

# MATLS 701/702 2016-17 Schedule

| Presenter           | Introduction          | Title  | Abstract  |
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| <b>SEPTEMBER 19</b> |                       |  |   |
| Carol F Glover      |                       | An SVET study of the throwing-power of in-coating corrosion inhibitor pigments                                       |   |
| <b>SEPTEMBER 26</b> |                       |  |   |
| Minghe Wang         | Xavier Michaud        | Abnormal magnetic behavior of electrodeposited nanocrystalline Ni-Fe alloys  | Studies of the structure and magnetic properties in a series of electrodeposited nanocrystalline Ni-Fe alloys have been carried out to understand the effect of composition and texture on the magnetic properties of the alloys. Magnetic measurements show that increasing Fe content increases saturation magnetization, while the coercivity is influenced by the individual texture components and their volume fractions. The texture of the alloys contains 18-37% volume fraction of nano-grains with main (100) texture component parallel to the growth direction of Ni-Fe alloys, with remaining 63%-82% of grains oriented randomly. Abnormal magnetic behaviour, expressed by partially inverted hysteresis loops with negative remanence, was observed for all alloys within the temperature range from 2K to 298K. The exchange interaction between the large magnetic moment of aggregated texture grains and the small moments of the adjacent randomly oriented grains is attributed to be the reason for the abnormal hysteresis loop shape in Ni-Fe alloys.   |
| <b>OCTOBER 3</b>    |                       |  |   |
| Alexandre Pofelski  | Christopher Pashartis | "Nanoscale strain characterization using Scanning Transmission Electron Microscopy (STEM) and Moiré interferometry". | Strain engineering is nowadays commonly used in the semiconductor field to boost devices performance. Changing locally the crystal periodicity enables to modify slightly the band structure, which can affect properties such as the carrier mobility or the band gap. Various methods exist to implement a specific strain field in a nanometer scaled device (epitaxy, thin film deposition, annealing, patterning, ...) which push the electron microscopy community to develop adapted characterization techniques to understand their mechanism. Multiple powerful techniques emerged based on different physics (diffraction, interferometry, direct imaging) and can be applied in current transmission electron microscopes. A novel technique using the interference between the aberration-corrected probe scanning grid and the crystal lattice to get relative deformation maps will be presented. A theoretical overview will be first outlined including practical aspects on how to record and process the data. Then, strain results on AlGaN/GaN Light Emitting Diode (LED) devices using STEM Moiré interferometry will be presented and briefly discussed. Finally, its performance with regards to |

comparable strain characterization techniques and potential developments will be explored.

**OCTOBER 17**

Ameya Kadrolkar

Yousef Tabatabaei

"Comprehensive Mathematical Model for Oxygen Steelmaking"

The BOF process is an important process for production of liquid steel from pig iron. Multiple phases (slag, metal and gas) and reaction sites make measurement of various process parameters difficult. In order to overcome this issue, attempts have been made to develop mathematical models and reliably predict the end-point temperature and composition of steel. Each of these models had variable degree of simplifying assumptions, especially with regard to the site of refining reactions. The ultimate goal of the proposed research is to develop a comprehensive model of BOF steelmaking based on a fundamental mechanistic understanding of the process. This study will focus on the kinetics of different reactions in the two prominent reaction zones. The role of bloated droplets in the refining of the metal in the emulsion zone has come to prominence due to recent experimental findings. The current study intends to incorporate the bloated droplet theory in the emulsion zone and evaluate its importance for process modeling of oxygen steelmaking. Some of the preliminary results include a heat balance model and a dynamic flux dissolution model. An explicit heat balance model to calculate the temperature profile of metal and slag phases has been developed. The simulation results are consistent with those obtained from 200 tonne oxygen steelmaking converter. The flux dissolution sub-model has been modified to make it truly dynamic. A procedure for coupling of the existing kinetic model with thermodynamic model (FactSage, Cell Model and Thermo-Calc) simultaneously has been introduced to predict the amount of dissolved lime with respect to the saturation concentration of CaO.

