical Property Measurements of Molten Slag Systems Using Brookfield Viscometry and Aerodynamic Levitation

Lily Ren, Dr. Aziz Bogno, Dr. Jonas Valloton, Dr. Hani Henein, Dr. Florian Kargl
University of Alberta, Institut für Materialphysik im Weltraum, Deutsches Zentrum für Luft- und Raumfahrt

The thermophysical properties of slag materials play a significant role in numerous metallurgical processes. It quantifies the flow properties of the slag, the degree to which the slag affects refractory attack, the amount of entrained metal in the slag, the mass transfer at the slag-metal interface, the heat transfer phenomena through the slag, and the thermodynamic activities of the slag components. The viscosity of molten slag heavily relies on its composition, temperature, and experimental condition. A literature review of viscosity measurements of SiO_2-FeO/Fe_2O_3-CaO slag systems and their viscosity models was carried out and will be presented. Apparent viscosities of the SiO_2-FeO/Fe_2O_3-CaO slag were measured by adapting the Brookfield DV2T viscometer into an induction furnace operating at 1400 - 1650 °C under an Ar atmosphere. The measured viscosities from this work will be compared with the viscosity values obtained using the Aerodynamic Levitation method. The prepared slag was characterized using Differential Scanning Calorimetry, X-ray diffraction, and ICP-MS to determine the phases and final compositions in the sample.

11:20 – 11:40

The Effect of Boronizing on Hardness, Wear and Corrosion Properties of Steels Used in Potash Processing Facilities

Chao Peng, Oguocha, I.N.A., Odeshi, A.G, Evitts, R.W.
University of Saskatchewan

Steels are widely used in potash processing but they show unsatisfactory performance under severe corrosion and wear conditions. Boronizing heat treatment is a good method to improve surface properties of steels used in potash processing. In the present study, AISI 1018 and AISI 316L steels were case-boronized at termperatures of 850 °C, 900 °C and 950 °C for 4 h, 6 h and 8 h. The effect of boronizing conditions on boride layer thickness, hardness and boride phase evolution were investigated using hardness, surface roughness and thickness measurements, X-ray diffraction, optical microscopy and scanning electron microscopy. The wear and corrosion resistance of the boronized steels were evaluated using a pin-on-disc wear testing apparatus and electrochemical corrosion measurements, respectively. The results obtained from this research will be presented at the conference.

11:40 – 12:00

Microstructural Evolution During Heat Treatment and Mechanism of Wear of Conventional and 3D Printed Ti6Al4V Titanium Alloys

Niyousha Azgomi and Solomon Boakye-Yiadom
York University

Medical Grade Ti6Al4V is one of the alloys used as hip and knee implants due to its biocompatibility, strength, toughness and good corrosion resistance. Recent efforts due to advancement of metal 3D printing has seen an increase in the number of 3D printed Ti6Al4V titanium alloys used as implants. Even though metal 3D printing has great advantages including ability to easily print complex shapes and parts, the properties of 3D printed Ti6Al4V titanium alloys are still under investigation. The aim of this study is to understand the effect of heat treatment on the micro-structural evolution, hardness and mechanism of wear of conventional and 3D printed Ti6Al4V titanium alloy. It is demonstrated that the micro-structural integrity of the Ti6Al4V alloys is a function of both the manufacturing process and the temperature/duration for heat treatment.

12:00 – 13:00 (FSC Lobby) Lunch

13:00 – 14:20 (FF303) Embury Symposium V

Session Chair: H. Zurob

13:00 – 13:20

The Ductility of Al-Mg-Si-Mn-Fe Alloys

Warren J. Poole and Mojtaba Mansouri Arani
The University of British Columbia

The ductility of Al-Mg-Si-Mn-Fe extrusion alloys is an important property which affects the forming of automotive parts and the in-service behaviour, e.g. crash performance. The precipitation of Mg-Si particles on the grain boundaries during quenching and artificial aging can reduce the fracture strain of the material due to i) strain localization at the grain boundary associated with the formation of a precipitate free zone adjacent to the grain boundary, and ii) reduction of the cohesive strength of the grain boundary. In this study the effect of quench rate and aging treatment on strain distribution within the grains and across the grain boundaries has been quantified using high resolution digital image correlation. The results show the degree of strain localization at the grain boundary is dependent on the cooling rate after the solution treatment. The localization correlates with the width of the precipitate free zone and the cohesive strength relates to the density of precipitates on grain boundaries.

