32nd CANADIAN MATERIALS SCIENCE CONFERENCE 2021

June 1, 2-4, 2021

FINAL PROGRAMME

version May 28

Hosted *Virtually* by Queen's University

Contents

Chair's Welcome

Dear Canadian Materials Science Community and International Guests:

It is with great honour that I welcome you to CMSC 2021, the 32nd Canadian Materials Science Conference, which incorporates the 70th Metal Physics and the 45th Metal Chemistry meetings. The conference theme this year is "community", to reflect on a very trying 2020 for all, which saw the postponement of this meeting for the first time in its history. Thanks to technology, built and running on the back-bone of semi- and metal conductors, insulators and light optic materials, we are able to safely meet together in a new yet familiar way to discuss materials science, see old friends, and make new ones, while the pandemic continues to impact our world. The program sessions include theoretical and experimental work on new and mature materials, features keynote lectures by the D.K.C. Memorial Award winner and the Metal Chemistry and Metal Physics award recipients. There is a pre-conference workshop on Irradiation to Simulate Reactor Conditions, and a student-only-session on Materials Commercialization. There is also a special symposium, Solute-Defect Interaction 2, in honour of Professor Emeritus Shig Saimoto with contributions from researchers from around the globe. CMSC is an important building block for many of our student researchers, who will will have their first conference experience here, interacting and testing their ideas with the community. CMSC is possible thanks to the continuing trustee role of MetSoc, the had work of the Organization Committee (p.3) and especially Candace Chabot for putting thoughts into action, and with the financial support of our industrial sponsors (p.4), who continue to believe in the importance of this meeting today to help solve the problems of tomorrow.

The history of this conference is evident, Hutchison, MacDonald, Basinski, Toguri, Brimacombe ….but it's future is brighter thanks to all of you, the community.

Enjoy the meeting.

Sincerely,

Brad Diak
CMSC2021 Chair
Queen's University, Kingston, Ontario

Important Information

Overview - After postponing for the first time since its inception in 1951, the 32nd Canadian Materials Science Conference (CMSC 2021) runs virtually this year in a live format. CMSC 2021 follows the tradition of previous conferences in this series held at different universities across Canada. It provides a collegial forum for students and researchers to discuss recent advances in the field of fundamental and applied materials chemistry, materials physics and materials engineering to promote a better understanding of the processes that determine the structure and properties of engineering materials at different length and time scales.

The conference features a pre-conference workshop, award lectures, special student-only session on entrepreneurship, two interactive poster sessions, and an international symposium on solute-defect interactions.

This event is organized in cooperation with the Metallurgy and Materials Society (MetSoc).

Virtual Platforms - The pre-conference workshop on June 1 will be presented using a video meeting interface, while the rest of the conference will run using the avatar-based platform from Virbela (www.virbela.com). *Information regarding accessing and using the avatar-based platform will be provided for registrants before the conference.*

Registration – You must be registered for the conference in order to participate. Please visit https://www.cmscconf.org/registration/.

Schedule – All scheduled events are based on Kingston Ontario local time, EST (GMT/UTC – 4). Since attendees are participating from different time zones, please use the internet to check Kingston Ontario time with your time.

Presentations - *Invited* and *keynote* talks are 25 minutes + 5 minutes questions; *Regular* talks are 12 minutes + 3 minutes questions; *Award lectures* are 50 minutes + 10 minutes questions. All presentations are live in the Virbela environment via file upload or screen share at time of event. Special training for presenters to use the presenter tools will be offered before the conference start – it is highly recommended presenters attend such events.

Posters – Posters are uploaded to individual virtual poster (web) boards at the venue on the day of the session. Posters must consist of one single page formatted as 16:9. File format can be a single graphic image files: .bmp, .gif, .jpg, (transparency is not preserved on a web board) or a pdf. [**Important**: images larger than 1500x1500 pixels cannot be uploaded. Virbela recommends that images be approximately 1000x1000 pixels in resolution. Images may be resized using Windows Paint3D or squoosh.app and should appear similarly to their larger counterparts when uploaded.]

Questions – Contact cmsc2021@queensu.ca about program and metsoc@cim.org about registration.

Organizing Committee

Conference Chair	**Brad Diak,** Queen's University
Conference Vice-Chair	**Yu Zhou**, University of Toronto
Logistics	**Candace Chabot**, Queen's University
MetSoc of CIM	**Brigitte Farah**, Managing Director **Victoria Woo**, Administrative Coordinator **Dimitrios Filippou**, Secretary, CMSC Liaison, Rio Tinto
Programme Committee	**Laurent Béland**, Queen's University **Kevin Daub**, Queen's University **Brad Diak**, Queen's University
Poster Sessions	**Olga Gopkalo**, Queen's University
Programme Design	**Megan Tucker**, Queen's University
Student Liaisons	**Sean Farrell**, Queen's University **Alex Pysklywec**, Queen's University **Matthew Thoms**, Queen's University
NexGen Materials Entrepreneurs Session Organizer	**Boyd Davis**, Kingston Process Metallurgy
Irradiation Workshop Organizers	**Laurent Béland**, Queen's University **Mark Daymond**, Queen's University
SDi2 Organizers	**Bradley Diak**, Queen's University **Marek Niewczas**, McMaster University **Chadwick Sinclair**, University of British Columbia

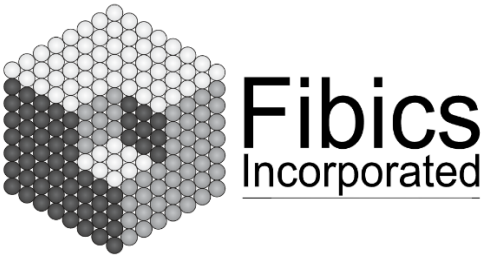
Sponsorship

The Organizers acknowledge the generous financial support of:

Best Student Poster Awards, Session 2

Best Student Presentation Awards

Irradiation of Materials Workshop



DKC MacDonald Memorial Lecture and Best Student Characterization Presentation Award

Kingston Works

Solute-Defect Characterization 2 Symposium and Student Poster Awards, Session 1

Conference Schedule at a Glance All times from Kingston, Ontario EDT (GMT/UTC-4).

EDT (GMT-4)	1-Jun Info Session	1-Jun Workshop	2-Jun Auditorium One	2-Jun Auditorium Two	3-Jun Auditorium One	3-Jun Auditorium Two	4-Jun Auditorium One	4-Jun Auditorium Two	EDT (GMT-4)
08:30h			**Conference Welcome**						08:30h
08:45h			SDi2 Introduction						08:45h
09:00h			SDi2 - 01		SDi2 - 13	Mech. Prop. 01	SDi2 - 21	Matls. Char. 06	**09:00h**
09:15h									09:15h
09:30h			SDi2 - 02		SDi2 - 14	Mech. Prop. 02	SDi2 - 22	Matls. Char. 07	09:30h
09:45h		Welcome				Mech. Prop. 03		Matls. Char. 08	09:45h
10:00h			SDi2 - 03		SDi2 - 15	Mech. Prop. 04	SDi2 - 23	Mals. Char. 09	10:00h
10:15h	**Virtual Practice Time Session 1** 10-12h	Topic 1						Matls. Char. 10	10:15h
10:30h			SDi2 - 04		SDi2 - 16	Mech. Prop. 05	SDi2 - 24	Matls. Char. 11	10:30h
10:45h						Mech. Prop. 06		Matls. Char. 12	10:45h
11:00h				Electrochem. 01	SDi2 - 17	Mech. Prop. 07	SDi2 - 25		**11:00h**
11:15h		Topic 2				Mech. Prop. 08			11:15h
11:30h				Electrochem. 02	**Interaction/Break-time at**		SDi2 Closing Remarks		11:30h
11:45h				Electrochem. 03	**Auditoriums/Main Hall/Welcome Area**		**Auditoriums/Main Hall/Welcome Area**		11:45h
12:00h		Topic 3		Electrochem. 04	Phase Trans. 01	Matls. Char. 01	Funct. 01	Additive 01	**12:00h**
12:15h				Electrochem. 05					12:15h
12:30h				Electrochem. 06	Phase Trans. 02	Matls. Char. 02	Funct. 02	Additive 02	12:30h
12:45h		Break			Phase Trans. 03	Matls. Char. 03	Funct. 03	Additive 03	12:45h
13:00h			SDi2 - 05		Phase Trans. 04	Matls. Char. 04	Funct. 04	Additive 04	**13:00h**
13:15h					Phase Trans. 05		Funct. 05	Additive 05	13:15h
13:30h			SDi2 - 06		Phase Trans. 06	Matls. Char. 05	Funct. 06	Additive 06	13:30h
13:45h		Topic 4			Phase Trans. 07		Funct. 07	Additive 07	13:45h
14:00h			SDi2 - 07	Comp. 01	**Interaction/Break-time at**		**Interaction/Break-time**		**14:00h**
14:15h					**Auditoriums/Main Hall/Welcome Area**		**at Auditoriums/Main Hall/Welcome Area**		14:15h
14:30h			SDi2 - 08					**CNL: Activities**	**14:30h**
14:45h		Topic 5		Comp. 02				**& Opportunities**	14:45h
15:00h			SDi2 - 09	Comp. 03		**Student Entrepreneurs**		*general information session*	15:00h
15:15h				Comp. 04		*special student only session*			15:15h
15:30h				Comp. 05			**Interaction/Break-time at**		15:30h
15:45h		Topic 6		Comp. 06			**Auditoriums/Main Hall/Welcome Area**		15:45h
16:00h							**Metal Physics**		**16:00h**
16:15h			**Interaction/Break-time at**		**Interaction/Break-time at**		**Award Lecture**		16:15h
16:30h			**Auditoriums/Main Hall/Welcome Area**		**Auditoriums/Main Hall/Welcome Area**		Hatem Zurob		16:30h
16:45h							McMaster		16:45h
17:00h			**Metal Chemistry Award Lecture**		**DKC MacDonald Memorial Lecture**		Student Awards and		**17:00h**
17:15h			Mansoor Barati		Julia Greer		Conference Closing		17:15h
17:30h			U of T		Caltech				17:30h
17:45h									17:45h
18:00h									
18:15h									
18:30h			SDi2 - 10		SDi2 - 18	MSEP 01			
18:45h									
19:00h	**Virtual Practice Time Session 2** 19-21h		SDi2 -11		SDi2 - 19	MSEP 02			
19:15h						MSEP 03			
19:30h			SDi2 - 12		SDi2 - 20	MSEP 04			
19:45h									
20:00h									
20:15h									
20:30h									
20:45h			**POSTER SESSION #1** **Main Hall** 120 min		**POSTER SESSION #2** **Main Hall** 120 min				
21:00h									
21:15h									
21:30h									
21:45h									

LEGEND

Abbreviation	Session Full Name
SDi2	*Solute-Defect Interaction*
Electrochem.	*Applied Electrochemistry and Degradation of Materials*
Matls. Char.	*Materials Characterization*
Phase Trans.	*Phase Transformation Fundamentals*
Mech. Prop.	*Mechanical Behaviour and Structure-Property Relationships*
Comp. Matls.	*Computational Materials Science*
Funct.	*Funct. and Emerging Materials*
Additive	*Additive Materials*
MSEP	*MSE Pedagogy*

Award Lectures

D.K.C. MacDonald Memorial Lecture

June 3, 17h

The MacDonald Memorial Lecture remembers the achievements of David Keith Chalmers MacDonald, born in Glasgow in July 1920. From an early age, he demonstrated considerable ability in mathematics and physics, and he graduated from Edinburgh University with first class honours. During the Second World War, owing to deficient eyesight, he served at the Military College of Science at Bury, where his remarkable talents for original research combining experimental and theoretical aspects became apparent.

In 1951, the year of the first Canadian Metal Physics Conference (the direct predecessor of the Canadian Materials Science Conference), MacDonald came to Canada. He and others associated with the National Research Council (NRC) soon became prominent and regular attendees at this annual conference. It was at the National Research Council that MacDonald developed an intense interest in the solid state at extremely low temperatures. He produced many papers of the highest quality during his tenure at the NRC. In 1957, MacDonald was diagnosed as having a rare neurological ailment that would lead to gradual debilitation of his limbs, and eventual death. His reaction was characteristic of his personality, and he increased the pace of activities to make the most of the time remaining. During this difficult period, the NRC, under Dr. Steacie, assisted him by providing special nursing and transportation services.

Keith MacDonald passed away in 1963. His honours included election to the Royal Society at a relatively young age, recipient of the Gold Medal of the Canadian Association of Physicists an honorary Professorship at the University of Ottawa, five books published, as well as the high esteem of his colleagues. MacDonald enjoyed a sense of achievement that is usually attained only at a more advanced age. He died a stricken but not unhappy man. It is no exaggeration to say that his contributions to metal physics in Canada set a standard that is yet to be surpassed.

The D.K.C. MacDonald Memorial Lecture has been a prominent feature of the Conference since 1964, and conference attendees have enjoyed Memorial Lectures presented by some of the leading figures in Materials Science, both from a Canadian and global perspective.

(photo credit: Rapid Grip and Batten Ltd of Ottawa)

2021 Recipient: Prof. Julia Greer, California Institute of Technology

Materials by Design: Three-Dimensional (3D) Nano-Architected Meta-Materials

Creation of extremely strong and simultaneously ultra lightweight materials can be achieved by incorporating architecture into material design. Dominant properties of such metamaterials are driven by their multi-scale nature: from characteristic microstructure (atoms) to individual constituents (nanometers) to structural components (microns) to overall architectures (millimeters+). To harness the beneficial properties of 3D nano-architected meta-materials, it is critical to assess their properties at each relevant scale while capturing overall structural complexity.

Our research is focused on the design, synthesis, and characterization of nano-architected materials using nanofabrication and additive manufacturing (AM) techniques, as well as on investigating their stimulus-driven response as a function of architecture, constituent materials, and microstructure. These "meta-materials" exhibit superior and often tunable properties, i.e. resilience against impact, recoverability, failure suppression, anisotropic stiffness; nano-photonic response (PhCs); new electrochemical degrees of freedom (Li-ion batteries), and shape memory response (SMPs) at extremely low mass densities, as well as lend themselves to novel functionalities (hydrogel-enabled synthesis) which renders them useful and enabling in technological applications. We strive to uncover the synergy between atomic-level microstructure and nano-sized external dimensionality, where competing material- and structure-induced size effects drive overall response. My talk with focus on additive manufacturing via function-containing chemical synthesis to create nano- and microarchitected metals, ceramics, multifunctional metal oxides, and shape memory polymers, as well as demonstrate their potential in some real-use applications. I will describe how the choice of architecture, material, and external stimulus can elicit stimulus-responsive, reconfigurable, and multifunctional response.

BIOGRAPHY

Greer's research focuses on creating and characterizing classes of materials with multi-scale microstructural hierarchy, which combine three-dimensional (3D) architectures with nanoscale induced material properties. We develop fabrication and syntheses of micro- and nano-architected materials using 3D lithography, nanofabrication, and additive manufacturing (AM) techniques, and investigate – among others – their mechanical, biochemical, electrochemical, electromechanical, and thermal properties as a function of architecture, constituent materials, and microstructural detail. We strive to uncover the synergy between the internal atomic-level microstructure and the nano-sized external dimensionality, where competing material- and structure-induced size effects drive overall response and govern these properties. Specific topics include applications of 3D nano- and micro-architected materials in in chemical and biological devices, ultra lightweight energy storage systems, filters for purification and chemically-assisted separation, damage tolerant fabrics, additive manufacturing, and smart, multi-functional materials.

Greer obtained her S.B. in Chemical Engineering with a minor in Advanced Music Performance from MIT in 1997 and a Ph.D. in Materials Science from Stanford, worked at Intel (2000-03) and was a post-doc at PARC (2005-07). Julia joined Caltech in 2007 and currently is a Ruben F. and Donna Mettler Professor of Materials Science, Mechanics, and Medical Engineering at Caltech. Greer has more than 150 publications, has an h-index of 62, and has delivered over 100 invited lectures, which include 2 TEDx talks, the multiple plenary lectures and named seminars at universities, the Watson lecture at Caltech, the Gilbreth Lecture at the National Academy of Engineering, the Midwest Mechanics Lecture series, and a "IdeasLab" at the World Economic Forum, and was recently selected as Alexander M. Cruickshank (AMC) Lecturer at the Gordon Research Conferences (2020). She received the inaugural AAAFM-Heeger Award (2019) and was named a Vannevar-Bush Faculty Fellow by the US Department of Defense (2016) and CNN's 20/20 Visionary (2016). Her work was recognized among Top-10 Breakthrough Technologies by MIT's Technology Review (2015). Greer was named as one of "100 Most Creative People" by Fast Company and a Young Global Leader by World Economic Forum (2014) and received multiple career awards: Kavli (2014), Nano Letters, SES, and TMS (2013); NASA, ASME (2012), Popular Mechanics Breakthrough Award (2012), DOE (2011), DARPA (2009), and Technology Review's TR-35, (2008). She is an active member of scientific community through professional societies (MRS, SES, TMS), having organized multiple symposia, been chosen as Conference Chair (MRS, 2021; GRC 2016), served on the Board of Directors for Society of Engineering Science (SES) and on government agency panels: DOE's Basic Research Needs workshop on setting Priority Research Directions (2020), National Materials and Manufacturing Board through National Academies (2020), and DoD's Bush Fellows Research Study Team (2020). Greer is the Director of the Kavli Nanoscience Institute at Caltech and serves as an Associate Editor for Nano Letters and Science Advances. She is also a concert pianist who performs solo recitals and in chamber groups, with notable performances of "Prejudice and Prodigy" with the Caltech Trio (2019), "Nanomechanics Rap" with orchestra MUSE/IQUE (2009), and as a soloist of Brahms Concerto No. 2 with Redwood Symphony (2006).

Metal Chemistry Award

June 2, 17h

The Metal Chemistry Award was conceived by Professor H. Hancock of the Technical University of Nova Scotia in 1988 to recognize outstanding contributions to metallurgical chemistry as epitomized by the inaugural winner, Professor L.M. Pidgeon of the University of Toronto. Since the time of its inception, the award has included recipients from universities, industry and government laboratories engaged in research activities ranging from hydrometallurgy, molten salt chemistry, corrosion and fundamental physical chemistry bearing upon smelting and refining processes.

2021 Recipient: Prof. Mansoor Barati, University of Toronto

Thermodynamic Lens: A Metallurgist's Best Tool

Thermodynamics emerged as a field of science over a century ago but its application dates back to early civilizations. While it is founded on a few "old" and established laws, its application continues to bring about radical changes in our lives. In the age of sustainability, thermodynamic is once again at the fore of breakthrough innovations that aim to address our grand challenges: clean energy supply, green production, and living better with less resources. In this lecture, through several examples of metallurgical research in the speaker's lab, it will be argued that thermodynamics is not just a scientific field to explain an observed phenomenon but a powerful engineering tool to relay upon for developing novel technologies and processes.

BIOGRAPHY

Mansoor Barati is Gerald R. Heffernan Chair and Professor in Sustainable Materials Processing at the University of Toronto. His research is centered on reducing the environmental footprint, and lowering the consumption of energy and resources in the metals industry, as well as development of high quality materials for renewable energy systems. He joined the University of Toronto after one year at WorleyParsons and established Sustainable Materials Processing research lab where over 80 researchers have worked in the past 10 years. His research has been highlighted in about 200 publications and patents has been recognized by many awards such as CMQ Best paper award, JOM best paper award, Metallurgical and Materials Transaction B Editor's Choice Award, TMS Extraction & Processing Division Technology Award, Brimacombe award, and PEO Young Engineer medal.

Metal Physics Award

June 4, 16h

The Metal Physics Award was conceived by Professor T.S. Hutchison of the Royal Military College of Canada to recognize achievements in fundamental physics of importance to the understanding of metals as materials. At the time of its first award to Z.S. Basinski in 1977, the advancement of dislocation theory was the very essence of the kind of achievement the award was intended to recognize. Although the Award since that time has been awarded for excellence in a much broader range of research achievement including advancement in non-metallic materials.

2021 Recipient: Prof. Hatem Zurob, McMaster University

The Evolution of Microstructure in Steels- Role of Interfaces

Grain-growth and recrystallization kinetics are controlled by the grain boundary and its interaction with solutes and precipitates. The kinetics of phase transformations, including diffusional transformations, are sensitive to the interface mobility and interface's interaction with defects within the parent phase. In this presentation, the kinetics and thermodynamics of grain boundaries and ferrite/austenite interfaces in steel are reviewed. Recent experimental observations and modelling efforts will be reviewed. Special emphasis will be placed on how to incorporate experimental data into models for interface motion, knowing that these models do not include many of the complexities of the real interface. The examples considered include grain-growth in high Mn alloys, recrystallization in microalloyed steels, ferrite growth during austenite decomposition, and dynamic precipitation of ferrite.

BIOGRAPHY

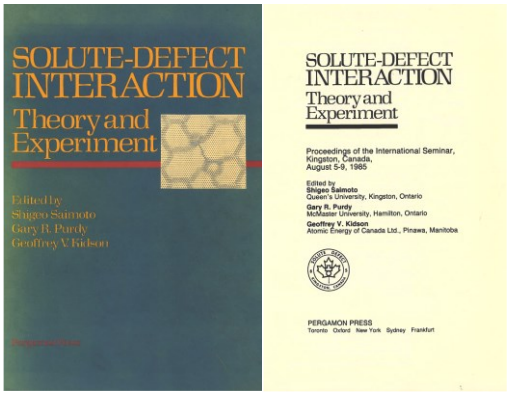
Dr. Zurob obtained his Ph.D. from McMaster University in 2003. He held post doctoral fellowships at the Grenoble institute and Technology and Oxford University prior to joining McMaster as an Assistant Professor in 2005. He was promoted to Associate Professor in 2012 and Professor in 2017. Dr. Zurob is presently serving as Chair of the Department of Materials Science and Engineering.