**OCTOBER 24**

Brian Jamieson

Kinetics of Manganese Reductive Alloying with Carbon and Silicon

Corporate Average Fuel Economy (CAFE) standards are pushing automotive manufacturers to seek novel methods of reducing fleet fuel emissions. Steel producers are aiming to address this with the commercial introduction of high manganese steels; 3rd Generation Advanced High Strength Steel (AHSS) is alloyed with around 4-11wt%Mn, while 2nd generation Twinning Induced Plasticity (TWIP) steels are composed of approximately 22wt%Mn. Currently the only commercial producer of TWIP steel is known to be using a reductive alloying approach to address the economic concerns of high manganese steel. This study seeks to determine the feasibility of manganese reductive alloying, using different reductants (specifically carbon and silicon in the present work). The outcome of this study will provide industrial partners with useful data regarding the kinetics of these reduction mechanisms, specifically as it relates to processing speed and composition limitations of various target steels. The study was carried out in a high temperature vertical tube furnace under a variety of composition and temperature changes; discrete data was generated

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|                   |                     |  | via a series of quenches at different times and used to generate a continuous kinetic function. The rate control step for silicothermic reduction appeared to be manganese diffusion control in the slag; SiO gas generation was observed along the slag-metal interface and is believed to hinder the rate of reaction by blocking the effective boundary layer volume; this could imply that mixed control is responsible. Literature review and lab work shows that the carbothermic system is likely to have two control stages; the faster stage is governed by MnO diffusion in the slag and the slower stage a chemical reaction involving CO nucleation and escape.  |
| <b>OCTOBER 31</b> |                     |  |  |
| Tai Xi Zhu        |                     | Gas Escape Rate Modeling from Droplet Swelling in BOF Steelmaking  | In BOF steelmaking, hot metal is refined into steel. When oxygen is jetted onto the surface of the liquid metal at supersonic velocities in BOF, it propels metal droplets into slag, creating the so-called metal-slag-gas emulsion. After the initial stage the droplets formed react with the slag causing CO gas to nucleate. If this gas nucleates inside the droplet it causes the metal droplet to swell. This swelling results in a much lower density allowing the droplet to remain suspended in the slag until swelling stops and the droplet falls back into the metal bath. Early studies have shown that up to 50% of furnace metal had been observed in this "emulsion" system, and more recently workers have shown that droplets are decarburized to a greater extent than the metal bath. Therefore, present work of developing a model for droplet swelling to determine residence time in the BOF steelmaking. Specifically, to model the gas escape component.  |
| <b>NOVEMBER 7</b> |                     |  |  |
| Sara Filice       | Nilushi Kariyawasam | Investigating Problematic Microstructural Features Causing Initiation of Hydrogen Induced Cracking in Linepipe Steel | <p>The aim of this research is to identify problematic microstructural features in a sour service X60 grade of linepipe steel (0.026 wt% C, 0.14 wt% Si, &lt;0.007 wt% P, &lt;0.0005 wt% S, 1.3 wt% Mn, &lt;0.15 wt% V+ Nb+Ti) that leads to initiation of hydrogen induced cracking (HIC). Through-thickness variations in the steel microstructure are to be characterized across multi-length scales using bulk extraction coupled with X-ray diffraction (XRD), light optical microscopy (LOM), scanning electron microscopy (SEM), and transmission electron microscopy (TEM); the latter two coupled with X-ray energy dispersive spectroscopy (EDS). Key features under study include the composition, shape, and distribution of inclusions as well as type and extent of interphase boundary, quarterline and centerline segregation.</p> <p>Specimens with a diameter of 10 mm and thickness of 1 mm were machined from the 1/4, 1/2, and 3/4 depths of X60 steel sheet to undergo hydrogen thermal desorption testing in an As2O3 solution using a current density of -0.5 mA/cm2 and -2 mA/cm2. Hydrogen permeation testing will then follow, using specimens with the size of</p> |