13:20 – 13:40

PSP Modeling for HPDC Mg

(INVITED)

Jeff Wood
Western University

This talk traces the results of 15 years of research and development efforts to improve the predictability of the mechanical response of HPDC magnesium components. Considerably more expensive than steel, HPDC magnesium alloys remain competitive in the automotive industry due to the economies afforded by part consolidation. The resulting geometric complexity, however, leads to local variations in solidification conditions which, in turn, creates a variety of common microstructural defects. Understanding the range of these defect structures, the conditions under which they are formed, and their impact on the resulting mechanical behaviour has led to the creation of a suite of numerical tools that enable the prediction of local mechanical properties based on the numerical simulation of the casting process. It is this capability that has significantly improved the ability to optimized the design of magnesium high-pressure die-castings.

13:40 – 14:00

Flow Stress and Electrical Resistivity in Pure Al at 4K

(INVITED)

Marek Niewczas
McMaster University

In-situ measurements of electrical resistivity during tensile deformation of pure Al polycrystals at 4K, and in samples with intermittent annealing between 4K and 298K, were conducted to follow the relationship of the flow stress and the density of dislocations stored in the metal. The data is assessed against general constitutive relationship of the form $\tau = \mu b \rho^{n}$, with n and constants. The Taylor law, $\tau = \mu b \rho^{1/2}$, describes the flow stress adequately in monotonically deformed Al however, it distorts stress - dislocation density dependence considerably in samples subjected to intermittent annealing, characterized by a higher rate of defect production and a lower rate of flow stress increase. The results are interpreted in terms of the interaction processes of mobile dislocations with different types of stored defects that determine the flow stress and work hardening of Al at 4K.

14:00 – 14:20 Discussion

13:00 – 14:20 (FF317) Computational Materials Science II

Session Chair: H. Zhang

13:00 – 13:20

Fracture ab initio: A Force-based Scaling Law for Atomistically Informed Continuum Models

(INVITED)

Johannes J. Möller[1], Erik Bitzek[1], Hamad ul Hassan[2], Alexander Hartmaier[2], Rebecca Janisch [2]

[1] Department of Materials Science and Engineering, Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany

[2] ICAMS, Ruhr-University Bochum, Germany

In fracture mechanics, established methods exist to model the stability of a crack tip or the kinetics of crack growth on both the atomic and the macroscopic scale. However, approaches to bridge the two scales still face the challenge in terms of directly converting the atomic forces at which bonds break into meaningful continuum mechanical failure stresses. Here we use two atomistic methods to investigate cleavage fracture of brittle materials: (i) we analyze the forces in front of a sharp crack and (ii) we study the bond breaking process during rigid body separation of half crystals without elastic relaxation. The comparison demonstrates the ability of the latter scheme, which is often used in ab initio density theory calculations, to model the bonding situation at a crack tip. Furthermore, we confirm the applicability of linear elastic fracture mechanics in the nanometer range close to crack tips in brittle materials. Based on these observations, a fracture mechanics model is developed to scale the critical atomic forces for bond breaking into relevant continuum mechanical quantities in the form of an atomistically informed scale-sensitive traction separation law. Such failure criteria can then be applied to describe fracture processes on larger length scales, e.g., in cohesive zone models or extended finite element models.

13:20 – 13:40

Ab-initio Driven Multiscale Modeling of Austenitic FeCrMn and Marval X12 Steels

(INVITED)

Vsevolod Razumovskiy[1], Hemantha Kumar Yeddu[2], Carola Hahn[1], Jürgen Spitaler[1], Lorenz Romaner[1]

[1]Materials Center Leoben Forschung GmbH

[2]New Castle University

Fundamental understanding of mechanical properties and microstructural characteristics of austenitic and maraging steels is of great practical importance for knowledge-based design of new materials. Here, we present the outcome of our investigation of the microstructure evolution of the Marval X12

steel and the solid solution strengthening in austenitic FeCrMn steels. Using the 3D elastoplastic phase-field model and density functional theory calculations we show that increasing carbon concentration in Marval X12 steel leads to formation of mixed martensite morphology and investigate the effects of composition and temperature changes on the magnetic state, elastic properties and stacking fault energies of Fe[10-16 at.%]Cr[12-32 at.%]Mn steels that are later used to evaluate the effect of the solid solution strengthening by Mn and Cr using modified Labusch-Nabarro model calculations. The effect of Cr and Mn alloying on the stacking fault energies is calculated and discussed in connection to possible deformation mechanisms.