The aim of Dr. Zurob's research is to understand and control microstructure development in engineering materials with the goal of optimizing mechanical properties. The applicant has made significant contributions to the areas of thermomechanical processing, recrystallization modeling, functionally-graded materials, austenite decomposition and structure-property relationships. Dr. Zurob is the recipient of several prestigious awards including the Sawamura Award and Guimaraise Award of ISIJ and the Best Young Researcher Award of Internationally Recrystallization and Grain Growth Conference. In addition, Dr. Zurob is a dedicated educator who was recognized by several teaching awards at McMaster. Dr. Zurob is also an active participant in professional societies including ASM, TMS and ASM Materials Camps Canada**.**

Special Symposium

Solute-Defect Interaction 2: Theory, Experiments and Modeling

In 1985 Shigeo Saimoto, Gary Purdy and Geoffrey Kidson hosted an international symposium entitled Solute-Defect Interaction: Theory and Experiment at Queen's University in Kingston, Canada of which the proceedings were published in the following year. The range of speakers and topics was exceptional and expanded the topic from the classical mind-set of linear elasticity, classical thermodynamics and random solutions.



Since that time the development of finer experimental probes, higher resolution detectors and their mainstream availability in experimental techniques like atom probe, synchrotron, electron microscopy, and the explosion of computational tools from EAM to DDD tied to a better visualization of microstructure has revealed a far more complicated landscape than envisioned. How solute atoms move, are trapped, and freed is critical to the processing and stability of modern alloys.

Thirty six years later the symposium Solute-Defect Interaction 2: Theory, Experiments and Modeling, is held as part of the 32nd Canadian Materials Science Conference. The symposium brings together a range of invited speakers to discuss the current state-of-the-art and the challenges in this field. Abstracts of the talks include "homework readings" for the participants to prepare for the presentations.

The honorary chairman of the symposium is Emeritus Professor Shig Saimoto.

Symposium Organizers

Bradley Diak (Queen's University), Marek Niewczas (McMaster University), Chadwick Sinclair, (University of British Columbia)

Extra Events

June 1, 08:45h – 16:30h

Pre-Conference Workshop* - Irradiation of Materials: how to simulate reactor conditions using ion beams

Organized by Laurent Béland and Mark Daymond, Queen's University

Ion irradiation is an increasingly popular alternative to neutron irradiation, used to study the effect of radiation on materials' properties, in the context of nuclear power generation. Its advantages include shorter irradiation times to reach an equivalent dose (roughly 1000 times faster), and lesser activation of the materials (which facilitates handling of the materials for characterization).

In this workshop, the participants will learn about fundamental, theoretical and applied aspects of ion irradiation of materials; proton irradiation in particular. Instructors include faculty in Queen's University's nuclear materials group, as well as an invited instructor: Roger E Stoller, retired distinguished scientist at the Oak Ridge National Laboratory.

* Must register for separately from conference.

June 3, 14:30h – 16h

Student-Only Session - NexGen Materials Entrepreneurs: A flight plan to get your materials start-up off the ground.

Organized by Boyd Davis, Kingston Process Metallurgy

This session gives tangible direction to budding entrepreneurs with an idea for a materials product while show-casing the world class ChemTech ecosystem in Kingston. A number of short presentations along the start-up commercialization path will be followed by a Q&A session and the possibility for one-on-one breakouts for individual advice.

June 4, 14:30h – 15:30h

The materials science of tomorrow, today: developments and opportunities at the Canadian Nuclear Laboratories

Organized by Katie Sutherland, Talent Advisor & Mike Welland, Research Scientist; Canadian Nuclear Laboratories

As Canada's national nuclear laboratory, CNL is in the midst of a revitalization with exciting developments towards siting a Small Modular Reactor by 2026, and constructing the largest active research facility in Canada. This presentation covers a status update of CNL, description of the combined experimental-theoretical approach to materials science research underway, and how you may join us.

Activities by Day

Tuesday June 1, 2021

Pre-Conference Workshop (must register for separately)

Irradiation of Materials: how to simulate reactor conditions using ion beams

Ion irradiation is an increasingly popular alternative to neutron irradiation, used to study the effect of radiation on materials' properties, in the context of nuclear power generation. Its advantages include shorter irradiation times to reach an equivalent dose (roughly 1000 times faster), and lesser activation of the materials (which facilitates handling of the materials for characterization).

In this workshop, the participants will learn about fundamental, theoretical and applied aspects of ion irradiation of materials; proton irradiation in particular. Instructors include faculty in Queen's University's nuclear materials group, as well as an invited instructor: Roger E Stoller, retired distinguished scientist at the Oak Ridge National Laboratory.

LOCATION: Virtual remote video conference

TIME ZONE: All times in EDT (GMT/UTC-4), or Kingston, Ontario time.

09:45h, Welcome and Introduction to the Workshop

10-11h, Introduction to neutron- and ion-induced damage. Types of defects, effects on mechanical properties, concept of radiation dose and primary knock-on atom. Some differences between ion and neutrons – *Mark Daymond, Queen's University*

11-12h, Calculating irradiation dose and ion-range: how to use SRIM. - *R. Stoller, Oak Ridge National Laboratory* (see: *www.srim.org*)

12-12:30h, Calculating induced activity of sample by irradiation. Demonstration of Queen's Java activation calculator – *Matt Topping, Queen's University*

12:30-13:30h, Break

13:30h-14:30h, Characterization of irradiation induced defects. – *Zhongwen Yao, Queen's University*

14:30h-15:30h, Computer Models for Irradiation. – *Laurent Béland, Queen's University*

15:30h-16:30h, Ion-irradiation in comparison to neutron-irradiation: a critical assessment. - R. Stoller, *Oak Ridge National Laboratory*

Virtual Campus Practice Time

Registered conference attendees can log-in to the virtual event campus one day before the conference to build their avatar and explore the environment. Attendees can join the campus anytime once they are given access, but two sessions are specifically set-up with technical support on site.

10h – 12h, Event Campus
Session I

19h – 21h, Event Campus
Session II

Wednesday June 2, 2021

08:30h – 08:45h, Auditorium 1

Conference Welcome

08:45h – 11h, Auditorium 1

Solute Defect Interaction 2, Session 1

Chairs: S. Saimoto and B. Diak, Queen's University

Paper ID	Title / Author(s) (Affiliation)
SDi2 - 01	Solutes Everywhere: High Entropy Alloys / Bill Curtin (Ecole Polytechnique Federale de Lausanne, Switzerland)
SDi2 – 02	Stacking fault energy in concentrated alloys / Maryam Ghazasaeidi, Mulaine Shih (The Ohio State University, USA)
SDi2 – 03	Interaction between screw dislocations and carbon in tungsten from ab initio calculations / Guillaume Hachet, Lisa Ventelon, François Willaime, Emmanuel Clouet (Université de Normandie, France)
SDi2 - 04	Parameterizing Solution Hardening Models by First Principles Calculations: BCC metals and complex concentrated alloys / Chris Woodward, Brahim Akdim, Satish I. Rao (Air Force Research Laboratory, USA; UES Inc, USA)

11h - 13h, Auditorium 2

Applied Electrochemistry and Degradation of Materials

Chair: S. Persaud, Queen's University

Paper ID	Title / Author(s) (Affiliation)
Electrochem. 01	**Keynote:** In-situ characterization of an Al-Li battery electrode using x-ray diffraction and electrochemical methods / Oles Sendetskyi, Mark Salomons, Steve Launspach, Michael Fleischauer (University of Alberta)
Electrochem. 02	Cracking behaviour in electrodeposited Ni-Fe-Cr coatings / Michel Haché, Yu Zou, Uwe Erb (University of Toronto)
Electrochem. 03	Pulse Electrodeposition of Pure Ni Coatings from Deep Eutectic Solvent and Study the Effect of Current Density on Microstructure, Current Efficiency, Corrosion and Hardness Properties of the Coatings / Mehry Fattah, Sylvie Morin (York University)
Electrochem. 04	Derivation of the fundamentals of the stress effects on corrosion potential and Kelvin potential of X52 steel in 0.01 M NaHCO3 solution / Yicheng Wang, Y.Frank Cheng (University of Calgary)
Electrochem. 05	Novel Method for Surface Chemistry Dynamics Analysis of HSS Steel Induced by Deep Cryogenic Treatment / Patricia Jovičević-Klug, Matic Jovićević-Klug, Bojan Podgornik (Institute of Metals and Technology, Ljubljana, Slovenia)
Electrochem. 06	**Keynote:** Rapid Production of Magnetite Scales / Darren Feenstra, Joseph Kish (McMaster University)

13h – 15:30h, Auditorium 1

Solute Defect Interaction 2, Session 2

Chair: C. Sinclair, University of British Columbia

Paper ID	Title / Author(s) (Affiliation)
SDi2 – 05	Solute-Defect Interaction to Improve Metal Processing and Material Properties / Shig Saimoto (Queen's University)
SDi2 – 06	A revision of Labusch's statistical theory of solid solution hardening / Bjorn Holmedal, Tomás Mánik (Norwegian University of Science and Technology, Norway)
SDi2 – 07	Does it Add Up? Dislocation Motion Through Aluminum Alloy Solute Fields at 78 K / Bradley Diak, Olga Gopkalo (Queen's University)
SDi2 – 08	Placing recent observations of solute strengthening, dynamic strain aging, and serrated flow in Mg alloys within a historical and theoretical context / Mohammed A. Shabana, Jishnu J. Bhattacharyya, and Sean R. Agnew (University of Virginia, USA)
SDi2 - 09	Polytypes precipitates in Mg single crystals / Marek Niewczas, A. Kula (McMaster University; AGH University of Science and Technology, Poland)

14h – 16:15h, Auditorium 2

Computational Material Science

Chair: P. Saidi, Queen's University

Paper ID	Title / Author(s) (Affiliation)
Comp. 01	**Keynote:** Crystal plasticity modeling of stress-assisted diffusion of hydrogen atoms in zirconium matrix / Hamid Abdolvand (Western University)
Comp. 02	Capturing Dislocation Half-Loop Formation and Dynamics in Epitaxial Growth using the Structural Phase-Field Crystal Method / Salvador Valtierra Rodriguez, Nathaniel Quitoriano, Matthew Frick, Nana Ofori-Opoku, Nikolas Provatas, Kirk H. Bevan. (McGill University; Canadian Nuclear Laboratories)
Comp. 03	A computational framework to predict transport of radiation-induced point defects in concentrated solid solution alloys; with the focus on Ni(x)Fe(1-x) alloys / Keyvan Ferasat (Queen's University)
Comp. 04	Pressure effect on diffusion of carbon at the 85.91 <100> symmetric tilt grain boundary of alpha- iron / Md. Mijanur Rahman, Fedwa El-Mellouhi, Othmane Bouhali, Charlotte S. Becquart, and Normand Mousseau (University of Montreal)
Comp. 05	**Keynote:** Machine learning accelerated discovery of single atom catalysts based on bidirectional activation mechanism / Zhi Wen Chen (University of Toronto)

17h - 18h, Auditorium 1

Metal Chemistry Award Lecture

Thermodynamic Lens: A Metallurgist's Best Tool, *Mansoor Barati*, University of Toronto

Chair: A. McLean, University of Toronto

18:30h – 20h, Auditorium 1

Solute Defect Interaction 2, Session 3

Chair: M. Niewczas, McMaster University

Paper ID	Title / Author(s) (Affiliation)
SDi2 – 10	Strain rate effect on hydrogen behavior in aluminum alloys during deformation / Keitaro Horikawa (Osaka University, Japan)
SDi2 – 11	Revisit the work hardening mechanism of TWIP steels: carbon atoms vs. deformation twins / Mingxin Huang (University of Hong Kong, Hong Kong)
SDi2 – 12	Inertial Contributions to Dislocation Drag in Alloys / Chad Sinclair (University of British Columbia)

20h - 22h, Main Hall

POSTER SESSION 1

Poster #	Title / Author(s) (Affiliation)
W01	Is Pickling Necessary for Stainless Steel Rebar? / Fook Yee Yang, Carolyn Hansson (University of Waterloo)
W02	Hydrogen Induced Cracking (HIC) API-5LX80 steel used in oil and gas transmission pipelines / Mohammad Maroufkhani (École de Technologie Supérieure), Saeed Reza Allahkaram, Fatemeh Jafari (University of Tehran)
W03	Non-local crystal plasticity modeling of neutron irradiated zirconium alloys / Omid Sedaghat, Hamidreza Abdolvand (Western University)
W04	A better model for interatomic interactions in Zirconium / Yu Luo (Queen's University)
W05	Improving atom-scale models of clay minerals using machine learning / Karim Zongo, Laurent K. Béland, Claudiane Ouellet-Plamondon (École de Technologie Supérieure; Queen's University)

Poster #	Title / Author(s) (Affiliation)
W06	First principles calculation of structural, electronic and thermo-electric properties of ScNiBi Half-Heusler / Amina Touia (Belhadj Bouchaib University of Ain Temouchent, Algeria)
W07	A first principles computational study of equiatomic Zr-Fe-Nb alloy / Aditya Kamath (Queen's University)
W08	Modelling of circumferential and radial hydrides interaction in zirconium alloys / Alireza Tondro, Ivan Ho, Hamidreza Abdolvand (Western University)
W09	Process optimization of superfer 52 cold rolled sheets / Santanu Saha, Sri S. Ravi Varma (Mishra Dhatu Nigam Limited (MIDHANI), India)
W10	Thermal embrittlement of maraging steel 250 extruded tubes / Ram Reddy Kanthala, Savitha Upadhyayula, K. Rajasekhar, D. Gopikrishna (Mishra Dhatu Nigam Limited (MIDHANI), India)
W11	Effect of hot rolling process parameters on toughness of tungsten containing high strength steel, Savitha Upadhyayula, Ram Reddy Kanthala, K. Rajasekhar, D. Gopikrishna (Mishra Dhatu Nigam Limited (MIDHANI), India)
W12	Correlation between fracture strain and yield stress for an age hardenable aluminum alloy / Megan Tucker, Bradley Diak (Queen's University)
W13	Evaluating the tensile properties of LPBF SS316L: Influence of the specimen dimensions / Nicolas Wawrzyniak, Paul Provencher, Priti Wanjara, Mathieu Brochu, Myriam Brochu (McGill University; Polytechnique Montreal)
W14	Enhancement of Young's modulus in a heterostructured aluminum-silicon automotive alloy / Soumya Dash, Dejiang Li, Xiaoqin Zeng, Daolun Chen (Ryerson University)
W15	Strength-ductility synergy in an Al-Cu-Mg alloy with a bimodal grain distribution / Sohail Mazher Ali Khan Mohammed, D.L. Chen, Z.Y. Liu, D.R. Ni, Q.Z. Wang, B.L. Xiao, Z.Y. Ma (Ryerson University)
W16	Fabric selection for the production of bespoke bras / Josephine Bolaji, T. Krawchuk, Patricia I. Dolez (University of Alberta)
W17	On the Extrinsic Transition in the Hall-Petch Behavior of Nanocrystalline Nickel Cobalt Alloy Electrodeposits / Jonathan Kong, Jonathan McCrea, Jane Howe, Uwe Erb (University of Toronto)
W18	The Mechanical and Failure Properties of Wired Glass / Marco Montoya, Doug Perovic, Thomas Coyle, Jane Howe (University of Toronto)
W19	Onsite DL-EPR Testing and Metallographic Assessment of Lean Duplex Stainless Steel Aseptic Storage Tanks / Luis Henrique Guilherme (ACW Engineering, Brasil), Dirk L. Engelberg, Assis Vicente Benedetti (The University of Manchester, UK; State University of São Paulo, Brasil)
W20	Parameter Effectiveness and Mechanical Behaviour Analysis of Inconel 625 fabricated through Laser Powder Bed Fusion / Jonathan Lewis, Clodualdo Aranas (University of New Brunswick)
W21	Mechanical behaviour of high-performance fire protective fabrics and the effect of hydrothermal ageing / Ankit Saha, Md. Saiful Hoque, Hyun-Joong Chung, and Patricia I. Dolez (University of Alberta)

Thursday June 3, 2021

09h – 11:30h, Auditorium 1

Solute Defect Interaction 2, Session 4

Chair: M. Niewczas, McMaster University

Paper ID	Title / Author(s) (Affiliation)
SDi2 – 13	Is 3D and 4D characterization needed for studies of recrystallization? / Dorte Juul Jensen (Technical University of Denmark, Denmark)
SDi2 – 14	Defect segregation in alloys: thermodynamics, kinetics and near atomic characterization Alisson Kwiatkowski da Silva, D. Ponge, B. Gault and D. Raabe (Max-Planck-Institut für Eisenforschung, Germany)
SDi2 – 15	A comparison of solute effects on moving grain boundaries and inter-phase interfaces / Gary Purdy, Hatem Zurob (McMaster University)
SDi2 – 16	Grain boundary phase transitions probed by tracer diffusion measurements / Sergiy Diviniski (University of Münster, Germany)
SDi2 – 17	Grain Growth in Polycrystals / Peter Voorhees (Northwestern University, USA)

09h – 11:30h, Auditorium 2

Mechanical Behaviour and Structure-Property Relationships

Chair: A.K. Pilkey, Queen's University

Paper ID	Title / Author(s) (Affiliation)
Mech. Prop. 01	**Keynote:** Using discrete element methods to generate digital materials: An application to direct reduction of chromite ore / Jason P. Coumans, David Carter, Laura Dickson, Nail Zagretdnov, Dogan Paktunc (CanmetMINING, Natural Resources Canada)
Mech. Prop. 02	Effect of processing conditions on the strength of pellets containing Ring of Fire chromite ore / David Carter, Laura Dickson, Dogan Paktunc (CanmetMINING, Natural Resources Canada)
Mech. Prop. 03	Irradiation Creep Behavior of Zirconium Alloys / Brodie Moore, Matthew Topping, Mark R Daymond (Queen's University)
Mech. Prop. 04	Characterizing 3D stress development in the vicinity of notch tips in polycrystalline zirconium / Karim Louca, Hamidreza Abdolvand, Darren Pagan (Western University)
Mech. Prop. 05	Effect of back stress on cyclic hardening of a heterostructured Al-Si automotive alloy / Soumya Dash, Dejiang Li, Xiaoqin Zeng, Daolun Chen (Ryerson University)
Mech. Prop. 06	Surface atomic diffusion-induced abnormal softening in metallic nanocrystals / Sixue Zheng, Scott X. Mao (University of Pittsburgh)
Mech. Prop. 07	Effect of carbon nanotube reinforcement in a bimodal-grained aluminum matrix nanocomposite / Sohail Mazher Ali Khan Mohammed, D.L. Chen, Z.Y. Liu, D.R. Ni, B.L. Xiao, Z.Y. Ma (Ryerson University)
Mech. Prop. 08	Hydrothermal Aging Behavior of Fire-Protective Fabrics- Effect on Mechanical Performance and Surface Condition / Md. Saiful Hoque, Ankit Saha, Hyun-Joong Chung, Patricia I. Dolez (University of Alberta)

12h – 14h, Auditorium 1

Phase Transformation Fundamentals

Chair: Levente Balogh, Queen's University

Paper ID	Title / Author(s) (Affiliation)
Phase Trans. 01	**Keynote:** Application of Diffusion Path Analysis to Understand the Mechanisms of Transient Liquid Phase Bonding in the Ni-Si-B System / E.D. Moreau, Stephen Corbin (Dalhousie University)
Phase Trans. 02	A new numerical model for simulating diffusion-controlled moving interphase boundary problems / Osamudiamen Olaye, Olanrewaju A. Ojo (University of Manitoba)
Phase Trans. 03	Numerical analysis of isothermal solidification behavior during diffusion brazing involving 2D and 3D movement of liquid-solid interphase boundaries / Oluwadara Afolabi, Olanrewaju A. Ojo (University of Manitoba)
Phase Trans. 04	Effect of synthesis method and reaction conditions on long-range and local structure of RE2Ti2O7 pyrochlore-type oxides (RE = Yb and Gd) / Farah Mahmood, Andrew P. Grosvenor (University of Saskatchewan)
Phase Trans. 05	On the effects of texture and grain morphology on hydrogen transport towards the notch tips and precipitating hydrides / Alireza Tondro, Hamidreza Abdolvand (Western University)
Phase Trans. 06	Combinative chemical analysis by functional surface nanodroplets / Zixiang Wei, Miaosi Li, Hongbo Zeng, Xuehua Zhang (University of Alberta)
Phase Trans. 07	Extraordinary Pb Whisker Growth from Bi-Mg-Pb Pools in Aluminum Alloy 6026 / Matic Jovičević-Klug, Patricia Jovičević-Klug, Bojan Podgornik (Institute of Metals and Technology, Slovenia)

12h – 14h, Auditorium 2

Materials Characterization I

Chair: Rosen Ivanov, Queen's University

Paper ID	Title / Author(s) (Affiliation)
Matls. Char. 01	**Keynote:** High Concentration Graphene Nanoplatelet Dispersions in Water stabilized by Graphene Oxide / Dominik P.J. Barz, Sreeman Mypati, Andrew Sellathurai, Marianna Kontopoulou, Aristides Docoslis (Queen's University)
Matls. Char. 02	Liquid Phase Shear Exfoliation of Graphite into Graphene Nanoplatelets using Graphene Oxide as Surfactant / Andrew Sellathurai, Sreeman Mypati, Dominik P.J. Barz, Marianna Kontopoulou (Queen's University)
Matls. Char. 03	Tuning the conductivity and electron work function of Spin-Coated PEDOT:PSS/PEO nanofilm for enhanced intramolecular adhesion / Raymond Setiawan (University of Alberta)
Matls. Char. 04	**Keynote:** High-Temperature Thermal Stability of Super-Tetragonal PbTiO3 Film / Mengsha Li, Chenyue Qiu, Stas Dogel, Hooman Hosseinkhannazer, Pingfan Chen, Jason Tam, Doug Perovic, Jane Howe (University of Toronto)
Matls. Char. 05	**Keynote:** Synchrotron Techniques for Materials Research / Feizhou He (Canadian Light Source)

14:30h – 16h, Auditorium 2

NexGen Materials Entrepreneurs: A flight plan to get your materials start-up off the ground.

This session gives tangible direction to budding entrepreneurs with an idea for a materials product while show-casing the world class ChemTech ecosystem in Kingston. A number of short presentations along the start-up commercialization path will be followed by a Q&A session and the possibility for one-on-one breakouts for individual advice.

