



Matls 701/702 Seminar Series Fall Term Schedule

**Thursday's at 2:00 p.m. – 2:40 p.m.
MS Teams**

ENGINEERING
Materials Science
& Engineering



Date	Speaker	Title
September 10	Orientation	
September 17	Health & Safety Training	
September 24	Hesham Hassan	Characterization of Confined Heteroepitaxy 2D Materials through Correlative Electron Microscopy and Atomic-scale Image Stitching
October 1	Bahareh Mobedpour	Microstructural and Mechanical Characterization of Bainitic Steels
October 8	Fan Xu	Interface Engineering for Highly Efficient and Stable Perovskite Solar Cell
October 15	Angshuman Podder	Modelling of Non-Metallic Steel Inclusions in Ladle Metallurgy Furnace
October 22	Saba Gol	Selective Oxidation of Medium-Manganese Steel
October 29	Chiara Micheletti	Resolving Bone and Bone Interfaces at the Nanoscale with Electron Microscopy
November 5	Mohamed Nawwar	Nanocomposite Materials for High Performance Supercapacitor Electrodes and Devices
November 12	Liza DiCecco	Scanning Electron Microscopy Imaging Applications of Room Temperature Ionic Liquids in the Biological Field
November 19	Kaelan Rorabeck	Nanocomposite Formations via Advanced Colloidal Techniques for Energy Storage in Supercapacitors
November 26	Kaustubh Kulkarni	Investigation of Functional Properties of Transition-metal Silicides
December 3	Chen Gu	Advanced Microstructure Characterization in hot-rolled High Strength Steels
December 10	Himanshu Saini	Theoretical Investigation of Spin Transfer Torque in Weyl Semimetals
December 17	Coleton Parks	Analysis of High-Temperature Nickel Superalloy Brazing for Turbine Engine Repair

Hesham El-Sherif
Ph.D. Candidate



Matls 701/702 Seminar Series

Characterization of Confined Heteroepitaxy 2D Materials through Correlative Electron Microscopy and Atomic-scale Image Stitching

A new category of 2D materials has been recently realized through a confinement heteroepitaxy (CHet) fabrication method. In this technique, mono- to few-layers of metals can be intercalated between epitaxial graphene (EG) grown on silicon carbide (SiC) substrates. Then, the metal intercalation process can be followed by nitrogen or oxygen intercalation and co-reaction, which synthesizes various combinations of 2D III-V Nitride semiconductors or 2D metal oxides in a form of Van der Waals heterostructures. With combinations, CHet materials attract interest for many next-generation electronic devices.

However, the implementation of the CHet synthesis into devices is still challenging because the CHet layers are grown disconnected within the SiC terraces formed by the offcut of the substrate crystal. Also, there are many unwanted features on the as-prepared CHet surface that could eventually limit the device performance. Furthermore, the characterization of such atomically thick layers is also challenging to conduct and to understand the relationship between growth parameters and their quality and thickness distribution.

Here, various correlative electron microscopy approaches are introduced to understand the structure and chemistry of the CHet layers to push forward the characterization of the layers' quality and properties. In addition, we bridge the imaging scalability gap between atomic-resolution STEM in cross-section view and the plan-view SEM imaging contrast of the CHet layers' surface through stitching hundreds of atomic-resolution images, accelerating the growth-characterization optimization.

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Thursday, September 24th, 2020
2:00 p.m. – 2:40 p.m.
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**Bahareh
Mobedpour**
Ph.D. Candidate



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Microstructural and Mechanical Characterization of Bainitic Steels

New generation of Advanced High Strength Steels (AHSS) are required for weight reduction and improved safety in the transportation sector. These steels are highly value-added and strategic products which are at research and development stage. As such prior to commercial production and adopting a proper variant of these steels, the interplay between processing parameters, microstructure and properties should be determined. A potential candidate for new generation of AHSS is bainitic steels, which have demonstrated a good combination of strength and ductility due to their multiphase microstructure. While properties and mechanical behavior of bainitic steels depend on microstructural features such as phase fractions, morphology and texture. Bainitic transformation is still one of the least understood phase transformations and there is still lack of fundamental knowledge about the mechanical responses of bainitic steels with complex microstructure to different loading paths and service scenarios.

The present work aims to investigate the effect of microstructural features on mechanical properties of bainitic steels by using experimental characterizations. The results will be discussed and interpreted.