13:40 – 14:00

Computing and Modelling Solute-grain Boundary Interaction

(INVITED)

Liam Huber, R. Hadian, B. Grabowski*, J. Neugebauer
Max-Planck-Institut für Eisenforschung (MPIE)
***University of Stuttgart**

The segregation of solute elements to grain boundaries (GBs) is one mechanism by which even very small concentrations of alloying elements can play an out-sized role in microstructure evolution, and thus material properties. At atomic length scales, structural disorder at the GB leads to a wide variety of local environments for segregating atoms. Using classical molecular statics, we sample these environments at 38 different boundaries in Al for six different solute species, obtaining a distribution of segregation energies for each boundary. In addition to revealing shortcomings in the popular Langmuir-McLean model for solute GB concentrations, this rich dataset of 1.4 million segregation energies also provides an opportunity to use machine learning to represent solute-defect interactions. In a similar manner, we construct solute segregation distributions for free surfaces corresponding to each GB and demonstrate how these can be used directly with the Griffiths criterion to investigate embrittlement. Finally, we consider solute-solute interaction by direct calculation of select supercells with finite concentrations of solute. From these we calculate the thermodynamic stability of particular patterns of solute decoration, revealing so-called "defect phases".

14:00 – 14:20

Multi-Scale Modeling of Hot Tearing in DC Casting Aluminum Alloys

Niloufar Khodaei and Andre Phillion
McMaster University

The prediction of hot tearing in aluminum alloys has evolved considerably but the quantitative prediction of cracking in semisolids remains elusive. In this study, a new semi-quantitative micro/macro approach to hot tearing for DC casting is proposed. First, a pore fraction hot tearing model developed by Dou and Phillion, which includes the effect of shrinkage feeding and strain rate perpendicular as well as parallel to thermal gradient is applied to a thermomechanis model of DC casting for AA5182 with different casting speeds. Then, the solid–liquid geometry is generated using a 3-D granular solidification model known as GMS-3D, and finally, the meso-scale multi-physics model is applied to simulate semi-solid deformation. The results show that the multi-scale approach can predict the strain-stress behaviour of semi-solids, and accordingly the initiation of crack in semi-solid region as a precursor to hot tear formation.

13:00 – 14:20 (FF217) Emerging Materials and Processes II

Session Chair: G. Miyamoto

13:00 – 13:20

High-Performance, Room Temperature Hydrogen Sensing with a Cu-BTC/Polyaniline Nanocomposite Film on a Quartz Crystal Microbalance

Osama Abuzalat, Danny Wong, Simon S. Park, Seonghwan Kim
University of Calgary

In this article, we demonstrate a high-performance hydrogen sensor under ambient conditions by growing a Cu-BTC/polyaniline (PANI) nanocomposite film on a quartz crystal microbalance (QCM) using intense pulsed light. The QCM was first sputter coated with a 200 nm thin layer of copper. The copper layer was then oxidized by sodium hydroxide and ammonium persulfate. A solution containing the organic ligand (BTC) and PANI was then dropped and dried on the copper hydroxide surface of a QCM with intense pulsed light which resulted in Cu-BTC/PANI nanocomposite film on a QCM. The gas sensing performance of the Cu-BTC film and Cu-BTC/PANI composite film was compared under ambient conditions. It was found selectivity and sensitivity of the Cu-BTC/PANI nanocomposite film to hydrogen were significantly improved. In addition, a fast response time (from 2 to 5 seconds), operation at room temperature even in the presence of high relative humidity (up to 60%), good repeatability were achieved with the Cu-BTC/PANI nanocomposite film-grown QCM sensor.

13:20 – 13:40

Effect of Graphene and Carbon nanotubes on Wear Behaviour of Alumina-Zirconia Hybrid Nanocomposites

Solomon Duntu, Solomon Boakye-Yiadom, Mohammad Islam, Iftikhar Ahmad
York University
King Saud University, Saudi Arabia

Attractive properties of advanced ceramic alumina such as high temperature strength and hardness, chemical inertness, thermal and electrical insulation has merited wide applications in the medical, aerospace and material research industry. However, the known low fracture toughness of alumina has restricted its capacity to be adapted for high temperature structural applications such as parts of turbine engine and space rocket shields. In the present work, nano-scale Graphene(0.5vol%) and Carbon Nanotubes(2vol%) were dispersed uniformly within Alumina-Zirconia mixture using colloidal mixing followed by hot-pressing to form hybrid nanocomposites. The densities, fracture toughness, microhardness and wear properties of the final sintered nanocomposites were determined. Extensive characterization of the microstructures before and after mechanical testing such as wear test were analysed to define the influence of the various second-phase additives on wear response of the fabricated nanocomposites. Fracture toughness of the nanocomposites were determined using the crack extensions from Vickers indentation.