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|  |  | <p>80 x 95 x 2 mm<sup>3</sup>. This combination of testing will provide information regarding the type and potency of the various hydrogen traps in operation. Validation of the various hydrogen traps will be attempted by hydrogen charging subsized tensile samples in an NH<sub>4</sub>SCN solution while simultaneously being subjected to uniaxial tensile loading using a proof ring tensile test cell. The steel sample will undergo SEM analysis to characterize the initiation and propagation of cracks, and focused ion beam (FIB) milling will be used to acquire a TEM sample of the initiation site for TEM characterization.</p> <p>Keywords: Hydrogen Induced Cracking, X60 Sour, Inclusion Characterization, Thermal Desorption, Hydrogen Charging.</p> |
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| <b>NOVEMBER 14</b> |  |  |  |
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| <b>NOVEMBER 21</b> |  |  |  |
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| Mukesh Sharma |  | <p>Fundamentals of micro particle removal by liquid oxide</p> | <p>The ever increasing demand for cleaner steels, with a low inclusion content has highlighted the limits of our current knowledge for controlling and predicting inclusion removal during liquid steel processing. Key knowledge gaps in the inclusion removal area result from the complex nature of the problem associated with measuring and visualizing the phenomena being studied. There is uncertainty with respect to the dynamic changes that inclusions undergo and interpretation of the data collected to accurately predict inclusion dissolution mechanisms and kinetics in slags. Laser scanning confocal microscope (LSCM) allows for continuous in situ observation of micron-size samples in real time, at high resolution, under conditions relevant to the steelmaking process. In LSCM, a single particle (inclusion) is placed on the surface of a solid slag and the inclusion-slag system is heated to steelmaking temperature under inert atmosphere and the dynamic changes in inclusion size is measured to determine dissolution kinetics and mechanism.</p> <p>In the current work, results from in-situ dissolution of alumina inclusion in a ladle type slag at 1500, 1550 and 1600°C will be discussed. Interestingly, it is observed that non-spherical particles rotate as they dissolve, whereby the dimension of dissolving particle in all principal directions (X, Y and Z) can be recorded and analyzed. We believe that this measurement of dissolving particle in 3 dimensions provides data for a slightly better modelling approach than the conventional approach where the irregular inclusion is assumed to dissolve as an equivalent sphere. The inclusion dissolution kinetics in our work is assumed to be controlled by mass transfer in slag. Preliminary results in modelling the dissolution kinetics for this inclusion/slag system is presented along with a few interesting in situ observations.</p> <p>Keywords: dissolution kinetics, alumina, steel cleanliness, laser scanning confocal microscope</p> |
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| NOVEMBER 28    |             |  |   |
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| Xavier Michaud | Minghe Wang | "Characterization of Sodium Beta-Alumina Solid Electrolytes Using DC Coulometry" | <p>There majority of secondary (rechargeable) cells have a solid anode and cathode with a liquid electrolyte (S-L-S cells). Some of the cells that fall under this construction are the more common lithium-ion batteries, the lead-acid batteries, and Ni-MH batteries. There are three other "common" cell constructions. These are the all-solid cells (Li-metal batteries), all liquid cells (in development), and the liquid-solid-liquid cells (Na-S, Na-NiCl). The L-S-L are the primary focus of this work. However, what is learned from this study could potentially apply to other cell constructions.</p> <p>During the development of ultra-high surface area electrolytes for L-S-L cells, it was determined that standard methods of analysis, like AC impedance spectroscopy, might not be suitable. A new method is being implemented to separate the contributions of the interface and bulk resistances to the total cell resistance. Previous work has shown that up to 80% of the electrolyte was due to the interface. It is expected that with significant modification of the electrolyte interface, the interfacial resistance will be suppressed.</p> <p>The development of this new method is tested on sodium beta-alumina solid electrolyte. This electrolyte is well known and has been thoroughly characterized in the 70s and 80s. It is used in the Na-S and Na-NiCl cells which have been shown to have a high theoretical energy capacity. By further reducing the internal resistance, these cells would become more attractive to the energy market.</p> |

| JANUARY 2       |  |   |   |
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| Shooka Mahboubi |  | Oxide Scale Stability of Type 310S Stainless Steel in High Temperature Air-Water Vapour Mixture | <p>It is well-known that increasing the alloyed Cr-content can enhance the formation of a protective external Cr<sub>2</sub>O<sub>3</sub>-based scale that is desirable for alloys used as structural components in high temperature applications such as: steam boiler power plants, solid oxide fuel cells, nuclear reactors and geothermal power plants. However, Cr<sub>2</sub>O<sub>3</sub>-based scales are susceptible to volatilization in such environment, leaving behind less protective and Fe-rich oxide scales. In the current study, a steam-oxidation testing apparatus was built in order to study the stability of the Cr<sub>2</sub>O<sub>3</sub>-based scales formed on relatively high Cr-containing Type 310S stainless steel. Coupons were exposed at atmospheric pressure and 550 °C air-water vapor mixture with 200 mL/min flow rate for up to 1000 h. The oxide scale structure and morphology was then studied by means of gravimetric measurements and electron microscopy techniques. Results from this study were compared to those obtained in high pressure supercritical water condition (water at T&gt;374 °C and P&gt; 22 MPa in supercritical water-cooled nuclear reactors) to address the effect of pressure on the kinetics of Cr<sub>2</sub>O<sub>3</sub>-based scales formation. Mechanism of the Cr<sub>2</sub>O<sub>3</sub>-based scale</p> |