1. **Incubators and Accelerator in ChemTech** – *Sebastian Alamillo* (KPM-Accelerate)

You have the next big business idea and some chemistry – now what? This section will talk about what the first considerations are when starting up a chemistry/materials-based business, how to get your idea funded, and what the first resources student entrepreneurs can access in the current ecosystem. With stories from personal experience, this will be a brief overview of how-to set up your start-up foundations before continuing your technical development.

2. **Universities and Start-ups**- *Jason Hendry* (Queen's Partnerships & Innovation)
This session will discuss the challenges researchers/students encounter when trying to commercialize their academic research and what actions they can take to improve their chances of success. The session will also describe the university technology transfer process and what support can be provided to university-based start-ups.

3. **Product/Process Validation** – *Tim Clark* (GreenCentre Canada)
This section focuses on approaches to de-risking and validating chemical and material technologies – identifying the most critical challenges as early as possible and generating the right data to address them. Advice on how to organize a technology development roadmap and execute on it efficiently will be provided. There will also be a brief summary of tools and resources available to accelerate the process.

4. **R&D ScaleUp**– *Rupert Spence* (DuPont)
DuPont's Kingston Technology Centre is focused on commercializing new technologies though scale up evaluations and piloting. This talk will introduce common steps taken by DuPont in scaling new technologies, including the business and technical objectives at each stage and typical development issues.

5. **Case Study** – *Boyd Davis* (Kingston Process Metallurgy Inc.)
The rapid rise from concept to unicorn of Li-Cycle will be presented. The talk will show the support of the Kingston ChemTech ecosystem and the moves that the founders made to create the leading lithium-ion battery recycler in North America.

6. **Q&A** - *All*

17h - 18h, Auditorium 1

D.K.C. MacDonald Memorial Lecture

Materials by Design: Three-Dimensional (3D) Nano-Architected Meta-Materials, *Julia Geer*, California Institute of Technology

Chair: B. Diak, Queen's University

18:30h – 20h, Auditorium 1

Solute Defect Interaction 2, Session 5

Chair: C. Sinclair, University of British Columbia

Paper ID	Title / Author(s) (Affiliation)
SDi2 – 18	Solute segregation at precipitate-matrix interfaces in aluminium alloys / Laure Bourgeois, X. Tan, Z. Zhang, Y. Zhang, M. Weyland, P.N. H, Nakashima (Monash University, Australia; University of Antwerp, Belgium; Thermofisher Scientific, The Netherlands)
SDi2 – 19	Precipitation strengthening of Al alloys through room temperature cyclic deformation / Wen Wen Sun (Southeast University, China)
SDi2 – 20	Ultra-high strengthening of A2024 alloy by grain refinement and grain boundary segregation / Takahiro Masuda, Xavier Sauvage, Shoichi Hirosawa, Zenji Horita (Yokohama National University, Japan; Université de Normandie, France; Kyushu Institute of Technology, Japan; Kumamoto University, Japan; Saga University, Japan)

18:30h – 20h, Auditorium 2

MSE Pedagogy

Chair: T. Coyle, University of Toronto

Paper ID	Title / Author(s) (Affiliation)
MSEP 01	The development of Case Studies in the delivery of a Materials Engineering Process Design course / K. Meszaros, H. Henein, C. Lemelin (University of Alberta)
MSEP 02	The Remote Delivery of a Hands-On Materials Science Engineering Design Course with an At-Home Mechanical Testing Kit / Xinyue (Crystal) Liu, Scott Ramsay (University of Toronto)
MSEP 03	@Home Materials Science Lab Learning Modules / Lucas Ravkov, Brodie Moore, Matthew Thoms, Bradley Diak (Queen's University)
MSEP 04	Modules to support online delivery of an advanced ceramic course / Tom Coyle (University of Toronto)

20h - 22h, Main Hall

POSTER SESSION 2

Poster #	Title / Author(s) (Affiliation)
Th01	Evolution of stresses in deformation twins in the plastic zone using three-dimensional synchrotron X-ray diffraction / Karim Louca, Hamidreza Abdolvand (Western University)
Th02	Quantifying the recovery of Zr-2.5Nb cold-worked at 250 °C using diffraction / Thalles Lucas, Levente Balogh, F. Long, A. Barry, Mark R. Daymond (Queen's University)
Th03	Towards Diffraction Line Profile Analysis of Laser Powder Bed Fusion Manufactured Ni-Superalloys & pure Cu / Lucas Ravkov, Vahid Fallah, Levente Balogh (Queen's University)
Th04	Polycarbonate degradation under combined effect of ultraviolet and temperature / Sonya Redjala, Said Azem, Nourredine Ait Hocine (Mouloud Mammeri University, Algeria)
Th05	Synthesis of Non-Radioactive Bimetallic Oxides To Understand Fission Product Behaviour / Andres Lara-Contreras, M. Affan, J. Scott, E.C. Corcoran (Royal Military College of Canada)
Th06	Tribological degradation of molybdenum disulfide lubricating films under proton irradiation / Eric Nicholson, Peter Serles, Guorui Wang, Tobin Filleter, James W. Davis, Chandra Veer Singh (University of Toronto)
Th07	Production of vinyl ester resins of epoxidized cardanol using cinnamic acid: A study on the curing, mechanical, thermal and morphological characteristics / Iheoma Nwuzor, Obumneme Emmanuel Ezeani, Paul Chukwulozie Okolie (Nnamdi Azikiwe University, Awka, Nigeria)
Th08	Poly(vinyl alcohol) and Functionalized Ionic Liquid-Based Smart Hydrogels for Doxorubicin Release / Mohammad Muzammil Kuddushi, Naved Malek (S.V.National Institute of Technology, Surat, India)
Th09	Oxide limited laser colouration of copper gratings for angle dependent colour control / Graham Killaire, Jaspreet Walia, Arnaud Weck, Pierre Berini (University of Ottawa)
Th10	Influence of Nano-scale Graphene and Zirconia on Mechanical Properties of Alumina Matrix Nanocomposites / Solomon Duntu, Kenneth Hukpati, Iftikhar Ahmad, Mohammad Islam, Solomon Boakye-Yiadom (York University)
Th11	Synthesis and characterization of zirconolite ($CaZrTi_2O_7$) based glass-ceramic composite materials / Mehrnaz Mikhchian, Andrew P. Grosvenor (University of Saskatchewan)
Th12	Transient Oxide Formation and Oxide Spallation on IN738 at 1050◦C / Alex Lothrop, Qi Yang, Bingjie Xiao, Carman Lefebvre, Megan Walker, Xiao Huang (Carleton University)
Th13	Corrosion Performance of High Temperature Alloys in Molten Salt Mixtures for Next Generation Energy Systems / Isabella McDonald (McMaster University)
Th14	Decreasing the binder setting time in bioactive glass composites for bone tissue scaffolds / Marzieh Matinfar, John A. Nychka (University of Alberta)
Th15	Smart headband for rehabilitation following jaw reconstruction / Pradipika Natamai Vasudevan, Patricia I. Dolez, Hyun-Joong Chung, Daniel Aalto (University of Alberta)
Th16	Cold embossing of laser written diffractive optical elements on metals / Xitong Xie, Arnaud Wenk (University of Ottawa)
Th17	Synthesis of Synthetic Rock Materials Using One-Step Methods / Andrew Ansah, Andrew P. Grosvenor (University of Saskatchewan)
Th18	Development of Ring Forgings of 11Cr-10Ni-2Mo-1Ti PH Martensitic Stainless Steel for Rocket Motor Application / Bhavanish Kumar Singh, A. Panikishore, K. Rajasekhar (Mishra Dhatu Nigam Limited (MIDHANI), India)

Friday June 4, 2021

09h – 11:45h, Auditorium 1

Solute Defect Interaction 2, Session 6

Chair: C. Sinclair, University of British Columbia

Paper ID	Title / Author(s) (Affiliation)
SDi2 – 21	Lattice point defect-mediated semi-coherent precipitation in irradiated alloys / Lisa Belkacemi (Max-Planck-Institut für Eisenforschung GmbH, Germany)
SDi2 – 22	Early-stage solute clustering in the phase-field crystal model / Nana Ofori-Opoku (Canadian Nuclear Laboratories, Canada)
SDi2 – 23	The application of solid solution hardening in aluminum alloy design for elevated temperatures / Hiaou Jin (CanmetMATERIALS, Natural Resources Canada, Canada)
SDi2 – 24	Solutes partitioning at crystal defects in crept Ni-based superalloys: towards a better understanding for enhanced materials properties / Lola Lilensten, Aleksander Kostka, Sylvie Lartigue-Korinek, Baptiste Gault, Sammy Tin, Stoichko Antonov, Paraskevas Kontis (PSL Research University, France; Max-Planck-Institut für Eisenforschung, Germany; Illinois Institute of Technology, USA; Imperial College, UK; Institut de Chimie et des Matériaux Paris Est, France ; Center for Interface-Dominated High Performance Materials (ZGH), Germany)
SDi2 – 25	Industrial Consequences of Solute Defect Interactions related to Nickel and Titanium Alloy Production and Application / Bill MacDonald (Titanium Metals Corp. and Special Metals Corp., USA)

09h – 11h, Auditorium 2

Materials Characterization II

Chair: M. Topping, Queen's University

Paper ID	Title / Author(s) (Affiliation)
Matls. Char. 06	**Keynote:** Role of Iron-Intermetallics on porosity characteristics in Al-Si-Cu cast alloys / Ehab Elsharkawi (Saint Mary's University)
Matls. Char. 07	Particle and Solute Dispersion in a cast Al-Cu-Mg-Ag+TiB_2 Composite / Rosen Ivanov, D. Mayer, S. Farrell, M. Phaneuf, M. Gallerneault, Bradley Diak (Queen's University)
Matls. Char. 08	Effect of Heat Treatment on Hydrogen Trapping Capacity of Model Fe-C-Mn-Nb Steel / Sara Filice, Dmitrij Zagidulin, James Noel, Joseph McDermid, Joseph Kish (McMaster University)
Matls. Char. 09	Structural evolution of oxide inclusions in cold-spray Cu coatings / Jason Tam, Dominique Poirier, Jean-Gabriel Legoux, Jason D. Giallonardo, Jane Howe, Uwe Erb (University of Toronto)
Matls. Char. 10	Laser processing of TiAlN-PVD pre-coated Zircaloy-4 for nuclear applications / Lin Zhu, Pusong Wang, Arash Nikniazi, Linjiang Chai, Vahid Fallah (Queen's University)
Matls. Char. 11	The corroded refractory linings preparation technique at laboratory condition for thermomechanical investigation / Sina Darban, Ryszard Prorok, Jacek Szczerba (AGH University of Science and Technology, Poland)

Paper ID	Title / Author(s) (Affiliation)
Matls. Char. 12	Influence of Hydrothermal Aging on the Strength of Moisture Barriers used in Firefighters' Protective Clothing / Laura Munevar Ortiz, Patricia I. Dolez, John A. Nychka (University of Alberta)

12h – 14h, Auditorium 1

Functional and Emerging Materials

Chair: D. Barz, Queen's University

Paper ID	Title / Author(s) (Affiliation)
Funct. 01	**Keynote:** Dynamic defects, bacterial biofilms and medical device infections / Benjamin D. Hatton, Desmond van den Berg, Dalal Asker (University of Toronto)
Funct. 02	Ultra Elastic, Stretchable, Self-Healing Conductive Hydrogels with Tunable Optical properties for Highly Sensitive Wearable Sensors / Meng Wu, Hongbo Zeng (University of Alberta)
Funct. 03	Size Effects of Superhydrophobic Microtopographies to Limit Microbial Adhesion and Transmission / Desmond van den Berg, Dalal Asker, Benjamin D. Hatton (University of Toronto)
Funct. 04	Tuning Surface Interactions Favors the Regenerable Separation of Oil-in-Water Emulsions / Mingfei Pan, Lu Gong, Li Xiang, Wenshuai Yang, Wenda Wang, Ling Zhang, Wenjihao Hu, Hongbo Zeng (University of Alberta)
Funct. 05	Biological microfluidics for smart optical control in buildings / Raphael Kay, Kevin Nitiema, Charlie Katrycz, Benjamin D. Hatton (University of Toronto)
Funct. 06	Modelling the Thermal Behaviour of Flexible Electronic Textile Heaters Under Varying Top Boundary Conditions / Ikra Iftekhar Shuvo, Justine Decaens, Dominic Lachapelle, Patricia I. Dolez (University of Alberta)
Funct. 07	The Effect of Substitution the Sites of the methoxy group in Quinoxaline Dyes on the Driving Force of an Electron injection: Dye-Sensitized Solar Cells Applications / Adel Daoud, Ali Cheknane, Jean-Michel Nunzi, Afek Meftah, (Mohamed Khider University of Biskra, Algeria; Queen's University)

12h – 14h, Auditorium 2

Additive Materials and Processes

Chair: V. Fallah, Queen's University

Paper ID	Title / Author(s) (Affiliation)
Additive 01	**Keynote:** Development of aluminum alloys for additive manufacturing applications / Michael Benoit, Suming Zhu, Mark Easton (University of British Columbia)
Additive 02	On the effects of Additive Manufacturing process parameters on the Macroscopic and Microscopic behavior of Hastelloy-X / Ahmed Aburakhia, Ali Bonakdar, Marjan Molavi-Zarandi, Joe Keller, Hamidreza Abdolvand (Western University)
Additive 03	On the Welding Speed Dependency of Fusion Zone Microstructure in a Newly-Developed Co-based Superalloy / Hamid Abedi, Olanrewaju A. Ojo (University of Manitoba)
Additive 04	Heat Treatment of Dual-metal 3D-printed Iron- and Cobalt-based Alloys / Jubert Pasco, Clodualdo Aranas, Kanwal Chadha (University of New Brunswick)

Paper ID	Title / Author(s) (Affiliation)
Additive 05	Effect of beam wobbling on microstructure and mechanical properties during laser wobbling welding / Hanwen Yang, Adrian P. Gerlich, James Chen (University of Waterloo)
Additive 06	Microstructural Evolution and Mechanical Properties of Low Alloy Low Carbon Steel Fabricated through Pulsed Gas Metal Arc Welding Additive Manufacturing / Javad Mohammadi, O.A. Gali, A.R. Riahi (University of Windsor)
Additive 07	Oxidation Resistance of Additively Manufactured Inconel 718 by a Plasma Arc Process / Li Ming (Devin) Wang, Adria Barcelo Singh, Bingjie Xiao, Xiao Huang, Xia Hunag (Carleton University)

14:30h – 15:30h, Auditorium 2

The materials science of tomorrow, today: developments and opportunities at the Canadian Nuclear Laboratories

Organized by Katie Sutherland, Talent Advisor & Mike Welland, Research Scientist; Canadian Nuclear Laboratories

As Canada's national nuclear laboratory, CNL is in the midst of a revitalization with exciting developments towards siting a Small Modular Reactor by 2026, and constructing the largest active research facility in Canada. This presentation covers a status update of CNL, description of the combined experimental-theoretical approach to materials science research underway, and how you may join us.

16h - 17h, Auditorium 1

Metal Physics Award Lecture

The Evolution of Microstructure in Steels- Role of Interfaces, *Hatem Zurob*, McMaster University

Chair: M. Millitzer, University of British Columbia

17h – 17:30h, Auditorium 1

Student Awards and Conference Closing

Abstracts

Additive Materials and Processes

Additive 01

Development of aluminum alloys for additive manufacturing applications

Michael Benoit, Suming Zhu, Mark Easton,

University of British Columbia

Additive manufacturing (AM) of high strength Al alloys is a challenge due to their susceptibility to hot tearing or cracking during solidification. The objective of this presentation is to present recent work that has been done to understand the relationship between Al alloy composition, crack susceptibility, and crack mechanism during rapid solidification conditions characteristic of metal AM. Two different alloy systems are considered in this presentation – a 6xxx alloy with minor Fe additions and a 7xxx alloy with up to 6 wt% rare earth (RE) elements. Samples from both alloy systems were cast, and the surfaces of the samples were subsequently melted by a laser to emulate rapid solidification of metal AM. It was found that the addition of RE elements increased the susceptibility to solidification cracking, which was attributed to (i) a decrease in the liquid volume during the terminal stages of solidification, (ii) an increase in the grain size at the melt pool boundary, and (iii) reduced permeability of the mushy zone due to the formation of RE-containing particles. Conversely, minor additions of Fe were found to eliminate solidification cracks in the melt pool, which was attributed to a change in the type and amount of Fe-containing intermetallic phases. The experimental results were confirmed by a numerical index calculated from the composition-dependent temperature-fraction solid curve during solidification. It is concluded that the alloy composition can significantly impact the crack susceptibility and mechanism of high strength Al alloys during AM.

Additive 02

On the effects of Additive Manufacturing process parameters on the Macroscopic and Microscopic behavior of Hastelloy-X

Ahmed Aburakhia, Ali Bonakdar, Marjan Molavi-Zarandi, Joe Keller, Hamidreza Abdolvand

Western University

Additive manufacturing (AM) has opened the doors to design and manufacture engineering parts with complex geometries with almost no design restrictions. While this advancement has encouraged industry to employ geometrical anisotropy in their favour to achieve better performance in critical operational locations, it introduces microscopic anisotropy in the materials microstructure due to complex thermal exposure during the process. An in-situ uniaxial neutron diffraction experiment is done on a nickel superalloy, Hastelloy-X, to understand the evolution of internal strains. As well, a crystal plasticity finite element model is used to understand how different AM process parameters affect the microstructure and

performance of the AM components. Results suggest that the specific energy input (SE = p / vd) has an influence on the AM-built parts, where p is the laser power, v is the scanning speed and d is the hatch spacing. When the SE is low, partially melted particles might be present in the microstructure due to low energy density and they can be randomly distributed through out the microstructure. These particles act as nucleation's sites during solidification which lead to random texture in parts manufactured with low SE.

Additive 03

On the Welding Speed Dependency of Fusion Zone Microstructure in a Newly-Developed Co-based Superalloy

Hamid Abedi, Olanrewaju A. Ojo

University of Manitoba

The welding speed dependency of fusion zone (FZ) microstructure in the newly developed Co-based superalloy, CoWalloy1, is evaluated using numerical modeling. A 3D finite-element transient model with a cone-shaped volumetric moving heat source is developed using APDL coding in the ANSYS to simulate the gas tungsten arc welding (GTAW) process. The model reveals that the molten pool geometry and the FZ microstructure are strongly influenced by the welding speed. Decreasing welding speed leads to change the molten pool shape to elliptical, with increased width and a greater depth of penetration. In addition, the solidification behavior is investigated by using the model to predict the dendritic and grain structure in the FZ. The results show that increasing welding speed decreases the volume fraction of the columnar dendritic structure and promotes a fully equiaxed grain structure in the FZ of the alloy, which is crucial to hot cracking resistance. The newly developed numerical model is validated using experimental data.

Additive 04

Heat Treatment of Dual-metal 3D-printed Iron- and Cobalt-based Alloys

Jubert Pasco, Clodualdo Aranas, Kanwal Chadha

University of New Brunswick

The effects of heat treatment to a cobalt-chrome-molybdenum-based superalloy and maraging steel dual-metal component fabricated for the first time using laser powder bed fusion (LPBF) was investigated. The solutionizing heat treatment consists of heating the samples to 1148 °C for 6 hours, while the aging heat treatment will soak the samples to 490 °C for 6 hours. The ideal orientations of the dual-metal material were also established using an electron backscatter diffraction (EBSD) technique. A strong <110>||building direction (BD) fiber texture dominates the cobalt-based material, while the iron-based alloy exhibits <111>||BD and <100>||BD fiber textures. Diffusion calculations also suggest that negligible diffusion depths of Co, Cr, Fe, and Ni can be attained after applying both the LPBF process and the heat treatment. Furthermore, as-printed and heat-treated samples revealed a well-adherent interface wherein the two alloys fused without any sign of mixing and a relative density of 99.89% was achieved.

Additive 05

Effect of beam wobbling on microstructure and mechanical properties during laser wobbling welding

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University of Waterloo

Laser welding with beam wobbling was employed to weld X70 high strength low alloy pipeline steel. The influence of beam wobbling on weld surface morphology, fusion zone microstructure and microhardness was investigated. Grain refinement was achieved by the effect of stirring during wobble laser welding due to the beam oscillation, which appears to change the melt flow direction, disturb grain growth, and break up solidifying columnar grains. A refined microstructure with short broken dendrites was obtained within the fusion zone of wobble laser welded joints. The weld metal of the wobble laser welded joints exhibited higher hardness compared to conventional laser welded joints due to a finer microstructure. A softened region was found in the inter-critical heat affected zone caused by partial coarsening of bainite. The hardness of the softened region could be improved by increasing the welding speed (from 1.0 to 1.5 m/min) which led to a lower heat input and limited the growth of grains in the HAZ.

Additive 06

Microstructural Evolution and Mechanical Properties of Low Alloy Low Carbon Steel Fabricated through Pulsed Gas Metal Arc Welding Additive Manufacturing

Javad Mohammadi, O.A. Gali, A.R. Riahi

University of Windsor

Wire arc additive manufacturing has become an increasingly significant application in the large-scale production of complex components. However, the operation parameters have been discovered to affect the additive manufactured product's microstructure and properties. Pulsed gas metal arc welding-additive manufacturing (PGMAW-AM) was employed to produce layer by layer low alloy steel components. The results revealed that the heat input decreased by adjusting the weld wire feed. Lower heat input in each bead refined the microstructure. Microscopic studies showed that at the boundary between the build, the substrate, and the top layer, the microstructure consisted of allotriomorphic ferrite's epitaxial grain structure with bainite and acicular ferrite. This microstructure resulted from the higher thermal cycle and supercooling rate experienced within the fabricated wall. The mechanical properties revealed higher values of yield and tensile strength of the deposited part, demonstrating that the strength and toughness of weld layouts were improved.