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Thursday, October 1, 2020
2:00 p.m. – 2:40 p.m.
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Alex (Fan) Xu
Ph.D. Candidate



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Interface Engineering for Highly Efficient and Stable Perovskite Solar Cell

Organic–inorganic hybrid perovskite solar cells (OIHPSCs) have been widely considered as a promising candidate for the next generation of photovoltaics, due to their excellent absorption property, long diffusion length, etc. However, the commonly employed formamidinium (FA)- containing perovskite solar cells (PSCs) exhibit a severe phase instability problem, thereby limiting their commercial applications.

In this presentation, both phase stability and energy efficiency of FA-based PSCs were improved by treating the perovskite surface with pyrrolidinium hydroiodide (Pyl) salts, resulting in a 1D perovskite structure (PyPbI₃), stacked on the original 3D perovskite. By employing in situ XRD measurements, we revealed that the temperature-dependent phase transition activation barrier was enhanced after forming the 1D/3D structure, resulting in a prolonged transition time by 30–40-fold. From the first-principle calculations, we found the thermodynamic energy difference between two phases reduced from -0.16 to -0.04 eV after the stacking of 1D PyPbI₃, offering additional lifetime improvement. Moreover, the champion 1D/3D bilayer PSC exhibits a boosted power conversion efficiency of 19.62%, versus 18.21% of the control. Such 1D/3D bilayer structure may be employed in PSCs to enhance their phase stability and photovoltaic performance.

Angshuman Podder
Ph.D. Candidate



Matls 701/702 Seminar Series

**Modelling of Non-Metallic Steel
Inclusion in Ladle Metallurgy Furnace**

Abstract Coming Soon

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Thursday, October 15, 2020
2:00 p.m. – 2:40 p.m.
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Saba Gol
MAsc Candidate



Matls 701/702 Seminar Series

Selective oxidation of Medium-Mn Third-Generation Advanced High Strength Steel

Third-generation advanced high strength steels are being developed to facilitate vehicle lightweighting in order to improve their fuel efficiency without compromising passenger safety due to their excellent combination of strength, formability, toughness and fatigue resistance across a large variety of applications.. Medium-Mn steels are promising candidates to meet these demands. This presentation will summarize the selective oxidation results for a prototype Medium-Mn 0.15C-6.02Mn-1.05Al-0.97Si-0.07Mo 3G AHSS after CGL-compatible thermal processing as well as the design of thermal profile for a prototype Medium-Mn 0.2C-6.25Mn-1.04Si,1.08Al-0.51Mo-0.03Cr 3G AHSS. This work presents the investigations conducted to determine morphology, spatial distribution of the selective surface and subsurface oxides formed during the intercritical annealing process as a function of process atmosphere pO_2 .

XPS results indicated that increasing the process atmosphere resulted in a transition from the external to internal selective oxidation as well as holding the experimental steel at the intercritical temperature for longer times led to an increase in either the thickness of external oxides or depth of internal oxides.

Thursday, October 22, 2020
2:00 p.m. – 2:40 p.m.
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Chiara Micheletti

Ph.D. Candidate



Matls 701/702 Seminar Series

Resolving Bone and Bone Interfaces at the Nanoscale with Electron Microscopy

Bone is a hierarchical material whose structure at the nanoscale still needs to be fully unveiled. Thorough understanding of bone structure is fundamental for what concerns its mechanical properties and the effect of diseases on its functioning. Moreover, arrangement of bone at the interface with a biomaterial can provide insights on how new bone is formed and how to improve this process by properly designing implant materials.

Scanning transmission electron microscopy (STEM) is an exceptional tool to resolve bone and bone interfaces at the nanoscale. In this seminar, different examples on how STEM can assist in the characterization of healthy and diseased bone, both alone and in presence of biomaterials, will be provided. In particular, the use of STEM imaging, electron tomography and image processing software to understand the nanoscale structure of healthy bone will be analyzed. The combination of STEM with analytical techniques such as electron energy loss spectroscopy (EELS) to understand how bacteria infections affect bone structure will be discussed. Finally, the investigation of new biomaterials and therapeutics to improve osteoporotic bone growth using STEM electron tomography will be reported.

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Thursday, October 29, 2020

2:00 p.m. – 2:40 p.m.