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|                       |              |   | volatilization was also examined within the context of scale stabilization by the alloyed Cr content.   |
| <b>JANUARY 9</b>      |              |   |   |
| Christopher Pashartis |              | Localization and Disorder in III/V Semiconductor Alloys | Semiconductor alloys of III/V have been studied and suggested for use in 1.55 $\mu\text{m}$ telecommunication VCSELs (Vertical Cavity Surface Emitting Lasers) in an effort to prepare for the onset of a data bottleneck. To alleviate this issue, we proposed to study the amount of disorder or localization introduced into a material in order to engineer a new lasing medium. Optoelectronic properties of III/V semiconductor alloys are examined using first principles with a focus on the spatial localization of electronic states. Localization is compared at the band edges due to various impurities in a host GaAs structure including its impact on the photoluminescence line widths and carrier mobilities. By studying localization in the band edges we can predict how effective a given material is for use in lasers and solar cells.  |
| <b>JANUARY 16</b>     |              |   |   |
| Guest Speaker         |              |   |   |
| <b>JANUARY 23</b>     |              |   |   |
| Jieming Li            | Juan Wu      | Conducting Polymer-based Electrodes for Electrochemical | Electrochemical supercapacitors are currently under intensive investigation as advanced energy storage devices, which offer the benefits of high capacitance, high power density and good cyclic stability. Polypyrrole (PPy) is a promising electrode material because of high specific capacitance, high conductivity and low cost. Various strategies were developed for the fabrication of PPy nanoparticles and films. Advanced dispersants were developed for the dispersion of multiwalled carbon nanotubes (MWCNT) and fabrication of advanced PPy-MWCNT composites. The use of novel anionic dopants for chemical polymerization allowed good electrochemical performance and cyclic stability of electrodes with high active mass loading (around 30mg $\text{cm}^{-2}$ ). The specific capacitance of 3.21 F $\text{cm}^{-2}$ was achieved at a scan rate of 2 mV $\text{s}^{-1}$ for the PPy- MWCNT composites. |
| <b>JANUARY 30</b>     |              |   |   |
| Keyan Miao            | Linfeng Zhou | Dissolution of calcium aluminate in liquid oxide        | Calcium treatment by powder injection or wire feeding is a common technique used in steel refining to modify oxide and sulphide inclusions. However, insufficient or superfluous addition of calcium leads to incomplete or excessive modification of alumina inclusions and the formation of solid calcium aluminates or CaS, which are detrimental to the castability of steels. Removing inclusions from liquid steel to slag phase in the ladle, tundish or mold prior to casting can minimize inclusion content. It is therefore important to understand the inclusion-  |

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|                     |               |  | <p>slag interaction to improve the removability of inclusions from liquid steel.</p> <p>The work presented here focuses on calcium aluminate inclusions and their removal. The rate of calcium aluminate inclusion dissolution in CaO-SiO<sub>2</sub>-Al<sub>2</sub>O<sub>3</sub> slags has been measured using a confocal scanning laser microscope at three different temperatures: 1500, 1550 and 1600 oC. Particle dissolution rate is estimated from volume change using shrinkage core models (SCM), by converting area of irregular shape inclusions projected at the horizontal plane to radius of spherical particles with equivalent projected area. It is found that total dissolution time decreased with an increase in temperature. The potential rate controlling mechanism has been evaluated. The proposed SCM cannot predict the dissolution rate of calcium aluminate inclusions.</p>   |
| <b>FEBRUARY 6</b>   |               |  |  |
| Nilushi Kariyawasam |               |  |  |
| <b>FEBRUARY 13</b>  |               |  |  |
| Sheikh Jamil Ahmed  |               |  |  |
| <b>FEBRUARY 27</b>  |               |  |  |
| Linfeng Zhou        | Michelia Alba | Effect of Vanadium Addition on Deformation and Fracture Behavior of DP1200 Dual Phase steels | <p>Advanced high strength steels (AHSS) is one of the lightweight material solutions in response to the stringent regulation on fuel economy and greenhouse gas emissions in the automotive industry. Dual-phase (DP) steels that consist of a hard martensite phase embedded in a soft ferrite matrix are the most widely used AHSS due to their simple microstructure, robust thermo-mechanical processing and attractive mechanical properties. However, DP steels are prone to deform heterogeneously with strong strain partitioning between phases. The addition of Vanadium in DP steels can form nano-precipitates of vanadium carbide (VC) that strengthen the ferrite and thus reduce the strain partitioning. This paper presents the influence of VCs on the deformation and damage behavior of ferrite-martensite DP1200 steels with and without Vanadium at the microscopic level. In-situ uniaxial tension tests were conducted on DP steels with similar martensite volume fractions within a scanning electron microscope (SEM) chamber. Microscopic-digital image correlation (<math>\mu</math>DIC) was then employed to analyze the local strain partitioning between ferrite and martensite. Local damage events such as void formation at ferrite martensite island interfaces and in the martensite islands were observed and rationalized with the <math>\mu</math>DIC results.</p> |
| <b>MARCH 6</b>      |               |  |  |
| Cameron Wallar      |               |  |  |
| <b>MARCH 13</b>     |               |  |  |
| Eric (Weiwei) Zhao  |               |  |  |