Additive 07

Oxidation Resistance of Additively Manufactured Inconel 718 by a Plasma Arc Process

Li Ming (Devin) Wang, Adria Barcelo Singh, Bingjie Xiao, Xiao Huang, Xia Hunag

Carleton University

In this study, the oxidation behaviour of Inconel 718 manufactured using plasma arc process was investigated and compared to that of conventional wrought Inconel 718. The oxidation tests were carried out at 800 and 900 °C for up to 400 hours. From the weight change observation, the two forms of the alloy exhibited similar trend. However, from the cross-section analysis, it seemed that the wrought alloy formed thicker and less uniform Cr-rich scale than that on AM Inconel 718. And the chromia oxide began to show signs of instability on both types of material after exposure for 200 hours at 900°C. A Nb-rich layer was observed between the chromia and metal substrate on both types. However, this layer was more continuous and uniform on AM specimens. This Nb-rich layer also increased in thickness as temperature and time increased. It is believed that the cast structure and the more uniform composition in AM material supported more uniform chromia formation under oxidation environment.

Applied Electrochemistry and Degradation of Materials

Electrochem. 01

In-situ characterization of an Al-Li battery electrode using x-ray diffraction and electrochemical methods

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NRC-Nanotechnology Research Centre, University of Alberta

Aluminum electrodes offer the potential for high lithium-ion capacities at low costs, capacities of 2000 mAh/g (six times higher than graphite, the current commercial standard) can be accessed at moderate temperatures (above 40 °C) [1]. Nevertheless, challenges with capacity fade, electrolyte breakdown, slow diffusion and nucleation barriers still exist. Reports suggest that ionic liquids may be key to improved capacity retention of aluminum electrodes at room temperature. Elevated temperature operation can be used to overcome nucleation barriers and slow diffusion, but at the cost of increased rates of electrolyte breakdown. Here, we combine controlled temperature electrochemical (de)lithiation with x-ray diffraction for in-situ studies of electrode and electrolyte reactions to shed light on these problems. Our in-operando cell is based on commercially available ultra-high vacuum compatible Conflat flanges [2, 3] with beryllium windows and electrical feedthroughs to maintain commercially-relevant stack pressure and cell sealing. We will report on cell design and performance, including full-powder-pattern refinement of the Li-Al electrode material during electrochemical (de)lithiation. Such refinement of the diffraction patterns allows us to quantify the fractions of the phases formed as well as details of the crystal structure (e.g. solid solution vs. new phase). Electrode composition from pattern refinement will be compared to electrochemical methods to separate the effects of electrode phase transitions and electrolyte breakdown. Better understanding of phase formation in Li-ion battery electrode materials will enable more robust production and improved performance of the batteries on the market.

[1] M. Z. Ghavidel et al, Journal of The Electrochemical Society, 166 (16) A4034-A4040 (2019)
[2] M. D. Fleischauer et al, Journal of The Electrochemical Society, 166 (2) A398-A402 (2019)
[3] O. Sendetskyi et al., Journal of Applied Crystallography, In preparation (2021)

Electrochem. 02

Cracking behaviour in electrodeposited Ni-Fe-Cr coatings

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Interest in the synthesis of Ni-Fe-Cr through electrodeposition has historically stemmed from the alloy class' widespread use in high-performance engineering systems in the form of stainless steels and nickel-based superalloys. More recently, the development of the field of high-entropy alloys (HEAs) and multi-principal element alloys (MPEAs) towards improving mechanical properties over larger temperature scales has driven this interest. A common phenomenon observed in almost all chromium electrodeposits is crack formation. While the mechanism by which cracking occurs is reasonably well understood in hexavalent chromium (Cr6+), trivalent chromium (Cr3+), which is usually used for alloy plating, is a much less understood system. This study works towards characterizing the cracking phenomena in Ni-Fe-Cr electrodeposits, in hopes of clarifying their causes and how they are related to the synthesis parameters. A major focus of this work is on the time-dependency of post-deposition crack growth, a topic that is infrequently considered in literature.

Electrochem. 03

Pulse Electrodeposition of Pure Ni Coatings from Deep Eutectic Solvent and Study the Effect of Current Density on Microstructure, Current Efficiency, Corrosion and Hardness Properties of the Coatings

Mehry Fattah, Sylvie Morin

Department of Chemistry, York University

In this paper, choline chloride-ethylene glycol (ChCl:2EG)-based environmentally friendly deep eutectic solvent (DES), was employed to produce Ni nanostructured coatings with improved corrosion and hardness properties simultaneously on the surface of AISI 1045 medium carbon steel through square waves pulse electrodeposition method. Electrodeposition was carried out at different current densities ranging from 2 to 30 mA.cm-2. The effect of electrodeposition current density on microstructure, current efficiency, corrosion, and hardness properties of Ni coatings were studied and discussed by using scanning electron microscopy (SEM), X-ray diffraction (XRD), nanoindentation hardness measurements, and potentiodynamic polarization test. XRD results revealed Ni peaks at three crystalline planes of (111), (200) and (220) for all samples as expected, and all coatings prepared at different current densities were characterized by a nano-sized Ni microstructure. Thickness of the layers increased with increasing the current density, and intergranular space between Ni grains, as well as cracks appeared on the surface. A dendrite-like growth of the Ni coating was clearly observed in the cross-section image of the coating prepared at 16 mA.cm-2, and current efficiency decreased obviously. Potentiodynamic polarization tests in 0.6 M aqueous NaCl solution at room temperature showed that Ni coatings electrodeposited at lower current densities, had more positive corrosion potential and lower corrosion current density with respect to the substrate. The maximum measured hardness was related to the coating electrodeposited at 4

mA.cm-2 and equal to 9600 MPa which was two times of the hardness of the substrate (4500 MPa). The formation of a more porous and discontinuous coating layer resulted at higher electrodeposition current densities due to the intergranular space and cracks in the coatings. This morphology gave rise to the higher corrosion rate and lower hardness values.

Electrochem. 04

Derivation of the fundamentals of the stress effects on corrosion potential and Kelvin potential of X52 steel in 0.01 M NaHCO3 solution

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University of Calgary

Engineering structures such as pipelines usually operate under stressing conditions. With the combined effect of the corrosive environment and stresses, pipeline corrosion would be enhanced. The interaction of stress and corrosion on pipelines was defined as the so-called “mechano-electrochemical (M-E) effect”, which has been proven to be one of the most threatening problem in pipeline integrity. However, although experimental tests have provided substantial evidence to prove the stress corrosion interaction in corrosive environments, the pipeline corrosion thermodynamics in the presence of stress has not been defined theoretically and quantitatively.

This work studied the fundamentals of the M-E effect for pipeline corrosion, where electrochemical corrosion thermodynamics of an X52 pipeline steel under stresses is developed by derivation of corrosion potential and Kelvin potential as a function of stress, respectively. The originality and uniqueness of this work is, at the first time of its kind to the authors’ best knowledge, theoretical formula of stress-induced negative shifts of Kelvin potential, and the relationship between corrosion potential and Kelvin potential under stress condition are derived and verified with experimental measurements, respectively. Results demonstrates that both corrosion potential and Kelvin potential are shifted negatively with increasing plastic stress, which is attributed to enhanced corrosion reaction. Furthermore, it is found that Kelvin potential is more sensitive to stressing condition than corrosion potential. The effect of plastic stress on Kelvin potential dropping mainly due to the decrease of the electron work of exit. An applied stress accelerates active corrosion of the steel in a near-neutral pH solution by changing both the overvoltage of ion discharge and adsorption process on steel surface.

Electrochem. 05

Novel Method for Surface Chemistry Dynamics Analysis of HSS Steel Induced by Deep Cryogenic Treatment

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Institute of Metals and Technology, Ljubljana, Slovenia

The corrosion behavior of high-speed steel AISI M35 (E.N.1.3243,HS6-5-2-5) enriched with Cr,Mo,W, V and Co, was investigated in alkaline environment (seawater) in order to observe and analyze surface chemistry dynamics induced by deep cryogenic treatment (DCT). In this study, evolution of corrosion phases is used as an indicator for surface dynamics of individual chemical elements, such as O, N, S, Cl, Mn, Cr, Mo, W, V, Co, which can unravel the impact of DCT on steel microstructure and properties. Focused ion beam milling combined with scanning electron microscopy (SEM) and energy dispersive spectroscopy (EDS) mapping was employed to obtain accurate depth profiles. Additionally, mass spectra analysis was conducted with Secondary Ion Mass Spectrometry with Time over Flight (SIMS-ToF) configuration for higher mass and chemical resolution. SEM-Mapping revealed the increased concentration of alloying elements in the surface and corrosion layer of DCT treated steel. This indicates that the alloying elements dynamics are different for DCT sample as compared to the conventional heat-treated (CHT) one. Furthermore, after DCT a layer enriched with N and depleted of other elements, dubbed “ghost layer” forms within the material’s surface, which correlates to the improved corrosion resistance of the DCT treated AISI M35 steel. In addition, SIMS-ToF has revealed the hidden dynamic of VO-, CoO-, WO3-, CrO, SO2-, FeO2- of DCT sample and the relation to reduced localized corrosion mechanism (pitting). Finally, for DCT sample a profound formation of magnetite is found in the base portion of the corrosion layer, whereas for CHT sample such layering is not observed. To conclude, this research provides an in-depth and systematic study of DCT effect on alloys’ dynamic, performed via corrosion analysis to identify the governing mechanisms. DCT was determined to be an effective tool for modifying the surface chemistry and reactivity that reduces the corrosion propagation in tool steels.

Electrochem. 06

Rapid Production of Magnetite Scales

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Magnetite scales have been known to be typical corrosion product formed on carbon steel feeder tubes under operation in CANDU nuclear reactors. It is of significant interest to rapidly produce representative magnetite scales to test new refurbishment techniques. This research aims to identify a suitable surrogate method to provide a magnetite (Fe3O4) scale on a carbon steel substrate on an accelerated time-scale that exhibits a similar structure, composition, morphology and thickness to that formed on carbon steel feeder tubes during operation of a CANDU nuclear reactor. Both wet air oxidation (corrosion) and electrochemical deposition were considered for this purpose. Scales were characterized for structure and composition using X-ray diffraction (plan-view) and scanning electron microscopy (SEM) and associated techniques (cross-sectional view). The electrochemical technique was scaled up to produce thicker scales in a minimal amount of time. It was found that a combination of both techniques could rapidly produce a representative surrogate film.

Computational Materials Science

Comp. 01

Crystal plasticity modeling of stress-assisted diffusion of hydrogen atoms in zirconium matrix

Hamidreza Abdolvand

Western University

The diffusion of hydrogen atoms into the zirconium lattice and formation of a brittle phase known as zirconium hydride has been a long-standing problem in nuclear industry. This diffusion can be affected by the formation of localized stress hotspots at the grain scale. Here, a crystal plasticity finite element model is developed to simulate stress-assisted-diffusion of hydrogen atoms and precipitation of hydrides. The results of the model are compared to electron backscatter diffraction measurements for hydride phase fractions in zirconium. It is shown that even in the absence of macroscopic loads, thermal residual stresses within zirconium grains can perturb the uniform distribution of hydrogen atoms by inducing large hydrostatic stresses in the vicinity of grain boundaries. Such stress concentrations can further affect the sequence of hydrides nucleation.

Comp. 02

Capturing Dislocation Half-Loop Formation and Dynamics in Epitaxial Growth using the Structural Phase-Field Crystal Method

Salvador Valtierra Rodriguez, Nathaniel Quitoriano, Matthew Frick, Nana Ofori-Opoku, Nikolas Provatas, Kirk H. Bevan

McGill University / Canadian Nuclear Laboratories: Computational Techniques

A structural phase-field crystal (XPFC) model is employed to simulate the process of defect nucleation in mismatched heteroepitaxial growth. We focus specifically on the formation of subcritical dislocation-half-loops and their subsequent evolution to form a mismatch defect along with two threads. The XPFC method employs a mean-field density field that resolves atomistic features but evolves on diffusional time scales. It is used to investigate different degrees of mismatch at the million atom" level and the half-loop dislocation behavior exhibited by the model is shown to be consistent with experiments reported in the literature. We also capable of capturing the strain energy accumulated by the mismatched epitaxial layer which yields another way of assessing the strain throughout the solid, both globally and locally Through this approach we are able to provide insights into the dislocation half-loop nucleation stage and its relation to both the conditions of the substrate employed and other defects present in the epitaxial layer. This approach can help in the understanding of dislocation nucleation events and help to control nucleation and result in high-quality, lattice-mismatched devices. This could potentially provide a useful computational tool in the design of semiconductor electronics to simulate the conditions leading to dislocation defects in epitaxially grown materials.

Comp. 03

A computational framework to predict transport of radiation-induced point defects in concentrated solid solution alloys; with the focus on Ni(x)Fe(1-x) alloys

Keyvan Ferasat

Queen's University

We present an Atomic kinetic Monte Carlo (AKMC) method to simulate point defect diffusion, benchmarked by molecular dynamics (MD) and the kinetic Activation Relaxation Technique (k-ART). It accurately predicts diffusion coefficients. Our simulations in Ni(x)Fe(1-x) indicate this method accurately predicts diffusion coefficients and show vacancy and self-interstitial defects have a non-monotonic dependency of diffusion coefficient to chemical composition. Our calculations indicate that composition dependence of migration energies is at the origin of the vacancy's non-monotonic behavior. In contrast, the difference between formation energies of Ni–Ni, Ni–Fe, and Fe–Fe dumbbell interstitials is at the origin of their non-monotonic diffusion behavior. Additionally, the migration barrier crossover composition–based on the situation where Ni or Fe atom jumps have lower energy barrier than the other one–is introduced. AKMC simulations indicate that the interplay between composition dependent crossover of migration energy and geometrical site percolation explains the non-monotonic concentration-dependence of atomic diffusion coefficients.

Comp. 04

Pressure effect on diffusion of carbon at the 85.91 <100> symmetric tilt grain boundary of alpha- iron

Md. Mijanur Rahman, Fedwa El-Mellouhi, Othmane Bouhali, Charlotte S. Becquart, and Normand Mousseau

University of Montreal

The diffusion mechanism of C in iron plays a vital role in carburization processes, steel fabrication, and metal dusting corrosion. Over the years, these mechanisms have been studied at ambient pressure. However, to date effect of pressure on the diffusion mechanism of C in grain boundaries (GBs) of iron has received much less attention and relatively little information is available. Using the kinetic activation-relaxation technique (k-ART), an off- lattice kinetic Monte Carlo algorithm with on-the-fly catalog building that allows to obtain diffusion properties over large time scales taking full account of chemical and elastic effects coupled with an EAM potential, we investigate the effect of pressure on the diffusion properties of carbon in 85.91◦ ⟨100⟩ symmetric tilt GBs of α-iron up to a pressure of 12 kbar at a single temperature of 600 K. More precisely, we explore the energy landscape and kinetic pathways. Then, diffusion coefficients are calculated to quantify the effect of stress on diffusivity. We show that, while the effect of pressure can strongly modify the C stability and diffusivity in the GB in ways that depend closely on the local environment and the nature of the deformation, isotropic and uniaxial pressure can lead to opposite and nonmonotonous effects regarding segregation energy and activation barriers. These observations are relevant to understanding of the evolution of heterogeneous materials, where variations of local pressure can alter the carbon diffusion across the material.

Comp. 05

Machine learning accelerated discovery of single atom catalysts based on bidirectional activation mechanism

Zhi Wen Chen

University of Toronto

Single atom catalysts (SACs) have provided new impetus to the field of catalysis due to their high activity, high selectivity, and theoretically full utilization of active atoms. However, the ambiguous activation mechanism prevents a clear understanding of the structure-activity relationship and results into a great challenge of rational design of SACs. Herein, by combining density functional theory calculations (DFT) with machine learning (ML), 126 SACs are explored to analyze and develop the structure-activity relationship for electrocatalytic nitrogen reduction reaction (NRR). A bidirectional activation mechanism with a new descriptor for catalytic activity is first proposed, which provides new insights for rational design of SACs. More importantly, a ML model is established for predicting the catalytic performance of NRR, validated by both DFT calculations and experimental works. The successful ML prediction in this work helps with accelerated design and discovery of new catalysts by computational screening with high practical significance.

Functional and Emerging Materials

Funct. 01

Dynamic defects, bacterial biofilms and medical device infections

Benjamin D. Hatton, Desmond van den Berg, Dalal Asker

University of Toronto

Medical devices such as catheters, prosthetic heart valves and reconstructive implants are susceptible to microbial biofilm colony formation and serious infection. If one were to mechanically deform an elastomer biomaterial (such as silicone), should that affect microbial growth? Recently we found that bacteria prefer the tensile (convex) side of bent silicone tubing, by about a factor of 3-4 times, over the compressive (concave) side. Why should this be? In general, there is not a very good understanding of microbial-surface interactions at early stages of growth. But we do know they're very sensitive to surface defects and roughness (scratches, grooves, etc). We have recently shown that elastomers such as silicone (polydimethylsiloxane, PDMS) or polyurethane form surface microcracks much more readily than has been previously recognized, and these surface defects become primary sites for initial microbial attachment. We show that even mild mechanical contact or deformation of PDMS materials, such as by surface wiping, is enough to generate these microcracks. The deformation of silicone tubing then appears to open up these microcracks, as dynamic defects that attract microbial surface attachment. This deformation effect of medical devices, to make them susceptible to infection, appears to be a previously unrecognized problem. Fortunately, we have also shown that infusion of silicone oil into PDMS elastomers (to make a highly non-adhesive silicone, iPDMS) can effectively block these defect sites and significantly reduce microbial attachment.

Funct. 02

Ultra Elastic, Stretchable, Self-Healing Conductive Hydrogels with Tunable Optical properties for Highly Sensitive Wearable Sensors

Meng Wu, Hongbo Zeng

University of Alberta

Wearable sensory devices have attracted considerable attention in both academic and industrial communities in recent years. Conductive hydrogels are of great significance for soft electronic sensors owing to their soft, flexible and biomimetic water-abundant natures, which can avoid mechanical mismatch with tissues and provide comfortable human-machine interaction experiences. Here, we have developed a novel ionic conductive hydrogel via one-pot polymerization of acrylamide and an amino-functionalized monomer in the presence of multiwall carbon nanotubes, aldehyde-modified F127 and LiCl. The dynamically cross-linked hybrid hydrogel demonstrates a wide spectrum of desirable properties, including excellent stretchability (1200%), skin-mimetic modulus, toughness, exceptional elasticity (recovery from 1000% strain), resistance to damage by sharp materials, self-healing property (636% stretchability after self-healing), high conductivity (3.96 S/m) as well as thermo responsiveness. The combination of these characteristics enables the hydrogel to be used as a durable, reliable and smart conductor to fulfill the increasing demands of modern electronics. When exploited as a strain and pressure sensor to monitor diverse human motions, the prepared hydrogel sensor shows excellent sensitivity and reliability. Particularly, the hydrogel sensor can detect detailed waveform change of human wrist pulses before and after exercise, suggesting its superior sensitivity compared to previously reported hydrogel sensors. The hydrogel was further integrated with an eye mask to monitor human sleep and showed high reliability for the detection of rapid eye movement (REM) sleep. This work provides new insights into the fabrication of multifunctional, smart and conductive materials, holding great promise for a broad range of applications like wearable sensors and soft robotics.

Funct. 03

Size Effects of Superhydrophobic Microtopographies to Limit Microbial Adhesion and Transmission

Desmond van den Berg, Dalal Asker, Benjamin D. Hatton

University of Toronto

Healthcare-associated infections (HAI) affect 1 in 20 patients admitted to a hospital and represent nearly 10% of total inpatient costs – amounting to an annual economic burden exceeding $35 billion to global health systems. In health care settings, indirect transfer of pathogens is dominated by the handling and contact of surfaces by individuals through touch contact, with importance placed on those deemed "high-touch contact" surfaces. Our objective is to engineer the surface of medical gloves to reduce rates of pathogen transmission to and from these surfaces. One strategy to reduce the fouling of surfaces is to limit the surface area available for microbial adhesion through surface topography. In this work, we investigate rates of microbial adhesion to superhydrophobic elastomers molded with micro- and nanopost arrays, where we test the role of micropost size relative to microbial cell size. This was achieved through the molding of microtopographies (generated via photolithography) ranging from 0.5 to 150 micrometers in diameter in a UV-curable polyurethane compound. After chemical functionalization to impart a superhydrophobic behaviour to these topographies, we found the adhesion of three bacterial strains (S. aureus, P. aeruginosa, and E. coli) and a yeast (C. albicans) could be reduced by factors of 10^3 to 1045. This approach also allowed for novel analysis of adhesion rates of microorganisms to limited areas, the potential mechanisms of their attachment to superhydrophobic surfaces, and the packing efficiency of bacteria on limited contact area surfaces. Through the proposed physical models investigated in this work, it is believed this mechanism could potentially apply to even smaller pathogens (viruses similar to COVID19) and further the understanding of the role surfaces play in healthcare environments and the propagation of infectious diseases.

Funct. 04

Tuning Surface Interactions Favors the Regenerable Separation of Oil-in-Water Emulsions

Mingfei Pan, Lu Gong, Li Xiang, Wenshuai Yang, Wenda Wang, Ling Zhang, Wenjihao Hu, Hongbo Zeng

University of Alberta

Developing antifouling membrane materials is of both fundamental and practical significance for separating surfactant-stabilized oil-in-water (O/W) emulsions, which has been conventionally achieved through the short-range hydration interaction from hydrophilic membrane surfaces as a physical barrier. In this work, we report a mussel-inspired antifouling coating formed by carboxyl and quaternary ammonium moieties bearing adjustable surface charge property, employing tunable long-range electrostatic interaction to achieve adaptive antifouling performance in response to the varying electrical characteristic of emulsions. The surface force measurement results showed that modulating the surface electrical properties of the coatings through varying the solution pH can effectively alter their electrostatic interactions with emulsions from attraction to repulsion, to enable emulsion repellence of the coatings. Such functional coatings were further applied on a PVDF membrane. An enhanced water permeability and

reusability was achieved to separate both the positively and negatively charged emulsions, demonstrating its adaptive antifouling performance for efficient and universal water treatment. This work provides fundamental insights into the antifouling mechanisms of membranes to O/W emulsions, as well as the facile advancement of functional materials with tunable surface interactions for various engineering and environmental applications.