MS Teams

Mohamed Nawwar

Ph.D. Candidate



MATLS 702 Seminar Series

Nanocomposite Materials for High Performance Supercapacitor Electrodes and Devices

Electrochemical supercapacitors (ES) are one of the modern energy storage systems for the applications of electric vehicles, electronic devices, and lit sources. To reach the max effect in these types of storage systems, optimization of power and energy densities should be applied. The storage mechanisms can be classified into two mechanisms; EDLCs and Pseudo capacitance. To optimize the advantages of (EDLCs) and pseudo capacitors, such as increase the conductivity, reduce resistivity, advanced stability and enhanced performance, a hybrid asymmetric supercapacitors with high areal capacitance should be developed.

Magnetite (Fe_3O_4) based composites are relevant candidate materials that could be used as an active material in the negative supercapacitor electrodes due to their high theoretical capacitance and low cost. However, the low conductivity and high susceptibility to agglomeration of Fe_3O_4 have significantly reduction effect on the capacitance especially at high active mass loading, which is an important parameter for the practical applications.

In this presentation, the application of conceptually new colloidal processing techniques and advanced dispersant agents will be discussed. Asymmetric hybrid supercapacitors depending on Fe_3O_4 based composites will be shown using different synthesis methods. Consequently, a multifunctional dispersing agent celestine blue dye and efficient in-situ synthesis method of mCNTs (Fe_3O_4 /CNTs) will be illustrated in addition to optimizing the higher mass ratio of the Fe_3O_4 /CNTs.

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Thursday, November 5, 2020

2:00 p.m. – 2:40 p.m.

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**Liza-Anastasia
DiCecco**
PhD Candidate



Matls 701/702 Seminar Series

Scanning Electron Microscopy Imaging Applications of Room Temperature Ionic Liquids in the Biological Field

Room temperature ionic liquids (RTILs), also referred to as molten or fused salts, are liquid at room temperature and composed of ions and short-lived ionic pairs. They are known for their attractive properties such as low vapor pressure, high ionic conductivity, non-combustibility, and capacity to dissolve many kinds of substances. However, only recently has the potential of RTILs as a preparation method for biological sample imaging in scanning electron microscopy (SEM) been explored. Applications of RTILs have been shown to provide improved or equivalent resolution and contrast compared to conventional preparation methods for biological SEM, which generally constitute dehydration, fixing, and/or coating or staining for biological samples. Preparing biological samples with RTILs for SEM usage involves simpler and shorter steps while their low vapor pressures enable samples wetted with ionic liquid solutions to be imaged under high vacuum conditions. These properties have provided new avenues for SEM applications involving hydrated biological materials, allowing samples to be observed in a more natural state, as well as novel mediums for *in situ* EM.

In this seminar, RTILs will be introduced in the context of an SEM preparation method for hard-to-image, soft and/or hydrated samples. Specific applications involving biological samples such as cell structures, bone, and biofilm observations will be discussed and interpreted. Notably, first-of-its kind work will be highlighted involving unfixed, hydrated bone imaged in SEM through an RTIL-based application method.

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Thursday, November 12, 2020
2:00 p.m. – 2:40 p.m.
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Kaelan Rorabeck
MAsc Candidate



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Nanocomposite Formations via Advanced Colloidal Techniques for Energy Storage in Supercapacitors

Our society's goal to reduce of carbon emissions while continuing to satisfy the increasing energy demand requires specialized technologies to meet specific needs. Electrochemical energy storage is a powerful tool used to develop efficacy in our grid system, unfortunately batteries perform poorly in high power demand applications. While traditional capacitors can be used, their low power density often becomes a limiting factor. Supercapacitors are an emerging technology that is bridging the gap between these classical electrochemical energy storage devices.

With the recent advancements in nanoscale materials science, Transition Metal Oxide (TMO) nanostructures and conducting polymers are under rigorous investigation to increase electrochemical performance of supercapacitors. In the Zhitomirsky group, we focus on testing new colloidal techniques and chemical surfactants to reduce agglomeration, which has led to increased BET surface areas and therein electrolyte permeability.

In this presentation, Salting Out and Butanol Extractions will be discussed and how the use of chemical surfactants can improve these extraction processes and promote improvements in electrochemical and capacitive properties of these nanocomposites by mesostructural manipulation.