13:40 – 14:00

KWN Modeling of Precipitation in a Friction Stir Welding Process

Olga Gopkalo, B.J. Diak, Frédéric De Geuser, Alexis Deschamps
Queen's University, SIMAP, Université Grenoble Alpes, Grenoble, France

The welding of heat-treatable aluminium alloys greatly impacts the pre-weld properties by the modification of the size and fraction of strengthening precipitates, and so it useful to understand and predict these changes. The Kampmann and Wagner numerical (KWN) model [Kampmann, Eckerlebe & Wagner, 1987] has been used to describe the precipitation kinetics in thermally processed aluminum alloys [Myhr, Grøng & Andersen, 2001]. The simplest model is based on the growth or dissolution of precipitates distributed in size classes and is adapted here to the solid state friction stir welding of an Al-Mg-Zn alloy, illustrating the time-dependent development of the different parameters related to the precipitation kinetics. The predictions of the model from the evolution of size and volume fraction of precipitates are compared to small angle X-ray scattering (SAXS) measurements. Model predictions are used to enhance physical insight into the range of material behavior in the observed experiments.

14:20 – 14:40 (FF 217, 303, 317) Coffee Break

14:40 – 16:00 (FF303) Embury Symposium VI

Session Chair: H. Zurob

14:40 – 15:00

Taxonomy, Design and Performance of Periodic Lattice Materials

(INVITED)

Frank W. Zok, Matt R. Begley, Ryan Latture, Amanda Ruschel
University of California, Santa Barbara

Additive manufacturing has enabled fabrication of previously-unimaginable lightweight lattice materials over length scales ranging from micrometers to meters. Despite this progress, many of the principles underpinning design, fabrication and performance of such materials remain to be established. This presentation will focus on recent developments and future challenges in this field. It will address strategies for identifying and classifying lattice topologies in a systematic manner; effects of topology on elastic and fracture properties of lattices; and roles of features – notably nodal fillets, free surfaces, and strut defects – on mechanical performance. Challenges in design and fabrication of multi-material lattices will also be discussed.

15:00 – 15:20

Advantages of Disorder in Cellular Solids

(INVITED)

Derek Aranguren van Egmond, Glenn Hibbard, Ben Hatton
University of Toronto

Structural cellular solids in nature, such as trabecular bone, corals, diatom frustules and plant stems, are typically disordered with respect to the cell size regularity. Intuitively, ordered honeycombs should have an advantage in both strength and stiffness, so why are they not more common in nature? What is the disorder (cell size variation) in natural cellular solids anyway? And could it actually give some evolutionary advantage?

Herein, we have generated 2D cellular panels with increasing structural disorder, to compare to an ordered hexagonal honeycomb of the same area fraction. These models were designed using stochastic Voronoi patterns, then 3D printed (MultiJet) and mechanically tested. We have defined a "regularity parameter" for the cell size variation. Uniaxial tension, compression and fracture experiments reveal significant crack path deviations and strain delocalization that is sensitive to disorder. In fact, we found enhancements in ductility and fracture toughness between 30-90% beyond that for the ordered honeycomb controls.

15:20 – 16:00 Discussion

14:40 – 16:00 (FF317) Computational Materials Science III

Session Chair: L. Romaner

14:40 – 15:00

Modeling Non-Equilibrium Microstructure Kinetics Using Structural Phase Field Crystal Theories

(INVITED)

Nik Provatas
McGill University

This talk will review closely connected density functional type theories that employ both short and long range, rotationally invariant, multi-point particle interactions. These give rise to a class of structural phase field crystal (XPFC) models. Results from recent XPFC modelling of solidification phenomena will be presented. We begin with multi-step nucleation pathways in nano-particle precipitation in liquids and solids. We then examine a proposed mechanism for second phase solids whose formation is triggered by voids in nano-confined liquid pools during rapid cooling. We then examine solute drag between structurally dissimilar crystalline solid phases in binary and ternary alloys. We end with a new formalism for a unified PFC-type theory that quantitatively captures the thermodynamics of solid, liquid and vapour phases. Latent heat effects on recalescence are demonstrated in the context of PFC theory.