Funct. 05

Biological microfluidics for smart optical control in buildings

Raphael Kay, Kevin Nitiema, Charlie Katrycz, Benjamin D. Hatton

University of Toronto

We propose that marine organisms can serve as a model for the design of buildings. Antarctic Krill, a shallow-swimming decapod, can change colour by dispersing and contracting pigments throughout the cells within its skin. This multicellular microfluidic mechanism enables switchable optical absorption and transmission at the organism's surface, helping to regulate harmful ultraviolet solar exposure through active fluidic shading. Buildings require equally-active solar control, operating in highly dynamic environments, where temperature and light intensity fluctuate across hourly, daily, and monthly timescales. Inadequate solar control is a major source of building inefficiency, and the resulting heating and cooling energy loads are responsible for roughly one third of the energy and greenhouse gas footprint of the globe. In our work, we suggest that microfluidic biological principles can scale to the length scales of building facades. We have developed large area (30x30cm2) fluidic devices, where pigmented fluids are digitally-manipulated within a confined volume, to control optical light transmission and colour. Differential pigmentary control enables highly reconfigurable operation, helping to achieve 50% savings in annual heating and cooling energy usage over comparable typologies in simulation. This millifluidic platform establishes precise and responsive building behaviours analogous to living tissue.

Funct. 06

Modelling the Thermal Behaviour of Flexible Electronic Textile Heaters Under Varying Top Boundary Conditions

Ikra Iftekhar Shuvo, Justine Decaens, Dominic Lachapelle, Patricia I. Dolez

University of Alberta

Joule heating textiles have been developed for different kinds of applications, including automotive car seats, de-icing blankets, and wearable heating jackets. The inherent flexibility and versatile form factor of heating textiles offer large opportunities for the broad adoption of these smart textiles. However, their market growth is limited by challenges in terms of quality, including variation in response time and uniformity of surface heat distribution. In this study, we have developed two mathematical models to describe the dynamic heating and cooling behaviours of a textile nonwoven heater made of silver-coated nylon and polyester fibers, encapsulated between two polyurethane films. The robustness of the models was assessed by testing the textile heater with a series of boundary conditions: a polyvinyl chloride pouch filled with water, a nylon-polyester jacket, a wooden board, a ceramic plate, memory foam, artificial leather, and a rigid cardboard. In each case, the other boundary condition was provided by contact with a bamboo board. The heating-cooling behaviour of the heating textile was characterized by supplying it with a constant power in the range of 10-12 W; then the power was switched off after 1 hour. The temperature of the heater was recorded over a period of 1800s, using a thermocouple affixed to its top surface. The temperatures recorded during heating and cooling were successfully fitted using the mathematical equations developed. A good agreement with R2 values of ~99% was obtained with all the top boundary conditions tested. This indicates the robustness of the fitting equations to describe the heating and cooling behavior of the heating textile. The adjustable parameters of the fitting equations can be used to compare the performance of different joule heating textiles and predict their dynamic behaviours. Moreover, the parameters could be also used to develop criteria to characterize the heating efficiency of smart heating textiles.

Funct. 07

The Effect of Substitution the Sites of the methoxy group in Quinoxaline Dyes on the Driving Force of an Electron injection: Dye-Sensitized Solar Cells Applications

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Using Time-Dependent Density Functional Theory (TD-DFT) calculations, we simulated here different Quinoxaline derivatives dyes, coded as $Q_{1\text{-}1}$, $Q_{1\text{-}2}$, $Q_{1\text{-}3}$, $Q_{1\text{-}4}$, $Q_{1\text{-}5}$, and $Q_{1\text{-}6}$, for n-type dye-sensitized solar cells (n-DSCs). All the structures have the same backbone, with two oxygens in fixed positions and different numbers and positions for the Hydroxyl group. Excitation energies and absorption spectra of different dyes have been predicted. The effect of different numbers and positions of oxygen atoms and hydroxyl groups on the Optical and Electronic properties of free dyes has been the main focus of research. DSC characteristics such as Light-Harvesting

Efficiency (LHE), electronic injection driving force (ΔG_{inj}), and dye regeneration spontaneity (Greg) have all been investigated as a result of this variation. The results show that the $Q_{1\text{-}2}$@TiO_2 interface has the maximum electronic injection (ΔG_{inj}) of -2.4356237 eV and LHE of the sequence of 0.6683. Finally, our study reveals the important effect of the Hydroxyl group on electrochemical properties.

Materials Characterization I

Matls. Char. 01

High Concentration Graphene Nanoplatelet Dispersions in Water stabilized by Graphene Oxide

Dominik P.J. Barz, Sreeman Mypati, Andrew Sellathurai, Marianna Kontopoulou, Aristides Docoslis

Queen's University

The preparation of aqueous graphene nano platelet (GNP) dispersions is a challenging task due to their tendency to agglomerate. In contrast, graphene oxide (GO), an oxidized form of GNP, has amphiphilic characteristics which allow it to disperse in an aqueous milieu without the addition of a surfactant. Therefore, we utilize GO as a dispersing agent to prepare highly-concentrated aqueous GNP dispersions, which can be used for various applications. The nature of the dispersed phase is investigated by various material characterization methods. Furthermore, we measure the zeta potentials of the dispersed phased as well as the contact angles of dispersions on different substrates. The latter data are used in the extended Derjaguin–Landau–Verwey–Overbeek theory to gain insight into the interactions that determine dispersion stability. We find that the stability of such dispersions mainly depends on the pH value as well as the ratio of GO and GNP concentrations. The rheology of the dispersions is investigated and different nematic phases are identified. Finally, highly-concentrated dispersions are used for printing of graphene films on a flexible substrate. After reduction of the minor GO fraction, the films have a high conductivity of more than 4500 S m−1.

Matls. Char. 02

Liquid Phase Shear Exfoliation of Graphite into Graphene Nanoplatelets using Graphene Oxide as Surfactant

Andrew Sellathurai, Sreeman Mypati, Dominik P.J. Barz, Marianna Kontopoulou

Queen's University

In this study, graphene nanoplatelets (GNP) are prepared using graphene oxide (GO), a derivative of graphene, as the dispersing agent in the liquid phase shear exfoliation of raw flake graphite. Graphene oxide has similar properties to that of graphene, however, it contains functional groups such as epoxides, hydroxyls and carboxyls. This added functionality makes GO amphiphilic and a suitable dispersing agent in water. In order to prepare stable GNP dispersions during exfoliation, the sheets need to overcome the van der Waals attractive forces and π-π interactions. Preliminary research shows that more widely stable GNP dispersions can be achieved by adjusting the pH of dispersions to 10. The major variables influencing the exfoliation of graphite are: the concentration of GO and graphite, along with shear rate, and time. Using dimensional reasoning and according to the factorial design of experiments, we obtain a correlation to optimize the GNP yield by a response surface methodology. The exfoliated GNP content in the dispersions is determined from UV-vis spectroscopy, via a GO/GNP standard calibration curve. Furthermore, the exfoliated GNP is characterized using, atomic force microscopy, Raman spectroscopy, X-ray diffraction, and X-ray photoelectron spectroscopy. Finally, the GO/GNP dispersions are then

concentrated and used to synthesize graphene hydrogels. The resulting hydrogels are used as an electrode material for making flexible supercapacitors and their performance is evaluated.

Matls. Char. 03

Tuning the conductivity and electron work function of Spin-Coated PEDOT:PSS/PEO nanofilm for enhanced intramolecular adhesion

Raymond Setiawan

University of Alberta

We report a novel phenomenon of increasing the adherence of PEDOT:PSS/PEO nanofilm for Si3N4 through cosolvent treatment by DMSO. By varying the w/w% ratio of DMSO, nanofilms with different conductivities were produced. AFM analysis showed that the adhesive force between its Si3N4 probe and the nanofilm increased by 35.8 % as the conductivity of the nanofilm was increased. The conductivity became saturated after the PEDOT:PSS to DMSO ratio reached a certain level. This study demonstrates that the variations in adhesive force are determined by two factors: 1) the difference in EWF between the nanofilm and counter-body Si3N4, and 2) the electrical conductivity of the materials involved. The former is the driving for establishing a dipole layer at the interface, while the latter determines the degree of ease to achieve the dipole layer. This study demonstrates an approach to tailor interfacial bonding for different types of material without atomic diffusion involved, which is promising for applications in various fields such as control of biomedical films on implants and functional films for electronic devices.

Keywords: PEDOT:PSS, adhesion force, conductivity, cosolvent, Variable Range Hoping Model.

Matls. Char. 04

High-Temperature Thermal Stability of Super-Tetragonal PbTiO3 Film

Mengsha Li, Chenyue Qiu, Stas Dogel, Hooman Hosseinkhannazer, Pingfan Chen, Jason Tam, Doug Perovic, Jane Howe

University of Toronto

Ferroelectric random-access memory (FeRAM) is a high-performance memory that combines advantages of traditional non-volatile memories and high-speed RAM. The computational information, 0 or 1, is represented by the spontaneous polarization direction of the ferroelectric thin film which is placed between two electrodes. As a result, the performance of FeRAM strongly dependents on the characteristics of ferroelectric materials. Normally the operational temperature of such materials is limited to $T < 0.5$ Tc (Curie temperature), since perovskites only exhibit a large tetragonality as well as an improved spontaneous polarization below Tc. Therefore, exploring new ferroelectric materials that can function in extreme environments (i.e. high temperatures) is of great importance to the applications of advanced devices.

In this project, we used pulsed laser deposition (PLD) to grow the PTO film on a NdGaO3 (NGO) substrate

with La0.7Sr0.3MnO3 buffer layer as the bottom electrode. Due to the PLD atmosphere with low oxygen pressure, the Pb-rich composite PTO film with the tetragonality of around 1.3 and the spontaneous polarization around 250 μC/cm2 is obtained. The secondary phase PbO shows nanocolumn morphology and is vertically aligned throughout the entire PTO film. Furthermore, in situ heating transmission electron microscopy (TEM) is a powerful tool to study the thermal stability of such functional materials. Herein, the heating experiments were performed using the Blazer heating holder (Hitachi High-Technologies Canada) equipped with MEMS based heating chip (Norcada Inc., Edmonton, Canada), on a Hitachi HF-3300 TEM. From the in situ heating experiments, the real-time structural evolution data reveals that the super-tetragonal PTO thin film can endure temperatures up to 600 degree in vacuum. The results of this study demonstrate the feasibility of applying this class of ferroelectric perovskites in functional devices that require high temperature stability.

Matls. Char. 05

Synchrotron Techniques for Materials Research

Feizhou He

Canadian Light Source

Every year thousands of researchers around the world travel to synchrotron light sources to carry out experiments for their researches. Statistics show that materials researches account for one third to half of the activities at a synchrotron, in areas such as engineering materials, nano-catalyst, energy materials, and novel electronic materials.
This talk will provide an overview of the research activities at the Canadian Light Source, the national synchrotron facility of Canada, with a few research highlights, such as non-destructive micro-CT imaging, in-situ/in-operando measurements of battery materials, and understanding the properties of materials at atomic level. These advanced imaging, spectroscopic and diffraction techniques are either impossible or very difficult without a synchrotron source.

Materials Characterization II

Matls. Char. 06

Role of Iron-Intermetallics on porosity characteristics in Al-Si-Cu cast alloys

Ehab Elsharkawi

Saint Mary's University

The effects of metallurgical parameters on the precipitation of the b-Al5FeSi phase, and porosity formation in Al-Si-Cu alloys were examined in detail. Microstructural characterization and phase identification were carried out using scanning electron microscopy, electron probe microanalysis coupled with energy dispersive X-ray (EDX) and wavelength dispersive spectroscopy (WDS) facilities, and thermal analysis. An image analyzer was used in conjunction with the optical microscope for quantification purposes. The results obtained showed that the size of the b-Al5FeSi platelets and their distribution, particularly at low cooling rates has a significant effect on characteristic of the porosity. Addition of strontium leads to fragmentation of b-platelets. This effect lessens with increasing iron concentration, and further strontium addition leads to the precipitation of Al2Si2Sr phase particles, instead. The porosity observed at any given studied alloy composition is depends on the permeability of the interdendritic regions as solidification proceeds.

Matls. Char. 07

Particle and Solute Dispersion in a cast Al-Cu-Mg-Ag+TiB2 Composite

Rosen Ivanov, D. Mayer, S. Farrell, M. Phaneuf, M. Gallerneault, Bradley Diak

Queen's University

The co-existing precipitate families in an Al-Cu-Mg-Ag+TiB2 alloy formed during solidification through a sand-casting procedure are reconstructed using FIB-SEM tomography and further analysed by TEM. Thermodynamic calculations show formation of a small solid fraction of Al3Ti at temperatures above 700 °C, followed by a wide freezing range for the primary α-Al and formation of a eutectic type of Al-Cu phase below 540 °C. The presence of solid TiB2 particles and formation of Al3Ti in the liquid lead to solidification of equiaxed α-Al grains rather than commonly observed dendrites. The low cooling rates of sand-casting and abundance of TiB2 particles results in their segregation to interfaces where they can agglomerate together with solutes, like Cu, rejected by the primary α-Al grains. The talk illustrates the characterization required in this complex cast-microstucture, which is needed to understand the role of homogenization and age-hardening heat treatments on Cu redistribution and precipitation of Ω and θ’ phases.

Matls. Char. 08

Effect of Heat Treatment on Hydrogen Trapping Capacity of Model Fe-C-Mn-Nb Steel

Sara Filice, Dmitrij Zagidulin, James Noel, Joseph McDermid, Joseph Kish

McMaster University

Supporting the development of HIC-resistant linepipe steel is crucial as pipelines are extensively used in the transportation of oil/gas that may contain high amounts of H2S [1]. In order to improve the reliability and safety of pipelines, a fundamental understanding of the HIC damage mechanism is necessary so that control measures can be implemented. Hydrogen absorption is well known to degrade mechanical properties and increase susceptibility to cracking and associated brittle fracture failure at stresses below the yield stress of linepipe grade steels [2,3]. The steel microstructure is widely recognized as a critical factor affecting HIC susceptibility, as microstructural features can affect the mobility of absorbed hydrogen by acting as traps [2]. Many features within the microstructure can act as hydrogen traps. However, this study focuses on strengthening precipitate particles, specifically the relative effects of size, size distribution, and volume fraction of Nb carbide and nitride precipitates.

Model Fe-C-Mn-Nb steel has been produced to elucidate the potency of Nb precipitate particles to serve as effective H traps. A spectrum of heat treatments was applied to vary the size, distribution and volume fraction of the Nb-bearing precipitates. Microstructure characterization was completed using TEM and bulk extraction replicas and SEM coupled with EBSD. Thermal desorption measurements were completed on all heat-treated samples to globally characterize the hydrogen trapping capacity of the Nb-bearing precipitates. Links were then made between the type, size, distribution and volume fraction and hydrogen trapping capacity.

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Matls. Char. 09

Structural evolution of oxide inclusions in cold-spray Cu coatings

Jason Tam, Dominique Poirier, Jean-Gabriel Legoux, Jason D. Giallonardo, Jane Howe, Uwe Erb

University of Toronto

Cold-spray is a metal coating deposition technique where micron size metallic powder particles (e.g., Cu) are accelerated to supersonic velocities by a carrier gas (e.g., He, N2) through a de-Laval type nozzle. Upon impact to the substrate, the powder undergoes severe plastic deformation and adheres on the surface, forming a solid coating. Since the feedstock powder will be exposed to ambient air during handling and processing, the particle surfaces will have a very thin layer of the metallic oxide which is inevitably co-deposited with the metal coating. The current study aims to uncover the structural evolution of oxide inclusions in cold-spray Cu coatings. Particularly, the microstructural evolution of the oxides in the Cu coatings after low temperature annealing and their influence on mechanical properties will be discussed.

It will be shown that the initially thin (< 50 nm) continuous oxide layer at the particle/particle interfaces begins to break up into individual particles after heat treating the material at 350°C for 1 hour due to capillary forces. Upon further annealing at 600°C for 1 hour, these oxides rapidly coarsen (Ostwald ripening) and leave behind large segments of oxide-free Cu particle/particle interfaces. Consequently, the ductility of the cold-sprayed Cu increases significantly with increasing annealing temperature.

Matls. Char. 10

Laser processing of TiAlN-PVD pre-coated Zircaloy-4 for nuclear applications

Lin Zhu, Pusong Wang, Arash Nikniazi, Linjiang Chai, Vahid Fallah

Queen's University

Zirconium and its alloys have widespread applications in nuclear industries though generally suffering from nodular corrosion and limited mechanical properties at high temperatures. To extend the service life of the Zircaloy-4 alloy, a method of enhanced surface coating on the zirconium alloy is proposed. TiAlN films with a high temperature oxidation resistance (~900℃) and wear resistance were applied on a Zircaloy-4 substrate using the Physical Vapor Deposition (PVD) technique with a thickness of ～5μm. Due to the difference in thermal expansion and elastic modulus, however, residual stress fields will be formed between coating and the base alloy affecting the interface stress load transfer and material performance, which leads to the necessity of laser treatment after PVD coating, i.e., to create metallurgical bonding. In this research, multiple laser treatments with different line energy densities were performed on TiAlN-PVD pre-coated Zircaloy-4 specimens. The suitable energy density range was investigated by cross-section inspection via SEM, EDX analysis and the use of relevant image analysis techniques, i.e., as to devise a parameter set (laser spot size, power and scan velocity) resulting in (1) a narrow metallurgical bonding with minimal dilution of TiAlN coating with the Zr substrate, as well as (2) the whole track geometrical and chemical uniformity.

Matls. Char. 11

The corroded refractory linings preparation technique at laboratory condition for thermomechanical investigation

Sina Darban, Ryszard Prorok, Jacek Szczerba

AGH University of Science and Technology, Poland

Refractories are a kind of high-temperature ceramic material. Generally, ceramics are fragile, and their tensile strength is significantly lower than compressive strength. Brazilian test, an indirect laboratory test, can be implemented to determine the tensile strength of ceramic materials due to efficient testing procedures. However, most of the investigations were allocated to the un-corroded samples; this research aims to prepare an appropriate corroded alumina-spinel sample for the Brazilian test, which needs optimum microstructure and physical condition characteristics. For this means, 1350 and 1450°C temperatures were chosen for corrosion tests based on thermodynamic calculations and hot stage microscopy results of industrial slag. Moreover, XRD and XRF techniques were utilized for phase and chemical analysis, respectively. Microstructure alternation investigated by SEM/EDS to evaluate the most-proper sample for thermomechanical investigations. The results showed that although the impregnation was achieved within microstructure, physical properties deteriorated, which is not desirable. Acknowledgments - The work was partially supported by the faculty of material science and ceramics and the European Commission's funding scheme, Marie Skłodowska-Curie Actions Innovative Training Networks in the frame of the project ATHOR - Advanced THermomechanical multiscale modeling of Refractory linings 764987 Grant.

Matls. Char. 12

Influence of Hydrothermal Aging on the Strength of Moisture Barriers used in Firefighters' Protective Clothing /

Laura Munevar Ortiz, Patricia I. Dolez, John A. Nychka

University of Alberta

The moisture barrier is an essential layer in firefighters' protective clothing because it prevents water penetration while allowing perspiration to escape. However, the performance of moisture barriers degrades over time because of exposure to the different conditions to which firefighters are exposed in service, including water from the environment and the firefighter perspiration. Therefore, the purpose of this study was to examine the effect of accelerated hydrothermal aging on the tear strength of moisture barriers.

Three moisture barriers used in firefighters' protective clothing were selected for the study. The specimens were immersed in containers filled with reverse osmosis water and thermally aged at 20, 80, 90, and 95°C for times between 6 and 1080 h. The aging temperatures were selected considering the conditions faced by firefighters. The residual tear strength of the fabrics was measured by trapezoidal procedure following the ASTM D5587-15 standard test method; however, due to limitations in fabric availability a slightly smaller specimen size (55 x 110 mm) was used. One-way analyses of variance were

carried out to analyze the influence of the aging time and temperature on the mean tear strength. Scanning electron microscopy was used to evidence any potential changes in the surface due to hydrothermal aging.

Different behaviors were observed for the three moisture barriers. In some instances, a decrease in tear strength was observed for the highest hydrothermal aging temperatures while the same condition did not affect other moisture barriers. In any case, the decrease in tear strength remained lower than 10% after 1080 h of hydrothermal aging. In one instance, the decrease in tear strength was possibly attributed to a degradation in the top polyurethane layer. These preliminary results demonstrate the importance of better characterizing and understanding the hydrothermal behavior of moisture barriers used in fire protective clothing.

Mechanical Behaviour and Structure-Property Relationships

Mech. Prop. 01

Using discrete element methods to generate digital materials: An application to direct reduction of chromite ore

Jason P. Coumans, David Carter, Laura Dickson, Nail Zagretdnov, Dogan Paktunc

CanmetMINING, Natural Resources Canada | Resources Naturelles Canada

Digital materials and digital rock physics has emerged as a valuable source of material property relationships and understanding of pore- and grain-scale processes which govern these properties. The generation of digital materials thus enables researchers to numerically investigate effective mechanical and hydraulic properties of materials and supplement laboratory investigations.

The direct reduction of chromite ore is a promising new technology actively researched as an alternative to conventional smelting. Direct reduction of chromite produces ferrochrome from chromite ore using a carbon reducing agent and flux without the high temperatures (1650 C) required to produce molten ore during smelting. During direct reduction at 1300 C, the pellets are comprised of solid ore and carbon (petroleum coke), and molten CaCl2 flux.

Chromite ore and petcoke particles comprise the structural skeleton of the pellet, whilst CaCl2 flux fills inter-particle pore space. Therefore, the disruption of the ore-petcoke structural framework by solid CaCl2 during the pelletizing process could result in structural weakness at temperature, affecting process efficiency. To investigate this, we present a numerical packing methodology that utilizes an open-source Discrete Element Method (LIGGGHTS) to generate digital pellets composed of ideal spheres. We systematically vary the mass percentages, grain sizes, and cohesion behaviour of the chromite ore, reductant (petcoke), and CaCl2 flux to generate a range of realistic pellet matrices. We then utilize a nearest-neighbour analysis to explore the microstructure of generated digital materials to intuit pellet feasibility and experimental design optimization. Preliminary results suggest small differences in CaCl2 particle size and cohesion reduces structural connectivity of the ore-petcoke skeleton for the mass fractions of flux used in direct reduction of chromite ore.