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Thursday, November 19, 2020
2:00 p.m. – 2:40 p.m.
MS Teams

Kaustubh Kulkarni
Ph.D. Candidate



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Investigation of Functional Properties of Transition-metal Silicides.

The downscaling of transistors and interconnects have been successfully used for more than 4 decades to enhance the density and performance benefits in integrated circuits significantly. This pitch scaling along with the advancements in manufacturing processes has remarkably improved the performance of the transistors. As the downscaling increases, the interconnects hold the larger share of the overall delay and cost of the integrated circuits today than in the past.

Materials used presently for interconnects such as Cu and W suffer from challenges like size effects, electromigration, control of interconnect dimensions, efficient processes for manufacturing and patterning at nano-dimensions, and integration of new processes and structures with the current technologies. These challenges need to be addressed to create interconnects with high yield and performance sufficient for ultra-large scale integration needs. The transition metals silicides (TMS) which include Co_2Si , CoSi_2 , TiSi_2 , and NiSi_2 offer possible replacements for these materials. They exhibit lower resistance at nanoscale dimensions, good process compatibility with Si, and little to no electromigration.

In this presentation, property characteristics important for the performance of materials used for interconnects will be discussed. Also, our efforts in the development of TMS' for interconnects and characterization of their structure and properties using theoretical and experimental approaches will be presented.

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Thursday, November 26, 2020
2:00 p.m. – 2:40 p.m.
MS Teams

Chen Gu
PHD Candidate



Matls 701/702 Seminar Series

Advanced Microstructure Characterization in hot-rolled High Strength Steels

HSLA usually contains 0.05–0.25% carbon content and small amounts of alloy elements (<0.1%), such as Nb, V, Ti and Al, which enhance the strength through the formation of stable carbides, nitrides or carbonitrides. The trend of improving the strength and maintaining or improving other properties has led to a major increase in research to develop HSLA, which provide increased strength with equivalent, or improved, ductility. It has been widely used in oil and gas pipelines, automobile components, storage tanks, construction and farm machinery, industrial equipment, etc.

However quantitative analysis of precipitates lacks due to the difficulty in quantifying the light elements, like C and N. And the characterization of cluster in HSLA steel is also difficult because of the limitation in conventional TEM. The role of cluster and transformation from cluster to precipitates are not completely understood.

In my project, I will use advanced techniques, such as, correlative use of APT and other EM, 4D-STEM and in situ TEM to conduct the quantitative analysis of precipitates and analysis the transformation from cluster to precipitate, the effect of micro-alloy and processing parameters on the mechanical properties and microstructure, strain field and phase transformation in HSLA steel.

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Thursday, December 3, 2020
2:00 p.m. – 2:40 p.m.
MS Teams

Himanshu Saini

Ph.D. Candidate



Matls 701/702 Seminar Series

Theoretical Investigation of Spin Transfer Torque in Weyl Semimetals

A multilayered structure consisting of two ferromagnetic layers that sandwich an insulator as a tunnel barrier is called a Spin-Transfer-Torque Magnetic Random Access Memory (STT-MRAM). The STT-MRAM technology provides exciting features for building a new non-volatile memory with access speed similar to a Dynamic Random Access Memory. Currently, the Fe-Co/MgO based MRAM gives the best performance. However, due to scalability, it is not possible to take the technology further, and hence the fundamental research is needed. Recently, Weyl semimetals have emerged as a new class of topological material characterized by gapless points (Weyl nodes) in the bulk while breaking the inversion or time-reversal symmetry. The spin-transfer torque can be significantly improved due to the strong spin-orbit interaction in Weyl semimetals, because of which they can provide a more effective means of manipulating magnetic textures.

In this presentation, ab initio characterization of Weyl semimetals is discussed. The theoretical methodology for calculating the Chern number (chirality or "monopole charge") associated with Weyl nodes is based on an extended Wilson loop method and a Berry phase approach. Furthermore, a theoretical analysis of spin-transfer torque in magnetic Weyl semimetals will be presented.

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Thursday, December 10, 2020

2:00 p.m. – 2:40 p.m.

MS Teams

Coleton Parks
Ph.D. Candidate



Matls 701/702 Seminar Series
**Analysis of High-Temperature
Nickel Superalloy Brazing for
Turbine Engine Repair**

Abstract Coming Soon

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Thursday, December 17, 2020
2:00 p.m. – 2:40 p.m.
MS Teams