15:00 – 15:20

Phase-field Modeling of Widmanstätten Growth

Hocine Lebbad[1], Benoît Appolaire[2], Yann Le Bouar[2], and Alphonse Finel[2]
[1]The University of British Columbia
[2]Université de Lorraine, LEM (CNRS/ONERA)

Widmanstätten structures are observed in various metallic alloys. They are caracterized by their acicular morphology and their singular kinetics which is linear in time in isothermal conditions. These structures are known to impact mechanical strength and fatigue properties, it is therefore crucial to control their growth. The present work aims at understanding their growth mechanisms as many open questions remain. A phase-field model coupling chemical and elastic effects has first been developed. We show that the anisotropic internal stresses caused by the phase transformation play a key role in determining the singular linear in time kinetics, the size and the shape of the Widmanstätten structures. Furthermore, we have demonstrated the ability of our phase field model to correctly describe the growth of acicular morphologies in titanium alloys. Then, we have developed specific phase-field models to analyse the consequences of two plastic relaxation mechanisms.

15:20 – 15:40

Introducing Density Shifts to Binary Alloy Phase Field Crystal Models

Matthew Frick and Nikolas Provatas
McGill University

Phase Field Crystal (PFC) models are simplified classical Density Functional Theories (cDFT) which combine atomistic length scales and diffusive time kinetics to explore defect moderated processes that occur on timescales unattainable by molecular dynamics. For simplicity, binary alloy PFC models have traditionally assumed that phases have equal bulk densities. In this work, we expand the PFC alloy formalism to allow for the incorporation of large density shifts between solid and disordered phases. The basis of our new approach is to employ the grand potential density to control thermodynamic pressure and to transition from an isochoric to isobaric ensemble of an alloy. As an application of this formalism we will explore the role of pressure on three example processes: pressure mediated pre-melting in grain boundaries, pressure-driven phase instability and pressure-driven grain boundary motion.

15:40 – 16:00

Modeling of Multi-pass Rolling During Thermo-mechanical Processing Using a Physically-based Model

Shenglong Liang, Hamid Azizi, Hatem S. Zurob
McMaster University

A physically-based model is developed to simulate thermo-mechanical processing of micro-alloyed steels. The model considers major restoration processes such as recovery, precipitation, recrystallization and grain growth in plain carbon and micro-alloyed steels and is capable of predicting properties such as grain size evolution during hot rolling process. The model was compared against both experimental metallography data and also grain size measurements using novel laser ultrasonic technique during hot working of micro-alloyed steels. Modeling of multi-pass rolling was also attempted by using the model, for both roughing and finishing regimes. Grain size evolution and mean flow stress can be predicted and compared with experimental data.

14:40-16:00 (FF217) Emerging Materials and Processes III

Session Chair: M. Xu

14:40 – 15:00

Synthesis and Characterization of pH Sensitive Copolymer for Targeted Oral Drug Delivery

Harish Chakrapani, Dr. João Soares, Dr. Hyo-Jick Choi
University of Alberta

pH-responsive polymers have been intensively investigated over the years due to their diverse applications in environmental decontamination, nutrient delivery/packaging, cosmetics, and pharmaceutical science. A pH-responsive swelling/shrinkage behaviour of encapsulation systems can be accounted for by the conformation change of polymer chains at different pH (i.e., extended or coiled). However, it is unusual to find their commercial applications due to several technical limitations such as incomplete protection of the encapsulated ingredients against harsh environmental conditions, weak response to pH change, and inefficient release behaviour. It is well known that one of the major technical challenges of developing an oral drug is mainly associated with the destabilization of

biopharmaceuticals in the acidic environment of the stomach (pH: 1-3). To this end, we synthesized pH-responsive poly(methyl methacrylate-co-methacrylic acid) copolymer [P(MMA-co-MAA; Mw ~25,000 Da, PDI ~1.5 -2] using free radical solvent polymerization. The prepared polymers were characterized by proton NMR, GPC, and FTIR, and employed to fabricate microparticles with pH-responsive macropores in the development of intestine-targeted drug delivery systems. The pH-responding release behaviour of the pored microparticles was examined by monitoring the time-dependent release profile of encapsulated 100-nm fluorescent nanoparticles in simulated gastrointestinal tract environment. Our pH-sensing polymer and microparticles will advance the current microencapsulation technology by solving key challenges in encapsulation, protection, and release of oral drugs and biopharmaceuticals.