Mech. Prop. 02

Effect of processing conditions on the strength of pellets containing Ring of Fire chromite ore

David Carter, Laura Dickson, Dogan Paktunc

Canmet MINING, Natural Resources Canada| Resources Naturelles Canada

The direct reduction of chromite (DRC) process shows potential as a more energy efficient technology for reducing chromite ore at approximately 1300 °C in either a rotary kiln or rotary hearth furnace than existing mature technologies. These mature technologies utilize a rotary kiln or travelling grate for pre-oxidation or pre-reduction (at approximately 1000 °C), in addition to an arc furnace a temperature greater than 1600 °C to completely reduce and melt the chromite ore. An especially important advantage of the DRC process is therefore that high degrees of chromite reduction can be achieved without melting the chromite ore, which can reduce the processing energy requirements by up to a third. To evaluate the feasibility of the direct reduction process, an understanding of pellet strength due to the pelletization process used, pellet composition, and as pellets are reduced is of great importance.

The unconfined compressive strength of various 12 mm diameter pellets that have been rolled or pressed and are composed of ground chromite ore (consisting of chromite; $(Mg0.4Fe0.6)(Al0.6Fe0.1Cr1.3)O4$ and minor clinochlore), calcined PETcoke, and $CaCl2$ as a flux was determined using a motorized force testing stand and gauge. As the flux content of pressed pellets increased from 0 – 30 wt% of chromite ore, dried pellet strength decreased 67% to between 1000 and 1700 kPa. This reduction in strength can be at least partially attributed to the cohesion between $CaCl2$ particles which lead to their clumping together. Cracks are therefore expected due to adhesive failure between $CaCl2$ clumps and well dispersed ore and PETcoke particles during compression. The strength of pellets reduced at temperatures above 1100 °C was between 150 and 490 kPa. As pellet strength decreases, operating conditions including pellet throughput, and dam height of a rotary kiln (if used) must be reduced, which will adversely affect process efficiency.

Mech. Prop. 03

Irradiation Creep Behavior of Zirconium Alloys

Brodie Moore, Matthew Topping, Mark R. Daymond

Queen's University

A nuclear power generator exploits high energy neutrons to heat water and spin a turbine. Zirconium based alloys are commonly used as structural components in a reactor’s fuel assembly due to their strength, corrosion resistance, and most importantly low neutron absorption cross-section. Even still, the interaction between the neutrons produced in a reactor and its structural components can have a dramatic effect on the material properties and performance. In-reactor creep behavior of materials is accelerated well beyond regularly understood ex-situ behavior and is referred to as “Irradiation creep”. Understanding irradiation creep in nuclear reactor structural components is of great importance to the nuclear industry; specifically influencing reactor safety, lifetime extension, and future reactor design. Investigating the creep behavior of these components proves to be a difficult task as experimental parameters such as neutron flux, stress, and temperature can vary greatly at different locations in the reactor. To assist in developing a mechanistic understanding of irradiation creep behavior an in-situ creep

rig has been developed at Queen's University's Reactor Materials Testing Laboratory. This rig, in conjunction with a linear proton accelerator, is used to emulate reactor irradiation conditions including flux and temperature whilst conducting creep experiments. Unlike conventional experiments in test reactors, in which strain rates are measured over many years, proton irradiation experiments can be conducted in a matter of days allowing for a systematic exploration of this multivariable scenario. Using this systematic approach, in-situ creep tests have been conducted on both Zircaloy-2 and CANDU reactor pressure tube material (Zr-2.5Nb). A test matrix of experimental parameters including proton flux, sample temperature, and stress was explored and the results will be discussed in comparison to neutron irradiation creep tests.

Mech. Prop. 04

Characterizing 3D stress development in the vicinity of notch tips in polycrystalline zirconium

Karim Louca, Hamidreza Abdolvand, Darren Pagan

Western University

Understanding the impacts of cracks and notches on material behaviour in ductile alloys is crucial for developing macro- and micro- predictive models. The impact of the microstructure near a crack can be detrimental to the material's fatigue behaviour specially in anisotropic crystal structures such as hexagonal-close packed (HCP) metals. In this study, synchrotron three-dimensional X-ray diffraction (3D-XRD) is employed to investigate the effect of a round notch on the grains stress states near the notch tips in a pure zirconium specimen. The measured microstructure and the shape of the notch is then imported into a crystal plasticity finite element (CPFE) model to simulate the polycrystal deformation. Stress distributions across the notch were investigated for different path angles to examine the microstructures effects on the stress concentrations. Furthermore, single crystal studies are provided to elucidate these distributions and explain the deformation mechanisms occurring ahead of the notch tips while varying crystallographic orientation.

Mech. Prop. 05

Effect of back stress on cyclic hardening of a heterostructured Al-Si automotive alloy

Soumya Dash, Dejiang Li, Xiaoqin Zeng, Daolun Chen

Ryerson University

Low-cycle fatigue properties are essential for the life prediction and design of load-bearing automotive structural components. Low iron-containing aluminum-silicon Silafont®-36 alloy has a high fatigue resistance than several other cast aluminum alloys when tested under strain-control in the as-cast condition. Due to its improved ductility, automotive manufacturers have selected it for the applications involving even shock tower components. Microstructural features generated during the high-pressure die-casting with minimum porosities and defects, leads us to understand its pragmatic cyclic deformation mechanisms. Internal stresses are generated during cyclic deformation of the alloy, namely, back stress and frictional stress which are produced due to the interaction of precipitates and intermetallic phases in the alloy with heterogeneous microstructures similar to that of particulate-reinforced metal matrix composites. Theses stresses were calculated from the mathematical conceptualization of the stress vs. strain hysteresis loops generated at each strain amplitude applied. The results were then correlated with the phenomenon of cyclic hardening for the alloy, which increased up to a total strain amplitude of 0.5% and then decreased. Fatigue-life of the alloy was also observed to be controlled by the generation of back and frictional stresses. These stress values at different strain amplitudes governed the low-cycle fatigue properties of the alloy. Details on this study will be presented at the conference.

Mech. Prop. 06

Surface atomic diffusion-induced abnormal softening in metallic nanocrystals

Sixue Zheng, Scott X. Mao

University of Pittsburgh

In metal materials, “smaller is much weaker” trends experimentally reported to date are generally believed to originate from Coble-type diffusional deformation process. Here, by using in situ nanomechanical testing in high-resolution transmission electron microscope, we found that the yield strength-size relationship of silver nanocrystal changed from a normal to an inverse Hall-Petch relation with decreasing the size scales. Surface diffusion-assisted dislocation nucleation, namely, coupled diffusive and displacive deformation mechanism, was discovered to be the dominant mechanism in the inverse Hall-Petch regime, manifested through both direct experimental evidence and molecular dynamics simulations. Large-scale diffusion of surface atoms activated by crystal slip was shown to induce abnormal softening in plastic flow process in silver nanoscale crystals. This work provides novel insights into the atomic-scale mechanisms of coupled diffusive and displacive deformation in small-sized metals.

Mech. Prop. 07

Effect of carbon nanotube reinforcement in a bimodal-grained aluminum matrix nanocomposite

Sohail Mazher Ali Khan Mohammed, D.L. Chen, Z.Y. Liu, D.R. Ni, B.L. Xiao, Z.Y. Ma

Ryerson University

Metal matrix nanocomposites reinforced with carbon nanotubes (CNTs) have long been considered as exciting prospects among the nanotechnology applications. However, after nearly two decades of studies in the area, question still remains about its practical significance. The uncertainty stems from factors including poor load transfer, interfacial reaction and dispersion that lead to processing challenges in such nanocomposites. In the current study, we present the effect of CNT reinforcement in a bimodal 2009Al alloy via microstructural and mechanical characterization. CNTs were ball milled along with 2009Al powders and later mixed with as-received 2009Al powder to attain bimodal grain distribution in the composite followed by thermomechanical processing. A significant improvement in the mechanical properties with acceptable ductility was achieved in the nanocomposite compared with the base 2009Al alloy fabricated by the same route. Several strengthening mechanisms including load-transfer, Orowan and thermal mismatch-induced dislocation strengthening contribute to the enhanced mechanical properties of the nanocomposite. Micromechanics and nano-scale models were implemented to predict the strength and elastic modulus of CNT reinforced metal matrix nanocomposites. The outcome of this study elucidates the improvement in the mechanical properties of the nanocomposite with a characteristic bimodal grain distribution.

Mech. Prop. 08

Hydrothermal Aging Behavior of Fire-Protective Fabrics- Effect on Mechanical Performance and Surface Condition

Md. Saiful Hoque, Ankit Saha, Hyun-Joong Chung, Patricia I. Dolez

University of Alberta

Fire-protective fabrics made from high-performance fibers are well known for protecting the wearer from various hazardous conditions such as extreme heat and temperature. However, apart from heat, fire-protective fabrics also are exposed to other deteriorating conditions such as ultraviolet light radiation, abrasion, and moisture. Among these damaging conditions, moisture, which could originate from the wearer's perspiration, weather, and fire extinguishing medium, is a concern as some of the high-performance fibers are sensitive to hydrolysis. This study exposed eight fire-protective fabrics composed of different blends of para-aramid, meta-aramid, polybenzimidazole (PBI), and polybenzoxazole (PBO) fibers to accelerated hydrothermal aging by immersing them in water at different temperatures between 60°C and 95°C for up to 1200 hours. The experimental data show that, after exposure to hydrothermal aging, some fabrics exhibit a significant loss in mechanical performance without showing any morphological changes. The residual strength data of each fabric were analyzed by the time-temperature superposition principle followed by the extraction of the activation energy from the Arrhenius plot. The analysis provides quantitative information to compare the resistance of different fabrics to hydrothermal aging and estimate their service life. Furthermore, water contact angle analysis revealed significant change in the water contact angle for some fabrics as a result of hydrothermal aging. The study provides an insight into the effect of a generally unnoticed hazard, i.e., hydrothermal conditions, on fire-protective fabrics. The results obtained from this study will serve as support for the development of end-of-life sensors and predictive models of the aging of fire-protective fabrics.

MSE Pedagogy

MSEP 01

The development of Case Studies in the delivery of a Materials Engineering Process Design course

K. Meszaros, H. Henein, C. Lemelin

University of Alberta

The University of Alberta undergraduate Material Engineering program includes two, fourth-year engineering design courses. The first of these courses is focused on metallurgical process design. In the curriculum, prior to the process design course, the undergraduate students have limited opportunity to learn how to approach open ended problems that have multiple possible feasible solutions. To assist the students, an active learning approach has been developed. Here a series of Case Studies (CS) in materials process design were developed and are similar to the assigned design problem but are shorter in scope. The students work in groups during class learning how to address their CS. Their proposed solution to the CS is then discussed in class. These CS provide an opportunity for students to learn about teamwork, professionalism, as well as how to manage time and meet deliverables. These CS exercises have enabled the students to tackle industry-based design projects provided by industrial facilitators. At various times throughout the course student learning is assessed through reporting, oral presentations, self-evaluations, and surveys. The data from the assessments over several terms suggests the positive role that active learning with CS plays in preparing undergraduate students for the challenges of an engineering career.

MSEP 02

The Remote Delivery of a Hands-On Materials Science Engineering Design Course with an At-Home Mechanical Testing Kit

Xinyue (Crystal) Liu, Scott Ramsay

University of Toronto

Laboratory work teaches students how technical knowledge is applied in practice and has long been recognized as a crucial component of a complete undergraduate engineering experience. Providing students with meaningful hands-on experience became more challenging in the remote learning environment during the COVID-19 global pandemic.
In the work being presented, a low-cost, open-source mechanical testing kit, the Miniature Mechanical Testing Kit (MMTK) was designed and implemented as a remote learning tool. The machine features a linear guide rail and a load cell, capable of testing components up to 500N. Custom designed printed circuit board (PCB) and user interface (UI) make the machine more user-friendly to operate. The kit includes all tools needed for assembly and troubleshooting, with step-by-step assembly manual provided to the users. The machine was launched as a lab kit in a third-year materials science engineering design class during the pandemic, to provide students with meaningful hands-on experience while learning from home. The students assembled the machine, used it to test samples, then designed and performed their

own experiments. The activities received generally positive feedback, and some interesting observations were made.

MSEP 03

@Home Materials Science Lab Learning Modules

Brodie Moore, Lucas Ravkov, Matthew Thoms, Bradley Diak

Queen's University

Many existing materials science and engineering laboratory activities have historically developed from research lab activities. Consequently there is a need for certain, usually expensive and possible dangerous tools and instruments to enable hands-on-activities from metallography (grinding media, chemical etchants, fume hoods, microscopes) to casting (furnaces, crucibles) to mechanical testing (testing frames) to structural/chemical analysis (x-ray diffraction), etc. The 2020 pivot to remote learning offered two paths to run an existing lab course, MECH-397 Materials Engineering Lab I, with a strong focus on phase transformations: (1) run the existing activities in the University labs remotely using video streaming; (2) create new activities that explore fundamentals to be done at home by the students. Motivated by Julia Ortonoy's "Goodie bags: A new route to hands-on chemistry learning through take-home mini-experiments [NA MES8 Conf. at MIT (2017)], and fading memory of the mail-order chemistry sets of the first half of the 20th century, four lab modules were developed for students to explore (i) microstructures and equilibrium phase diagrams; (ii) wettability and optics; (iii) crystal growth and microstructure; (iv) investment casting and resonance. Starting with a mail-out box of supplies at the start of a 12-weeks term, the students were given loose guidance by the TAs to play their way through the activities. The presentation will reflect on the learning experience from the student, TA and instructor perspectives.

MSEP 04

Modules to support online delivery of an advanced ceramic course

Tom Coyle

University of Toronto

Advanced ceramic materials play a crucial enabling role in many industrial sectors including energy, bio-medical, automotive, and aerospace. Therefore, knowledge of the unique properties of this class of materials is a key component of a materials engineering curriculum. These programs are often among the smallest undergraduate programs within an Engineering Faculty, and therefore it is difficult to regularly offer this type of specialized course. This project will create a set of online modules to support the teaching of specialized advanced ceramic materials topics, which taken together would constitute a stand-alone online course at the 4th year or introductory graduate student level, accessible through eCampus Ontario. Individual modules could also be incorporated into existing courses to add specialized content. Input is welcome concerning the content and format of the modules to improve compatibility with existing programs.

Phase Transformation Fundamentals

Phase Trans. 01

Application of Diffusion Path Analysis to Understand the Mechanisms of Transient Liquid Phase Bonding in the Ni-Si-B System

Stephen Corbin, E.D. Moreau

Dalhousie University

Diffusion path analysis was applied to the Ni-Si-B system to explain the deviation from classical transient liquid phase bonding observed when using multicomponent systems containing Boron as a melting point depressant. This was achieved using a combination of differential scanning calorimetry, SEM-EDS microstructural and chemical analysis and Thermo-Calc modeling software of Ni/Ni-Si-B couples. Compositional analysis identified differing distributions of B and Si across the braze joint which were mapped onto isothermal sections of Thermo-calc generated phase diagrams. Below 1093°C, the inevitable formation of diffusionally affected (DAZ) and isothermally solidified (ISZ) zones is a direct consequence of the need for phase equilibria in the Ni-Si-B ternary system and is predicted by diffusion path analysis. Above 1100°C, diffusion path analysis also correctly predicts a persistent liquid phase observed to occur through the melting of the DAZ (i.e. a γ-Ni(Si)-Ni3B eutectic reaction).

Phase Trans. 02

A new numerical model for simulating diffusion-controlled moving interphase boundary problems

Osamudiamen Olaye, Olanrewaju A. Ojo

University of Manitoba

A new explicit numerical model based on Leapfrog and Dufort-Frankel's explicit schemes is developed to study the kinetics of diffusion-controlled interphase-interface migration. The new model considers solute conservation and can be used in binary alloy diffusion systems with constant and varying diffusion coefficients. The stability and consistency analysis of the scheme indicates that the scheme is more stable, effective, and efficient than classical explicit models and can be appropriately used to study the phase growth/dissolution kinetics in diffusion-controlled systems. The new model is used to modify the classical Heckel's criteria for the dissolution of an unstable phase. Generally, unstable phases dissolve; however, classical Heckel's criteria show an unstable phase can grow before dissolution. This work further demonstrates that even when an unstable phase starts by first dissolving, it is possible for the phase to subsequently grow after the initial dissolution before undergoing the final dissolution when the solute diffusivity changes with concentration. The model is validated using the experimental data in Kirkendall et al. and found to be suitable for studying and understanding diffusion-controlled kinetics in systems where diffusivity is either constant or isothermally varies with concentration and time.

Phase Trans. 03

Numerical analysis of isothermal solidification behavior during diffusion brazing involving 2D and 3D movement of liquid-solid interphase boundaries

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Diffusion brazing has evolved as a promising technique for joining difficult-to-weld advanced materials. Existing theoretical modelling work on the kinetics of the process, for simplicity, apply assumptions such as; one-dimensional (1D) movement of liquid-solid interphase boundaries leading to symmetric treatment of the joint system, and constant diffusion coefficient. However, in reality, liquid-solid interphase boundaries can undergo two-dimensional (2D) or three-dimensional (3D) movement and diffusion coefficient can change with concentration and time. In this work, a hybrid explicit-fully implicit numerical simulation model, the results of which are experimentally validated, is used to study the kinetics of isothermal solidification in joint systems involving 2D or 3D movement of liquid-solid interphase boundaries while incorporating variable diffusivity. Contrary to general notion, it is found that, during the joining process involving 2D or 3D movement of interphase boundaries, there is a transition from the conventional evenly matched solidification behavior to a skewed solidification behavior such that the substrate in which solute diffusion occurs along the direction of decrease in curvature, exhibits superior extents of isothermal solidification, notwithstanding the absence of material dissimilarity or temperature gradient. This is attributable to solidification rates divergence which is induced by the curvature at the moving liquid-solid interphase boundaries. Furthermore, it is found that when interphase boundaries undergo 2D or 3D movement, not only the diffusivity, equilibrium concentrations at the interphase boundaries and initial substrate composition determine the kinetics of isothermal solidification, but also the type and degree of curvature at the moving interphase boundaries exact significant influence on the kinetics.

Phase Trans. 04

Effect of synthesis method and reaction conditions on long-range and local structure of RE2Ti2O7 pyrochlore-type oxides (RE = Yb and Gd)

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Nuclear reactors have the potential to be abundant sources of energy with a low carbon footprint. The nuclear industry in Canada is worth more than $6 billion and generates 16.6% of the country's electricity. A major drawback of adopting nuclear power is the disposal of radionuclides from spent nuclear fuel. Current plans for managing high-level waste (HLW) involve sequestration in borosilicate glass and potential disposal in geological repositories. However, there is considerable interest in using ceramic oxides, such as pyrochlores, as alternative nuclear waste forms due to the high chemical durability and waste loading capabilities of these materials compared to borosilicate glass. The ceramic method is often used to synthesize RE2Ti2O7 pyrochlore-type oxides and requires the use of high temperatures and long reactions times, making this process less economically feasible for large-scale production. Recently,

solution-based synthetic routes, such as coprecipitation and sol-gel methods, have been shown to require much lower reaction temperatures by reducing diffusion distances between precursors. This work studied the effect of low annealing temperature and reaction time on the structure of RE2Ti2O7. The effect of low temperature and short synthesis time on radiation damage resistance of these materials was investigated using heavy-ion implantation studies. Yb2Ti2O7 pyrochlore-type oxides are known to undergo temperature and radiation damage-driven phase transformation to the defect fluorite structure. Possible phase transitions in RE2Ti2O7 were investigated using phase analysis and Rietveld refinement of powder X-ray diffraction (XRD) patterns. The local structure of these materials were studied using X-ray absorption near-edge spectroscopy (XANES), and extended X-ray absorption fine structure (EXAFS). Changes to local structure in ion-implanted materials were investigated using glancing-angle (GA-) XANES.

Phase Trans. 05

On the effects of texture and grain morphology on hydrogen transport towards the notch tips and precipitating hydrides

Alireza Tondro, Hamidreza Abdolvand

Western University

Delayed Hydride Cracking (DHC) is dominantly accountable for hydrogen embrittlement and failure of zirconium alloys. DHC involves recurring processes of hydrogen diffusion, hydride precipitation and fracture of hydrides. The state of stress, through stress-assisted diffusion, is a crucial factor in redistribution of hydrogen atoms within the zirconium microstructure. During the operation of nuclear pressure tubes, a stress concentrator such as a service-induced flaw causes significant flux of hydrogen towards the flaw tip, increasing the probability of DHC initiation. This study uses a coupled diffusion-crystal plasticity finite element model to conduct a parametric study on the redistribution of hydrogen atoms near the service-induced flaws and precipitating intergranular and intragranular hydrides within the pressure tubes. The effects of texture, grain size, and flaw tip geometry on hydrogen transport are investigated. Also, the effects of parent grain orientation on hydride growth are studied. Results suggest that texture at the flaw tip can significantly affect the diffusion of hydrogen into specific regions such as triple points and grain boundaries. It is lastly shown that due to the state of hydrostatic stresses, the highest and lowest hydrogen concentrations take place respectively at the hydride tips and hydride sides. This is due to the tensile and compressive stresses forming respectively at the tips and sides of the hydrides, both of which result in axial growth of the hydrides.