| MARCH 20            |                 |   |  |
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| Evan Drew           | Adam Moniz      | The effect of strain ageing on plasticity in high strength steels | The influence of strain ageing on the mechanical properties, plasticity and fracture of quenched and tempered martensitic 300M was investigated. Tensile testing with variable strain rate and sample geometry determined that strain ageing has an appreciable impact on mechanical properties and final fracture of 300M. Digital image correlation (DIC) was utilized in order to visually distinguish differences in plastic flow produced by strain ageing. Fracture analysis was conducted using scanning electron microscopy (SEM) to identify differences in fracture morphology due to strain ageing. Inclusion and impurity analysis was conducted using SEM and INCA Feature software. A model by Brown and Embury is used to link particle size and distribution to failure strain and fracture mode. Models for dislocation evolution and locking based on fundamental theories are also produced and evaluated in an effort to relate mechanical behavior to dislocation population behavior.  |
| MARCH 27            |                 |   |  |
| Yousef Tabatabaei   | Ameya Kadrolkar | Transformation of inclusions in the Ladle Metallurgy Furnace      | <p>SEN clogging by solid alumina inclusions is a common problem during continuous casting of aluminum killed steel. These inclusion are mostly formed in the ladle due to deoxidation process which is necessary for continuous casting.</p> <p>Calcium treatment is a one of the promising methods to modify solid alumina inclusions to liquid or partially liquid spherical calcium aluminates which has been widely used in Al-killed steels for decades. However, injected calcium can also react with the dissolved sulfur to form calcium sulfide.</p> <p>The aim of this research is to investigate the mechanism, thermodynamics and kinetics of the oxide inclusion transformation during Ca treatment to provide a comprehensive model to predict and explain evolution of inclusions size, type and chemical development during secondary steel making. Furthermore, the competition of sulfide inclusions with alumina for calcium is taken into accounts. Finally, the results is compared and validated with data from the steel plant.</p> |
| APRIL 3             |                 |   |  |
| Mady Bhattacharyya  |                 |   |  |
| APRIL 10            |                 |   |  |
| Juan Wu             | Jieming Li      |   |  |
| APRIL 17            |                 |   |  |
| Maedeh Pourmajidian |                 |   |  |

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| <b>MAY 29</b>     |  |   |  |
| Daniella Pallisco |  | Effect of Starting Microstructure and Intercritical Annealing Parameters on the Microstructure and Mechanical Properties of a Medium-Mn Third-Generation Advanced High Strength Steel | Third generation advanced high strength steels (3G AHSS) are relatively cost-effective alloys with superior combinations of high strength and ductility that would facilitate vehicle light-weighting. The present work investigates the mechanical properties and microstructural evolution of a prototype 0.15C-6Mn-2Al-1Si 3G AHSS arising from heat treatments that are compatible with the continuous galvanizing process. The effects of starting microstructure and thermal processing parameters on the microstructural evolution of the alloy and resultant tensile properties within the context of established targets will be presented. |

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| <b>MAY 1</b>  |               |  |  |
| Daniel Osorio | James Tedesco |  |  |

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| <b>MAY 8</b>  |               |  |  |
| James Tedesco | Daniel Osorio |  |  |

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| <b>MAY 15</b> |  |  |  |
| Michela Alba  |  |  |  |

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| <b>APRIL 24</b> |  |  |  |
| Chao Zheng      |  |  |  |