15:00 – 15:20

Cellulose Nanofibers for Active Food Packaging of Fresh Produce

Karthik Ramachandran Shivakumar, Dr. Yaman Boluk, Dr. Phillip Choi
University of Alberta

Cellulose nanofibers are fibres of diameter <5 nm and length <1000 nm giving them a high surface area produced by catalytic chemical oxidation of native/ regenerated cellulose fibres with TEMPO method. By this process the polymer becomes monodisperse, has lower degree of polymerization and forms a transparent film with good barrier and mechanical properties. This has been studied extensively over the past two decades, but for the first-time cellulose nanofibers are being studied with Nano calcium hydroxide. This composite is made by drop growth of crystals of calcium hydroxide on cellulose nanofibers. It can be used for the bulk storage of fresh produce. The cardboard storage box can be coated by this material and the carbon dioxide produced by the fresh produce will be absorbed by the calcium hydroxide and forms calcium carbonate, by doing so the production of ethylene and other ripening agents in the food can be minimized and thus the shelf life of the produce could be increased. We are studying the uniformity of the formation of Nano crystals of calcium hydroxide on the surface of the fibres and conforming using FE-SEM, studying the extent of carbonation using thermogravimetric analysis on older films, also confirming the carbonation using FTIR. Our cellulose nanofiber and calcium hydroxide composite (Nano lime paper) will co-compliment the barrier property and carbon capture property of each other and advance the current passive packing technology into a newer smarter packing system or in other words it will act as an active package.

15:20 – 15:40

Sulfated b-Cyclodextrin Layer-by-Layer Films in Heavy Metals Detection

Jessica de Alemeida[1], Marystela Ferreira[2]
[1]State University of São Paulo (UNESP), [2]Federal University of São Carlos (UFSCar)

Nowadays, efforts have been made to monitor the environment of heavy metals contamination risk regions. In this scope, electrochemical sensors have been used for their precise and fast response. Thus, this work had as objective the development of a sensor built by a simple technique and composed of low-cost materials to detect and quantify cadmium and copper in hydric sources. We used the “Layer by Layer” technique, to build nanometric layers of poly(allylaminehydrochloride) and the sulfated b-cyclodextrin, by electrostatic interactions. The film was tested on the simultaneous presence of Cd2+ and Cu2+ at different concentrations and the same proportion. The obtained results allowed the quantification of the cadmium ions at an analytical range of 0.5 to 10.0 ppb, and copper at the analytical range of 0.5 to 8.0 ppm. These ranges were interesting, allowing the quantification of Cd and Cu at drinking water guideline concentrations of the World Health Organization.

15:40 – 16:00

Photocatalytic Degradation of Natural Organic Matters (NOM) by Plasmonic Photocatalysis Using UV-LED Controlled Periodic Illumination

Azar Fattahi, S. Kowalczyk, A. Kaur, R. Liang, N. Zhou, M. Servos
University of Waterloo

Plasmonic photocatalysis has recently come into focus as a very promising technology for high performance photocatalysis. It involves dispersal of noble metal nanoparticles into semiconductor photocatalysts and obtains drastic enhancement of photoreactivity under the irradiation of UV and a broad range of visible light. In addition Plasmonic photocatalysis create advance oxidation processes (AOPs) that can greatly improve the rate of disinfection and the range of organism targeted and also can be used to concurrently degrade numerous chemical contaminates including natural organic matter (NOM). NOM derives from decomposing plants and animal residues and microbial activities and is ubiquitous in surface and groundwater. In the current study, the effect of AgTiO2 nanocomposites as plasmonic photocatalysis on NOM investigated using UV-LED controlled periodic illumination.

16:15-17:15 (Angus 098) MacDonald Lecture

Dynamic Processes in Colloidal Crystals and Glasses

Frans Spaepen
School of Engineering and Applied Sciences, Harvard University, Cambridge, MA, USA

Colloidal particles in suspension form liquid, crystalline and glassy phases similar to those formed by atoms. Since the particles are “fat” (~1μm) and “slow” (~10Hz), they can be individually tracked in space and time by confocal microscopy. Dense colloidal systems therefore serve as "analog computers" to study the dynamics of condensed matter, and provide a direct look, at the particle level, of complex phenomena, such as phase transformations, atomic transport and plastic deformation.
Examples to be discussed include: crystal nucleation and growth from the melt; the formation of misfit dislocations in epitaxial growth; the custom design of grain boundaries; the interaction of dislocations and grain boundaries; the determination of the grain boundary stiffness from thermal fluctuations; and the deformation mechanisms of monodisperse glasses.
Using a recently developed method, based on coupling the colloidal crystals or glasses to a calibrated gel of known stiffness, it is possible to measure the stress during deformation, and to produce stress-strain curves. The features of those curves (elastic deformation, yield, plastic deformation, stress relaxation) can be related to specific defect motion in the samples.