Phase Trans. 06

Combinative chemical analysis by functional surface nanodroplets

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University of Alberta

Functional nanodroplet on a solid substrate surface has potential applications in highly sensitive chemical analysis, micro-reactor design, surface lubrication and among others. In this work, we form a multi-component surface nanodroplet by a simple one-step solvent exchange process. The droplets are stabilized on a solid substrate, enabling a combination of nanoextraction and the colorimetric reaction of chemicals from an immiscible phase. Due to the large surface area to volume ratio, the whole process is speeded up, completing in few minutes. The specificity of the component of the droplet makes it possible to distinguish targeted analyte from multi-component mixtures, e.g., a group of organic acids from oil medium. When an organic acid is extracted from an oil phase into the aqueous droplets, the acid dissociates and then releases protons to react with halochromic compounds contained in the droplets, leading to a visible decoloration of the droplets. The droplet discoloration time scale is specific to the droplet size, acid concentration, and acid types, enabling an effective discrimination of the acid mixtures even at the same pH value. To further demonstrate the advantage in practical application, the reactive nanodroplets were used to fast determine counterfeit alcoholic beverages from diverse spirits by using a simple mobile phone. Our approach may also be valuable for chemical analysis in the oil industry, food products and water quality monitoring.

Phase Trans. 07

Extraordinary Pb Whisker Growth from Bi-Mg-Pb Pools in Aluminum Alloy 6026

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Aluminum alloy 6026 is a widely used machinable alloy for applications in electrical components, automotive components, robotics and prosthetics. As these components are sensitive to surface changes and behavior of selected material, in this study the state of its surface was investigated over time in ambient conditions. The observations resulted in the first-time discovery of unique metallic whisker formations that were exerted from Bi-Mg-Pb pools found within the material. Further research of the unexpected phenomenon determined that the whiskers are composed of pure Pb and that their emergence is a result of internal stresses of the material. However, the stress does not only originate from residual stresses of the produced material (modified with heat treatment procedures and deep cryogenic treatment), but also forms due to the oxidation of Bi in the pools that results in significant material expansion and increased stresses. The observed whiskers displayed lengths up to 160 µm within the first 24 hours (average growth rate up to 0.6 nm s-1) after polishing the surface of the alloy. SEM investigation determined extraordinary faceted hillocks and unique whiskers that displayed more than 10-fold larger width than the area from where they emerged. Furthermore, the whiskers display a multicrystalline structure in the form of fused individual crystals with rotated crystal orientation, which were observed to grow in a step-wise manner. The TEM observation of whiskers revealed that the whiskers are in-fact

constructed of spherical Pb nanocrystals, with average size of 5 nm. The extraordinary whisker growth and nanocrystalline structure suggest a crystal growth caused by oriented attachment. Such observation and clear evidence of nanocrystalline formation of whiskers has until now not been reported. The new mechanism of whisker growth challenges current whisker growth theories and indicates a presence of a recrystallization process of the material during whisker growth.

POSTER SESSION 1

W01

Is Pickling Necessary for Stainless Steel Rebar?

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The mill scale on stainless steel reinforcing bars (rebar) is formed at high temperatures during manufacturing. This oxide layer, which is chromium-rich, is usually removed from the rolled bars by shotblasting and then the chromium-depleted layer adjacent to the mill scale is removed by pickling in an acid mixture of nitric acid, HNO3 and hydrofluoric acid, HF. The pickling process has both health and environmental safety consequences. Therefore, this project was aimed at determining whether the as-rolled bar would provide sufficient corrosion resistance and, if not, whether the shotblasting process alone would be sufficient. A potentiostatic rapid screening test was used to evaluate rebars of four different surface treatments to evaluate their corrosion performance. It was found that the as-rolled bars provided the same level of corrosion resistance as the shotblasted-and-pickled bars in this test, but the shotblasted-only specimens exhibited active corrosion. Further tests are ongoing to investigate the cause of the corrosion and to determine if similar behaviour would occur in longer-term tests giving the steel time to naturally passivate in concrete mortar before encountering chlorides.

W02

Hydrogen Induced Cracking (HIC) API-5LX80 steel used in oil and gas transmission pipelines

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One of the most important corrosion degradations in the oil and gas industry is hydrogen-induced cracking (HIC) The purpose of this paper is to provide a comprehensive review of the HIC corrosion problem during oil and gas transportation. The study has been conducted to evaluate HIC resistance and the type of crack formed in the steel pipeline in the H2S environment by performing a HIC corrosion test based on NACE-TM0284 standard on base metal, heat affected zone (HAZ), and weld metal. Using an optical microscope (OP) and scanning electron microscope (SEM) to observe the cracks. The results showed that HIC resistance in base metal is lower than the HAZ and weld zone. Besides cracks contained considerable quantities of aluminum oxides obtained by Energy-Dispersive X-ray Spectroscopy (EDS).

W03

Non-local crystal plasticity modeling of neutron irradiatied zirconium alloys

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Western University

α-zirconium, with hexagonal close packed (HCP) crystal structure, has been widely used in the core of various nuclear reactors due to its low neutron absorption cross section and good corrosion resistance. In a nuclear reactor, zirconium alloys are exposed to an intensive neutron flux resulting in a phenomenon known as irradiation damage, which has some effects on the deformation mechanism of the alloy over the service time. In this study, a dislocation based non-local crystal plasticity finite element (CPFE) model is developed to simulate the effects of crystal anisotropy and polycrystal microstructure on the localized stresses that develop as a result of neutron irradiation. The results of the model are firstly compared to the previously published measurements of growth strain in both annealed single crystals and annealed as well as cold worked polycrystalline α-zirconium specimens irradiated with neutrons. The distributions of growth strain within and across the grains of the polycrystals are critically analyzed. It is shown that due to heterogeneous distribution of the dislocation line densities at the crystal level, a noticeable non-uniformity in growth strain is observed, particularly at grain boundaries as well as on slip bands.

W04

A better model for interatomic interactions in Zirconium

Yu Luo

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Powerful prediction from force field of Zirconium can be fed into predictive models at larger length and time scales (like radiation damage modeling, dislocation dynamics, finite element method). It was shown that there is lack of force field to build accurate association between certain complex defect structures and system energy in Zirconium. A Python framework was built to generate embedded-atom method force field based on quantum mechanics data. Density functional theory is utilized to calculate the system energy of associated atomic structures. The pairwise terms and the embedded terms of the force field were parametrized via particle swarm optimization to link non-linear association between atomic structures and system energy. With this trained potential, various physical properties in Zirconium were predicted and validated with density functional theory calculations. Compared with the existing potential, this potential displayed advantages in the predictions of point defects migration, stacking fault energy, and free surface energy, etc.

W05

Improving atom-scale models of clay minerals using machine learning

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Bentonite clay is a geomaterial with numerous interesting physicochemical properties. Notably, it shows promise as a buffer material for underground long-term storage of radioactive waste. The material is predominantly composed of smectite montmorillonite, as well as considerable quantities of other minerals such as quartz, illite, feldspars, and others. Understanding this material at the atomic scale is can help understand how minute changes in the environment or potential release of radio-isotopes would affect a spent fuel long-term repository. I will present a model to describe the interatomic interactions within the main components of bentonite clay via machine learning. Specifically, I will introduce the moment tensor potential (MTP), how it will be adapted to describe clay minetral, and present a first set of results, involving an interactomic model of slilicon and silica, that constitute the backbone of clay minerals.

W06

First principles calculation of structural, electronic and thermo-electric properties of ScNiBi Half-Heusler

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The structural, electronic, and thermo-electric properties of ScNiBi Half-Heusler have been studied using a full potential linearized augmented plane-wave (FP-LAPW) method implanted in the WIEN2K code. The results of the calculations presented in this work were obtained through the use of different approximations GGA-PBE, GGA-PBEsol , GGA-WC and mBJ-GGA. The electronic band structures exhibit that the ScNiSb alloy has a small indirect gap. This means that the ScNiBi is semiconductors. The variation of the thermal conductivity, power factor, figure of merit ZT, Seebeck Coefficient and electrical conductivity, as a function of temperature have been obtained.

W07

A first principles computational study of equiatomic Zr-Fe-Nb alloy

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In this computational study, we studied the crystallographic structure of equiatomic Zr-Fe-Nb alloys. We used electronic density functional theory and Metropolis Monte Carlo calculations. The calculations indicate that this equiatomic ternary alloy forms a thermodynamically stable ternary hcp compound--Zr(Fe,Nb)2--described by the hP12 crystal structure. The calculated lattice parameters match those determined by recent experimental measurements. This study improves our understanding of the Zr-Fe-Nb phase diagram, which is important in the context of nuclear power applications, where Zr alloys are abundantly employed.

W08

Modelling of circumferential and radial hydrides interaction in zirconium alloys

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Hydride precipitation in zirconium alloys is a major concern in the nuclear industry due to the deterioration to the integrity and strength of the zirconium microstructure. This study focuses on investigating the interaction of zirconium hydrides at the grain scale using a coupled diffusion-crystal plasticity finite element model. For this purpose, two hydrides are embedded within a zirconium single crystal in parallel and perpendicular arrangements, replicating the formation of hydrides in circumferential and radial direction of pressure tubes. The distance between the two hydrides are varied to understand the relationship between hydride distance, hydride orientation, and hydride tips stress concentrations. It is shown that as distance is decreased between two forming hydrides, stress and stress fluctuations increase due to the interaction of the respective local stress fields. Such increases in stress concentrations can further affect hydride propagation and cause two neighboring hydrides to potentially join. Results suggest that parallel hydrides interact at higher separation distances than perpendicular hydrides due to the alignment of the growth direction in parallel configuration. It is also shown that parallel hydrides interact the most at separation distances < 30 um, and that the effects of hydride interaction are practically negligible at distances > 45um. Similarly, results for perpendicular hydrides indicate that interaction occurs mostly at separation distances < 15 um and interaction is practically negligible at distances >20 um.

W09

Process optimization of superfer 52 cold rolled sheets

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Superfer 52, equivalent to 36HXTIO8M of GOST 14117-85, is a wrought non-magnetic corrosion resistant Iron-Nickel base superalloy. This solid solution strengthened alloy is further strengthened by precipitation hardening with additions of Titanium and Aluminium through formation of coherent intermetallic compounds such as γ' phase Ni3(Al,Ti) and non-coherent phases like carbides. The alloy Superfer 52 posses significantly high yield strength values due to the combination of solid solution strengthening by high Mo & Cr, precipitation hardening by γ' phase & M23C6 and M6C carbides. Due to very high yield strength, this alloy is widely used in manufacturing of elastic sensitive elements like Belleville / Disc springs where large compressive forces act but the deflections are limited and are operated at higher temperatures up to 400℃.
Processing of Superfer 52 is extremely difficult due to poor workability and very narrow range of hot processing window because various grain refinement and carbide precipitation mechanisms trigger below 1070℃. Poor workability leads to surface cracking during forging and hot rolling. Hence, a study was taken up to optimize hot working parameters for forging and rolling. This was further extended to achieving mechanical properties by making use of process annealing parameters, percentage of cold reduction and final heat treatment. Higher process annealing temperature combined with higher soaking times resulted in good workability during cold rolling. Two different process annealing cycles were carried out with three different % cold reductions and mechanical properties evaluation and micro structural studies were carried out in solution treated condition, solution treated plus aged condition and direct aged condition.

W10

Thermal embrittlement of maraging steel 250 extruded tubes

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Maraging steel 250 is characterized by excellent combination of ultra high strength and toughness properties hence widely used in special applications. Purity and processing conditions are the two major important parameters in production of very high fracture toughness products. Thermal embrittlement is the major phenomena which deteriorates the toughness of the alloy. Extrusion of this alloy requires very high temperatures and sometimes lower working depending on the final size of the product. Finish temperatures of the process will also be very high due to faster process. This set of processing conditions will make the steel more susceptible to embrittlement through Ti carbide precipitation. Thermal embrittlement of maraging steel 250 extruded tubes was monitored as a function of processing conditions by evaluating impact, fracture toughness properties. Parameters of interest were working temperature, % reduction and cooling rate during extrusion. The extent of embrittlement and its effect on toughness was characterized by optical and scanning electron microscopy techniques. The severity of embrittlement is found high with higher finish temperatures, low reductions and slower cooling rates. Quenching after

extrusion is beneficial to the impact and fracture toughness as it avoids the precipitation of Titanium carbides/carbonitrides which causes the embrittlement. Thermal embrittlement of the extruded tubes results in change in the fracture mode from transgranular to intergranular. The impact toughness of embrittled tubes was observed in the range of 10-15J whereas fracture toughness was in the range of 65-80MPa√m. Thermal cycling treatments were performed to compensate embrittlement which has improved the toughness slightly by grain refinement. A high temperature solution treatment in the range of 1100-1200°C was also applied to re-dissolve the Ti(C,N) precipitates formed during the extrusion process and significant improvement in toughness was observed.

W11

Effect of hot rolling process parameters on toughness of tungsten containing high strength steel

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Maraging steels are low carbon Fe-Ni-Co-Mo based steels that exhibit combination of high strength and good toughness through the formation of intermetallics such as Ni3Mo, Ni3Ti in tough bcc martensite matrix. Tungsten containing maraging steel belongs to the clan of maraging steels that is hardened by the formation of intermetallic precipitates such as Ni3W and Ni3Ti. This alloy exhibits superior yield strength in combination with higher impact toughness and finds applications in defence sectors.
The alloy was vacuum melted and processed to realise 45Ø bars. The finish temperatures during hot rolling affect the microstructural evolution in these steels. Further, these steels were prone to thermal embrittlement which deteriorates the impact toughness as the material is cooled in the temperature range 1200-800°C. Hence, it is important to understand the combined effect of these two phenomena on microstructure to achieve desired mechanical properties. The present work aims to understand the effect of finish rolling temperatures (1200-800°C) on impact toughness. The effect of cooling rate was also studied by subjecting the bars to air cool and water quench and evaluating their impact toughness. The samples were characterized for microstructure using optical and scanning electron microscopy. Further, the effect of ageing parameters on impact toughness was also studied.
The microstructure shows lath martensite which is typical of maraging steels. The hot rolled product with higher finish rolling temperatures showed better impact toughness compared to the ones finish rolled at lower temperatures. The lower impact toughness was attributed to thermal embrittlement due to the formation of Ti(C, N). An attempt has also been made to improve the toughness of embrittled material by subjecting the material to higher temperature solution annealing to dissolve the Ti (C,N). Ageing temperature and time were fine tuned to achieve superior impact toughness.

W12

Correlation between fracture strain and yield stress for an age hardenable aluminum alloy

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Magnesium and silicon (Si) containing 6xxx series aluminum alloys are of interest to the automotive industry for light weighting applications due to their formability, high strength, and better surface finish compared to other aluminum alloys. These characteristics are largely controlled by the chemistry and microstructure. Correlations between fracture strain and yield stress have been observed previously for a range of 6xxx series aluminum alloys with different microstructures [Langille et al, MSE A 705 (2017) 196-199]. The purpose of the present work is to determine the sensitivity of this correlation for Al-Mg-Cu alloys with different Si chemistries and aging conditions built on a matrix containing iron-based dispersoids. Three aluminum alloys were tested, having a nominal composition of Al-0.35Mg-0.2Cu (wt%) with 0.9, 1.1, or 1.3 wt% Si. The materials were received in a rolled condition and were solutionized and processed to be in a naturally aged, pre-aged 1, pre-aged 2, or naturally aged and paint baked state. ASTM E8 standard sample blanks were uniaxially tensile tested at room temperature to determine the stress-strain behaviour from yield to fracture. Fracture strains were determined from the fracture surface areas. A single linear correlation was observed between yield strength and fracture strain for all chemistries and aging conditions. The yield strength is controlled by the grain size, distribution of solid solution, second phase particles and dislocation density. The contribution of the inter-obstacle spacing was calculated to characterize the strengthening due to clusters in the starting microstructures. The interplay between Si addition and heat treatments modifies the inter-obstacle spacing, where the uniform strain increases, and the fracture strain decreases with decreasing inter-obstacle spacing. The role of inter-obstacle spacing on nano-void nucleation will be discussed.

W13

Evaluating the tensile properties of LPBF SS316L: Influence of the specimen dimensions

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This study takes place in the context of additive manufacturing (AM) of metals. Local part geometry affects the cooling rates induced in the laser powder bed fusion (LPBF) process. This leads to heterogeneous solidification structures, and thus to local variations of the mechanical properties. The specimen dimensions specified by the ASTM-E8 standard are too large to study small-scale heterogeneities of the tensile properties. Furthermore, such large specimens are inadequate for the limited volume of the building chamber. They also do not accurately represent the thin sections of AM parts. There is currently no industry standard for the characterization of local tensile properties across AM parts.

A tensile test methodology using as-built miniature specimens was developed. The properties of the scaled-down specimens were compared to those of ASTM-E8 subsize samples produced in the same LPBF build. The elongation at break (εbreak) of both geometries was statistically equivalent. However, the as-built miniature samples were less dense, possibly explaining a larger scatter of εbreak toward low values.

The ultimate tensile strength (UTS) of the small specimens was 10% lower than that of the standard samples. It was found that a decrease in UTS of around 6% originated from elements of the methodology. Metallographic observations as well as microhardness measurements showed that the sample dimensions influenced the microstructure, further reducing the UTS by about 4%.

W14

Enhancement of Young's modulus in a heterostructured aluminum-silicon automotive alloy

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Lightweight automotive grade aluminum (Al) alloys produced through vacuum-assisted high pressure die-casting (VA-HPDC) technology are expected to have better mechanical properties due to the controlled porosity amounts and fewer casting defects. Low iron (Fe) containing Silafont®-36 alloy constitutes silicon (Si) as its primary alloying element in order to ensure proper die filling by increasing the fluidity, and imparting the high machinability and integrity to the alloy. Magnesium and manganese are essential in the alloy system to improve the strength and fatigue properties and also help in replacing part of Fe which could lead to brittle intermetallic phases. Upon investigation of the microstructural characteristics and the deformation behavior of this Al-Si alloy, it was observed to have a rather interesting phenomenon of strengthening due to the presence of heterogeneous microstructure without anisotropy. Microstructures after deep-etching were observed to exhibit a fibrous-coral like network of strontium modified-Si, which was embedded in the Al matrix as particulate-like reinforcements. These Si particles, having rounded or elongated shapes with an aspect ratio of 2-4, were responsible for the composite-like behavior and enhanced Young's modulus (~78-88 GPa) as well as higher elongation (5-8%) values. The enhancement of Young's modulus could be understood via the rule of mixtures for composite materials based on the volume fraction of strontium modified-Si particles. Further details will be presented at the conference.

W15

Strength-ductility synergy in an Al-Cu-Mg alloy with a bimodal grain distribution

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A superior combination of strength and ductility in materials is necessary for their structural applications. Unfortunately, due to the long-standing dilemma of strength-ductility trade-off in materials science, the increase in strength tends to decrease ductility. The development of bimodal alloys is promising in resolving this issue and thus attracts a considerable interest. Here, we present a bimodal grain distribution of coarse grains (CG) and ultra-fine grains (UFG) in 2009Al alloy (Al-Cu-Mg) fabricated by combination of two-step ball milling and powder metallurgy. The ball milled powders were mixed with as-received powders to achieve a mixture of coarse and fine grains. Monotonic and cyclic deformation tests were conducted at ambient temperature to relate to the unique bimodal microstructure of the alloy. The alloy exhibited a high yield strength of ~553 MPa arising from the presence of UFG with a fairly good ductility

of ~10% due to strong back stresses. These exceptional properties are attributed to the unique bimodal grain structure which delayed the onset of plastic instability resulting in higher strength as well as larger uniform elongation and work-hardening rate. These studies shed light on the “strength-ductility” dilemma and can be extended to improve the mechanical properties of a wide range of materials.

W16

Fabric selection for the production of bespoke bras

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Introduction. Bespoke bras have the ability to provide a more functional, well fitted and supportive bra to those with atypical breast shapes/sizes. To achieve this, understanding and selecting the right material for the different parts of the bra is key because it ensures fabric optimization in the final product. In this study, we analyse the burst strength and stretch of knitted fabrics commercially available in order to drive the selection of the most suited fabric for application in areas such as the cup where good stretch and flexibility is required.
Materials & Methods. 18 commercially available knitted fabrics of varying weight and elastane content were studied. Burst strength was measured according to ASTM D6797. The fabric loss and recovery were evaluated using the ASTM D4964-96 standard with modified specimen dimensions (3 x 12 inches). All fabrics were conditioned at 65% RH and 21oC for a minimum of 72 hours prior to testing. Microscopic analysis was also done to understand the differences in the knit structures of the fabrics.
Results and discussions. The burst strength results ranged between 377N and 207N. These values are within an acceptable range for bra applications. The results of the unrecovered stretch and load at 80% extension in the warp direction indicate that the fabrics have a very high recovery rate. Microscopic analysis tells about the influence of knit structures on the burst strength and the unrecovered stretch.
Conclusion. The results obtained for a series of knitted fabrics lay the foundation for the identification of good candidates for the bra making. Having the right fabric will contribute to the comfort and support properties of bras, which will translate into an increase in customer satisfaction and product performance.
Acknowledgment: This research benefits from a grant from MITACS (Canada) and the company Simply Best Underpinnings Corp (Edmonton, AB).

W17

On the Extrinsic Transition in the Hall-Petch Behavior of Nanocrystalline Nickel Cobalt Alloy Electrodeposits

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The Hall-Petch relationship of metals and alloys has been investigated for more than half a century. This relationship relates the strength/hardness to the grain size of the material. On the other hand, a transition to inverse Hall-Petch behavior (i.e. decreasing hardness with decreasing grain size) was first observed for nanocrystalline metals in the late 1990's. In this study, the Hall-Petch relationship of an electrodeposited nanocrystalline nickel cobalt (NiCo) alloy was examined to determine the grain size effect on the microhardness of the material. A series of annealing treatments were performed on electrodeposited alloy at different temperatures to obtain grain sizes ranging from 18 – 240 nm. The hardness results show a regular Hall-Petch to inverse Hall-Petch transition of the alloy between grain sizes of 46 – 22 nm. We refer to this as the extrinsic regular to inverse Hall-Petch transition. This grain size is larger than for pure electrodeposited Ni in which the transition occurred at 12 nm in the as-prepared state (intrinsic Hall-Petch transition). Preliminary results suggest that the difference is likely due to the annealing treatment of the NiCo alloy compared to the as-deposited Ni. The intrinsic Hall-Petch to inverse Hall-Petch transition observed in pure Ni is due to changes in the dominant deformation mode from dislocation based to grain boundary mediated deformation as the grain boundary volume fraction increases. On the other hand, the extrinsic Hall-Petch to inverse Hall-Petch transition observed in NiCo alloy is likely due to the annealing treatment that may alter the grain boundary properties because of segregation of impurities and grain boundary relaxation. This stabilizes the grain boundary and inhibits grain boundary associated deformation.