18:00 (Sage) Conference Banquet

Thursday, June 13

8:00 – 9:00 (FSC Lobby) Breakfast

9:00 – 12:30 (FF303) Embury Symposium VII

Session Chair: C.W. Sinclair

9:00 – 9:30

Canadian Steel – Accelerating Into the Future

(INVITED)

David Overby
Stelco

The steel industry in Canada has been at the forefront of technical developments for decades. It continues to develop advanced processes and products, applying new fundamental understanding and adapting to changes in the regulatory landscape. Collaboration across geographic and technical boundaries will continue to be a key to success. In this presentation, we will consider some of the processes and products that appear to be on the horizon.

9:30 – 9:50

Perspectives and Prospectives in Vehicle Lightweighting: Many Faces of Advanced Steels

(INVITED)

Mohammad M. Gouné[1], T. Iung[2]

[1] ICMCB-CNRS, 87 Avenue du Docteur Schweitzer, 33608 Pessac, France

[2] Maizieres Automotive Products R&D, BP 30320, 57283 Maizières-les-Metz Cedex, France

Almost 60 % weight of the materials used to build a modern car are steel based. However, steel is under question since the automotive sector will undergo radical change in the short coming years. It will face a number of major challenges:

- more and more strict environmental and energy standards,
- the competition with other lighter materials such as aluminium, magnesium and carbon fibers,
- the emergence of both electrical and autonomous vehicles,
- and the digital revolution under way.

In a first part, we will take stock of the advanced steel in the automotive industry: the process involved, the microstructures formed and the resulting properties. In a second part, we will aim to provide elements of an answer to the following question: is steel in its many facets offers solutions for tomorrow's automobility? and how ?

9:50 – 10:10

Towards a Better Understanding of the Damage Properties of Dual Phase Steels

(INVITED)

C.P. Scott [a], B. Shalchi Amirkhiz [a], I. Pushkareva [a], F. Fazeli [a], S.Y.P. Allain [b]

[a] CanmetMATERIALS

[b] Institut Jean Lamour, UMR CNRS-UL 7198, France

Ferrite-martensite dual phase (DP) steels are the most widely used advanced high strength steels (AHSS) in cold stamped automotive body-in-white applications. This commercial success has been achieved despite their mediocre damage properties in stretch flange forming operations, when compared to most competing AHSS metallurgies. There has been a long debate on the origin of this susceptibility to damage, given the otherwise excellent formability of DP alloys. In 2007 Kang, Ososkov, **Embury** and Wilkinson published an important paper using digital image correlation (DIC) to map the microstrains in both ferrite and martensite phases for the first time. This led to new insights into the relations between strain partitioning, DP microstructure and micro-crack formation. Here, we will discuss some of our recent findings on the importance of the basic microstructure (martensite content, percolation limit, ferrite grain size), the phase strength ratio (martensite carbon content, stress spectrum, tempering) and the work hardening behaviour of the individual phases on DP damage properties.

10:10 – 10:30

Phase Transformations, Clustering and Strengthening in Modern Line Pipe Steels

(INVITED)

F. Fazeli[1], C. Scott[1], B. Shalchi Amirkhiz[1], Brian Langelier[2], H. Zurob[2], Muhammad Arafin[3]
[1]CanmetMATERIALS, Natural Resources Canada
[2]McMaster University
[3]EVRAZ INC. NA

Tightly specified thermomechanical controlled processing (TMPC) routes followed by accelerated cooling (ACC) are required to produce advanced line pipe steels. The microstructure of modern steels that meet stringent industry specifications for strength, low-temperature toughness and weldability consists of variants of low-carbon bainite. This paper discusses the kinetics of bainite transformation during accelerated cooling and tempering of fresh bainite during coiling. The main scope will be the microstructural features and strengthening mechanisms of bainite with a focus on the role of microalloying elements. Microalloying elements in solid solution shift bainite transformation temperatures whereas the formation of V-C and V-N clusters during coiling suppresses the softening of fresh bainite and contributes markedly to the final strength of coiled plates. Vanadium interactions with carbon atoms also influence the tendency of carbon segregation to dislocations, thus changing the initial yielding behaviour of tempered bainite. Some guidelines to exploit these findings for the development of advanced line pipe steels will be provided

10:30 – 10:50 (FF 303) Coffee Break

10:50 – 11:10

Role of Intermetallic Compound in Fracture of Al-steel Resistance Spot Welds

(INVITED)

Jidong Kang[1], Liting Shi[1,2], Xu Chen[2], David R. Sigler[3], Amberlee S. Haselhuhn[3], Blair E. Carlson[3]
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Multi-material solutions are increasingly employed in the automotive industry for structural lightweighting and fuel economy which pose challenges for joining dissimilar materials, particularly aluminum to steel. General Motors developed a novel resistance spot welding technique using multi-ring domed electrode and multiple solidification weld schedules to address these challenges. In aluminum-steel resistance spot welds (RSWs), an intermetallic compound (IMC) layer is formed at the

interface and its strength affects the fracture modes, i.e. interfacial vs. pull out fracture, in tensile shear specimens.
In this talk, we present a new formula to calculate critical weld nugget diameters to predict pull out fracture of Al-steel RSWs. This formula takes into consideration material inhomogeneity, in particular, the unique shear strengths of the IMC and the heat affected zone (HAZ). The shear strength of the IMC is directly measured using a newly developed mini-shear test while the shear strength of the HAZ is directly measured using an ASTM standard shear test that Dr. David Embury helped to develop many years ago. The calculated critical weld nugget diameters are then compared with experimental results to predict the fracture modes for a variety of stack-ups of aluminum to steel RSWs. The results are in excellent agreement with the observed experimental fracture modes.

11:10 – 11:30
Microstructure-Property Development during CGL-Compatible Thermal Processing of Medium-Manganese Third Generation Advanced High Strength Steels
(INVITED)

J.R. McDermid[1], K.M.H. Bhadhon[1], D.M. Pallisco[1], V. Patel[1], M. Pourmajidian[1], F.E. Goodwin[2]
[1]McMaster University
[2]International Zinc Association North Carolina, USA

A series of prototype C-6Mn-xSi-yAl-zSn alloys were investigated to determine the relative roles of transformation- and twinning-induced plasticity (TRIP and TWIP) in the development of third generation advanced high strength steel (3G-AHSS) target mechanical properties. The annealing treatments employed were compatible with the continuous galvanizing line (CGL) with the objective of ultimately producing Zn-coated substrates. It was determined that 3G-AHSS target properties could be achieved using relatively low peak annealing temperatures for annealing times of 120 s. The resulting large volume fractions of chemically stable retained austenite (γ_{ret}) allowed for a gradual transformation of $\gamma_{ret} \rightarrow \alpha'$ via the TRIP effect during deformation, thereby allowing for the maintenance of a high instantaneous work hardening rates such that the onset of necking was delayed such that the 3G UTS and total elongation targets were met. TEM examination of the chemically stable γ_{ret} also showed evidence of mechanical twinning during deformation, thereby providing additional plasticity enhancement. It was further determined that a 0.05wt% Sn addition to a model C-6Mn-2Si alloy resulted in successful reactive wetting by a conventional continuous galvanizing bath without significantly affecting mechanical properties. This paper will discuss the microstructural development, both in the bulk substrate and surfaces, which have resulted in these prototype C-6Mn-xSi-yAl-zSn alloys showing strong potential for the production of metallic coated 3G-AHSS.

11:30 – 11:50
Multi-scale Modelling of Phase Transformations in Steels

Matthias Militzer
The University of British Columbia

Computational materials science provides tremendous opportunities to formulate next generation phase transformation process models by bridging from atomistic scale to microstructure scale simulations. The austenite-ferrite transformation kinetics is governed by the migration of interfaces such that interface-based design constitutes a new frontier of alloy design. Atomistic-scale simulations are used here to gain quantitative insight into the interaction of alloying elements with interfaces. On the microstructure scale, phase field modelling is a powerful tool to describe microstructures with complex

morphologies, e.g. bainitic and Widmanstätten ferrite. The status of developing next generation process models will be reviewed by discussing challenges and opportunities for high-performance steels.

11:50 – 12:10
Concluding Remarks
David Embury