W18

The Mechanical and Failure Properties of Wired Glass

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Wired glass is a common construction material consisting of conventional annealed glass with an embedded steel mesh, used in buildings as a fire safety glass. When the glass fractures under the thermal stresses caused by a fire, the wire mesh holds the glass fragments in place, keeping the pane intact and minimizing the spread of the fire. However, this same property of wired glass has caused numerous injuries. In cases where glass fracture is due to human impact, the fragments held in place have resulted in severe lacerations to the victim, leading to life changing injuries and even death in some cases. Despite industry agreement that wired glass should not be used in areas where human impact is a concern, the material continues to be used in building construction. Nevertheless, there have been limited studies performed to characterize the fundamental properties of wired glass, such as its mechanical strength and failure properties. This study aims to fill in this gap by determining the modulus of rupture (MOR) values of wired glass through four point bend testing of glass samples in accordance with ASTM C158 Standard

Test Methods for Strength of Glass by Flexure. Fracture surfaces from the aforementioned samples were studied to determine how the wire mesh affects the fracture of the glass. Further testing in this study will involve determination of intrinsic MOR values and failure mechanisms using wired glass samples with carefully prepared surfaces to mitigate edge fracture initiation.

W19

Onsite DL-EPR Testing and Metallographic Assessment of Lean Duplex Stainless Steel Aseptic Storage Tanks

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Large aseptic tanks are widely used in the bio-processing industry for the storage of food-grade liquid products. These tanks are often made of grade 2101 lean duplex stainless steel, to prevent excessive corrosion damage during extended storage periods. However, localised corrosion has recently been observed at the internal surface of these tanks. To evaluate the susceptibility of the tank surfaces, on-site Double-Loop EPR (DL-EPR) tests were carried out to measure the local degree of sensitization (DOS). Assessment of microstructure susceptibility was augmented by onsite metallographic investigations. Field metallography was performed after etching the surface with a 10% (wt.) oxalic acid solution, with both inspection techniques applied to ten independent corrosion sites at the large bottom plate inside the emptied storage tank. DL-EPR measurements were obtained via a portable electrochemical mini-cell.

Most of the corrosion sites were observed along internal welds, both in the base metal and within weld regions, including the fusion line and weld face. The measured DOS for the base metal and weld face was, however, below 1%, indicating that the microstructure was not sensitized. Subsequent metallographic assessments revealed a clean microstructure, with only austenite and ferrite present in these regions. The weld fusion line contained large corrosion sites, with a DOS ranging from 11% to 20%. Onsite field metallography showed the presence of Widmanstätten-type austenite laths and secondary austenite (γ2) embedded within a matrix of larger ferrite grains The presence chromium nitride precipitates within ferrite grains possibly supported the observed local attack.

The application of on-site DL-EPR testing in combination field metallography is demonstrated here, with these techniques then easily be deployed for advanced inspection protocols of stainless steel industrial equipment.

W20

Parameter Effectiveness and Mechanical Behaviour Analysis of Inconel 625 fabricated through Laser Powder Bed Fusion

Jonathan Lewis, Clodualdo Aranas

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The aerospace industry can greatly benefit from manufacturing advantages provided by introducing additive manufacturing (AM). There are challenges facing this introduction, since the mechanical properties of fabricated components are highly sensitive to the specifics of the AM process used. An important alloy in the industry, Inconel 625 superalloy (IN625), and an important AM process, Laser Powder Bed Fusion (LPBF), were selected as the focal points of the present study. The effects of the processing parameters of the LPBF process on fabricated IN625 were investigated, along with the response of such samples to impact testing at a range of strain rates and temperatures using a Split-Hopkinson Pressure Bar (SHPB). The results show that increasing the laser power had the greatest effect on the porosity of samples, while the hardness was not significantly affected. The initial SHPB testing indicates that once the dynamic range was reached, strain rate does not greatly affect the stress/strain relationship for impact testing.

W21

Mechanical behaviour of high-performance fire protective fabrics

and the effect of hydrothermal ageing

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The outer shell fabrics of fire protective clothing are prepared from blends of high-performance polymer fibre such as p-aramid, m-aramid, polybenzimidazole (PBI), polybenzoxazole (PBO) and liquid crystal polyester (LCP). These fabrics are designed in such a way to withstand extreme temperatures and provide protection to firefighters against work hazards. The initial part of this study focusses on the mechanical behaviour of eight different outer shell fabrics to understand how they perform under tension and relate this behaviour with the fabric physical characteristics and fibre content. This provides insights for further improvement of these fabrics' performance. The second part of the work focusses on the degradation of these outer shell fabrics when exposed to accelerated hydrothermal ageing by immersing them in water at temperatures between 60°C and 90°C for up to 1200 hours. The residual tensile strength of the fabrics was measured for specimens collected after different exposure times. The effect of hydrothermal ageing was analyzed based on the fabric physical characteristics and fibre content. These results serve as the cornerstone for the development of end-of-life moisture sensors for fire protective fabrics.

POSTER SESSION 2

Th01

Evolution of stresses in deformation twins in the plastic zone using three-dimensional synchrotron X-ray diffraction

Karim Louca, Hamidreza Abdolvand

Western University

Hexagonal closed-packed (HCP) metals have been extensively used in various industrial sectors. Understanding the deformation mechanisms of HCP metals at the grain-scale is a necessity for developing predictive models that can be used for the performance or failures analysis of engineering components. One of the common deformation mechanisms in HCP metals is deformation twinning. In this study, average grain stresses and size of the tensile twins are investigated with respect to their parent grains. In-situ three-dimensional X-ray diffraction (3D-XRD) is used for capturing grains center-of-masses (COMs), orientations, strains, and volumes. The evolution of stresses in twin and parent pairs are studied in details, both at the early stages of plasticity and further into plastic zone in zirconium. The methods developed to detect twin-parent pairs and track down their stresses are also studied.

Th02

Quantifying the recovery of Zr-2.5Nb cold-worked at 250 °C using diffraction

Thalles Lucas, Levente Balogh, F. Long, A. Barry, Mark R. Daymond

Queen's University

It has been observed that dislocation structures which develop due to the plastic deformation and irradiation of metallic materials behave differently when subjected to annealing. This indicates that the underlying mechanisms through which these dislocations are annealed out seem to depend on whether they were created by plasticity or irradiation. The activation energy plays an important role in the kinetics of thermally activated processes and its value could provide insights about the driving force of the dislocation recovery. For that purpose, specimens extracted from an unirradiated Zr-2.5Nb pressure tube were cold-worked at 250 C, near the core temperature of CANDU reactors, to create a dislocation structure suitable for comparison with specimens irradiated under reactor operating conditions. The structure of this material was analyzed using X-ray diffraction, and the line profile analysis method Convolutional Multiple Whole Profile analysis (CMWP), was used to quantitatively characterize the microstructure. Using the rate of decay of the dislocation density as a function of temperature, the activation energy for recovery was successfully determined. The determined activation energy agrees within experimental uncertainty with the value reported in the literature for vacancy migration. The next step of the project aims to research and understand the contribution of vacancy migration to the overall recovery mechanism both for plastically deformed and irradiated Zr-2.5Nb. The presented results can help to build and validate predictive models of plasticity under reactor operating conditions.

Th03

Towards Diffraction Line Profile Analysis of Laser Powder Bed Fusion Manufactured Ni-Superalloys & pure Cu

Lucas Ravkov, Vahid Fallah, Levente Balogh

Queen's University

The advent of additive manufacturing (AM) techniques, in particular laser powder bed fusion (LPBF) manufacturing capable of processing metallic materials, has played a transformational role in the manufacturing industry. With the use of AM, arbitrarily complex geometries may be printed directly from a digital model, with reduced material waste, the lack of part-specific tooling, and the ability to manufacture multiple components simultaneously. In this study, LPBF manufactured samples of various Ni-Superalloys (IN718, IN625, Hastelloy-X) as well as pure Cu will be printed so to facilitate various materials characterization and mechanical tests. The materials being investigated are used as structural materials in proposed Small Modular Reactors (Ni-Superalloys) and Dark Matter Detectors (pure Cu), respectively.

Materials characterization will be conducted to identify a range of mechanical, microstructural, and radiological parameters for the LPBF manufactured samples. These parameters will then be related back to the processing conditions from which the samples were made. Proposed materials characterization experiments that will be carried out are: density (Archimedes method), optical microscopy (2D grain size measurements, 2D void characterization), micro computed-tomography (3D grain size measurements, 3D void characterization), SEM (precipitate orientation relationships, chemical variation), TEM (HAADF/HAABF – dislocation character/structures, diffraction – lattice parameter variation), X-ray Diffraction Line Profile Analysis (DLPA) – bulk characterization of dislocation density, sub-domain size, dislocation character), and background radiation emission evaluation (pure Cu only).

Th04

Polycarbonate degradation under combined effect of ultraviolet and temperature

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Mouloud Mammeri University, Algeria

Polycarbonate (PC) is an amorphous polymer widespread in commerce. Among its many interesting properties, we can mention, among others, transparency, impact resistance and low density. However, long exposure to the severs weather makes it fragile and translucent. The objectif of this study is to submit the PC to the simultaneous action of ultraviolet (UV) and temperature. The effects were highlighted by physico-chemical and thermal analyzes. Thus, molecular rearrangement and peaks shift have been revealed by X ray diffraction (XRD). A changes of the thermal properties was revealed by the thermogravimetric (TGA) and Differential Scanning Calorimetric (DSC).

Th05

Synthesis of Non-Radioactive Bimetallic Oxides To Understand Fission Product Behaviour

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Royal Military College of Canada

The Royal Military College of Canada (RMC) is committed to providing the Thermodynamic of Advanced Fuels – International Database (TAF-ID) with reliable thermodynamic data on the Sr-Mo-O and Ba-Mo-O chemical systems as literature data are limited. Hence, the synthesis of non-radioactive samples of the various compounds within those systems are required to study these systems safely. Attempts to prepare compounds described in current thermodynamic models have been made through solid-state synthesis (SSS) methods. Successful preparations of $SrMoO_6$, $SrMo_5O_8$, Ba_3MoO_6, Ba_2MoO_5, and $BaMo_3O_{10}$ have been achieved, but further purification of some samples is still required. Synthesis of the remaining compounds (i.e., $SrMoO_3$, Sr_2MoO_4, $Sr_3Mo_2O_7$, $BaMoO_3$, and $BaMo_2O_7$) is currently in progress through SSS methods.

Concurrently, the synthesis of complex and novel compounds (i.e., $SrMo_6O_{19}$, $SrMo_4O_{13}$, $SrMo_8O_{26}$, $BaMo_6O_{19}$, $BaMo_5O_{17}$, $Ba_3Mo_{18}O_{28}$) via wet chemistry methods are underway. Their study is crucial to determine their addition to current thermodynamic models. Successful preparation of precursor materials (i.e., $[(C_4H_9)_4N]_2Mo_6O_{19}$) has been achieved, and hydrothermal and solvothermal methods are being investigated to prepare such compounds. For thermodynamic characterization, Differential Scanning Calorimetry (DSC) and Thermo-Gravimetric Differential Scanning Calorimetry (TGA-DSC) techniques are used to assess enthalpy of melting, low-to-moderate temperature heat capacity, and transition temperatures. Method benchmarking tests using $SrMoO_4$ and $BaMoO_4$ found chemical interactions that require innovative solutions for accurate measurement of such properties. The use of non-reactive liners is being investigated at RMC. With the new experimental data for the various manufactured materials, current thermodynamic models available in the TAF-ID can be updated to describe accurately the thermochemical behaviour of the fission products comprising these chemical systems.

Th06

Tribological degradation of molybdenum disulfide lubricating films under proton irradiation

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University of Toronto

Molybdenum disulfide (MoS2) solid-state lubricating films are commonly used in spacecraft for their mechanical robustness and vacuum compatibility. Atomic oxygen exposure in low-earth orbit has been seen to compromise their tribological performance, and tribological failure of materials has resulted in several documented space mission failures. Deep space flights will be subjected to the Galactic Cosmic Radiation (GCR) spectrum, which is 85% protons, but no characterizations have been reported on the effect of proton irradiation damage on MoS2 lubricants. Irradiation testing of a space-grade MoS2 lubricating film has shown severe tribological performance degradation using friction force microscopy and nanoindentation to characterize the response to 500 eV protons. At a fluence of 3e23 H/m^2, the highest fluence tested, wear rate is elevated five-fold relative to virgin material, coefficient of friction is doubled, and the material is softened and made more compliant. X-ray photoelectron spectroscopy and Raman spectroscopy reveal the mechanisms of degradation to be the preferential removal of sulfur leading to amorphization of the structure and the formation of reactive sites. Damage effects are resolvable by our structural characterization methods at a fluence of 1e21 H/m^2, and mechanical property effects persist with decreasing fluence such that wear rate is still seen to be slightly increased at 1e19 H/m^2, the low fluence limit of our testing. Due to the low flux and high energy of GCR particles, these levels of damage are not expected to acutely impair deep space flight lubricant performance. However, the mechanisms revealed in this study are expected to be active in these fields, and fine sensitivity testing of specimens with controlled exposure to GCR on a future lunar-orbit research station can seek these signatures of damage to assess the magnitude of performance degradation in MoS2 lubricating materials.

Th07

Production of vinyl ester resins of epoxidized cardanol using cinnamic acid: A study on the curing, mechanical, thermal and morphological characteristics

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Over the years, industrial equipment have been shielded from marine organisms, wind, rain, sun beams and natural assault in the dirt utilizing petroleum derived coating materials. These coating materials have been noted to have dangerous effects, causing risks during processing and application. The high rate of radiating unpredictable volatile organic compounds (VOC) produced by these petroleum derived polymers which might be cancerous are likewise a reason for concern. Discharges of these compounds are typically controlled, however, not manageable and no longer adequate to meet end user's needs. Presently, environmental standards necessitate the removal or control of VOC at the most minimal levels. Therefore, considering the VOCs, rise in prices and high depletion of petroleum resources, the quest for alternative, non-toxic, economical, sustainable and renewable source of coating materials is a subject of extraordinary

interest. However, viable alternatives for polymer synthesis have appeared to originate from characteristic unlimited sources, such as, cashew nutshell liquid (CNSL). In this work, cardanol, a major component of CNSL was used to synthesize vinyl ester resins. The physicochemical characterization of the oil and resins were carried out using international standard methods. The molecular weight of the pure cardanol and resins were determined with GCMS. FTIR and TGA analysis were used to identify some functional groups and analyze the materials weight changes with stability relative to temperature. The results of the mechanical and thermal properties of the resins showed better performance and thermal stability. The chemical resistance properties of the resins showed improved performance when subjected to alkalis and acids, an indication of anti-corrosive property. The better performances of cardanol based vinyl ester resins obtained from this study justify and suggest their applicability in coatings both for anticorrosion and marine growth protection.

Th08

Poly(vinyl alcohol) and Functionalized Ionic Liquid-Based Smart Hydrogels for Doxorubicin Release

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The intrinsic limits of conventional cancer therapies prompt the development of an effective, safer, smarter and targeted drug carriers that improve the efficiency of the drug carrier, reduce the adverse effects of the drug on the healthy cells, and helps in preventing the cancer recurrences. This research aims to design a stimuli-responsive, self-healable, adhesive, and injectable polymeric hydrogel with ester functionalized ionic liquid (ILs) as one of the additives to improve the efficiency of the anti-cancer drug in encapsulation and localized delivery. The designed hydrogel responds to intracellular biological stimuli (e.g. acidic pH of cancerous cells and temperature), change the morphology through changing the shape and size of the gelator within the hydrogel matrix and release the encapsulated doxorubicin (DOX) at the tumor site efficiently. Molecular interactions, gel morphology, and mechanical strength of the hydrogel were characterized through state of the art analytical techniques, including small angle neutron scattering (SANS). Adhesive properties of the polymeric hydrogel were measured by lap-shear strength tests and biocompatibility and cellular drug uptake study on human breast cancer (MCF-7) and human cervical carcinoma cells (HeLa). The in-vitro cytotoxicity and drug release study showed that the hybrid hydrogel is more effective at killing the cancerous cells, and the targeted release of the DOX occurred at intracellular acidic pH. The polymeric hydrogel provides an efficient therapeutic approach for the encapsulation and release of the drug. Overall, the study offers a proof of concept to test the feasibility of the hydrogel system whether the hydrogel formulation helped or hindered the total cellular DOX trafficking.

Th09

Oxide limited laser colouration of copper gratings for angle dependent colour control

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University of Ottawa

In this report, the complex optical response of laser machined copper (99.98%) surfaces showing an array of perceived colours with varying degrees of angle dependence. These different colours are generated by raster scanning the copper surface using a 1030nm wavelength PHAROS laser with 300fs pulses with a repetition rate of 10kHz to generate different patterns onto the surface using AEROTECH 5D stage and galvo mirrors (AGV-10HPO). Through grazing angle Fourier transform infrared (FTIR) spectroscopy and Raman microscopy increased oxide content was found on samples with smaller linespacing thus higher pulse density. This increased oxide content coincides with a greater angle independence of the colours compared to the much lower oxide content found at larger line spacings. The surface itself shows many similarities despite vast differences in the colour with the underlying periodic microstructure shows a consistent periodicity and duty cycle for all samples with a decrease in amplitude of the features from 400nm for the smallest line spacings to roughly 100nm amplitude for the largest line spacings. Reflectance measurements performed using a ThorLabs warm LED source (MWWHF2-4000K) and CCS200 spectrometer show a shift in reflectance peaks observed by eye. The overall complex colour of the surfaces is attributed to a combination of the known colouring effects of thin copper oxide layers interfering with an underlying sinusoidal grating structure.

Th10

Influence of Nano-scale Graphene and Zirconia on Mechanical Properties of Alumina Matrix Nanocomposites

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York University

The inherent brittleness of monolithic alumina has consistently limited its potential for several structural applications such as engine turbine parts and high temperature space materials. The fracture toughness property of nanocrystalline alumina can be improved by the uniform dispersion of nanometer-sized second-phase particles in the alumina parent matrix. In the current work, alumina matrix nanocomposites were fabricated by homogeneous dispersion of Zirconia (4wt% and 10wt%) and Graphene(0.5wt%) using colloidal mixing followed by hot-pressing at 1600oC for 1 hour. The final microstructures depict extensive grain-refinement by the uniform dispersion of 0.5wt%Gn and 10wt%ZrO2 in the parent alumina matrix. This was generally due to the inhibition of the matrix grain growth caused by the interfacial graphene and ZrO2 particles at the matrix grain boundary. A study of influence of the microstructural features on the mechanical properties such as micro-hardness and fracture toughness was also carried out using the Vickers micro-hardness and Indentation fracture toughness (IFT) techniques. Generally, an improved hardness (up to 9.6%) and toughness value (~ 114%) were recorded with the addition of the 0.5wt%Gn. This was ascribed to the presence of tougher graphene particles and strong interfacial bonding between the graphene and the alumina matrix. Even though the fracture toughness was increased with the addition

of 10wt%ZrO2 (up to 163%), its microhardness decreased due to the presence of ZrO2 particles with lower hardness attributes than the matrix. Limited concentration of ZrO2 within the matrix with the addition of 4wt%ZrO2 yielded a higher hardness but relatively lower fracture toughness value. Fractured surface analysis also revealed the transgranular and intergranular mode of fracture demonstrated by the nanocomposites.

Th11

Synthesis and characterization of zirconolite (CaZrTi2O7) based glass-ceramic composite materials

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University of Saskatchewan

Zirconolite (CaZrTi2O7) based glass-ceramic composites are potential waste forms for nuclear waste sequestration due to their high chemical durability and the ability to immobilize a large variety of radioactive waste elements in either the glass phase or the crystalline structure. In this study, borosilicate and Fe-Al-borosilicate glass-ceramic composites containing crystallites of zirconolite were synthesized at different annealing temperatures and characterized using powder X-ray diffraction (XRD) and X-ray absorption near-edge spectroscopy (XANES). Powder XRD was conducted on both the zirconolite and glass-zirconolite composites (annealed either at 750 or 1100°C) in order to study the different phases in these materials. The effect of the glass compositions, zirconolite loading percentage, and annealing temperature on the local environment of Zr, Ti, Si, and Fe was investigated using XANES analysis. Examination of the Ti and Zr K-edge XANES spectra from the composite materials annealed at 750°C indicated no change in the local chemical environment of Ti or Zr in the glass-zirconolite composite materials as the glass composition was varied. However, the intensity of the pre-edge and main-edge features in the Ti and Zr K-edge XANES spectra from the composite materials annealed at 1100°C changed as a result of the loading percentage of zirconolite in the composite, variations of the glass composition, and the annealing temperature. The Si L2,3-edge XANES spectra collected from the composite materials (annealed either at 750 or 1100°C) have shown that the loading percentage of zirconolite in the composite materials, variations of the glass composition, and the annealing temperature can affect the local environment of Si in the glass-zirconolite composites. This study has allowed us to better understand how the local chemical environment of the glass-zirconolite composite materials changed as a result of a change in the synthesis conditions and glass composition.

Th12

Transient Oxide Formation and Oxide Spallation on IN738 at 1050◦C

Alex Lothrop, Qi Yang, Bingjie Xiao, Carman Lefebvre, Megan Walker, Xiao Huang

Carleton University

In this study, cast alloy IN 718 was oxidized at 1050◦C to study the transient oxidation behavior and remaining oxide(s) after a long term exposure. It was found that the initial oxide formed on the surface was characterized as TiO2; below which, a layer of Cr2O3 and limited amount of spinel formed after 4 hours. Cracks were observed within the Cr-rich oxide layer. Partial spallation occurred after 16 hours of exposure which led to exposed surface covered with either TiO2, Cr2O3 or a mixture of Al2O3+substrate+Cr2O3. No continuous alumina was observed during the 4-16 hours of exposure, instead, internal Al oxidation resulted in the formation of alumina stringers in IN 738. After extended exposure of 1000 hours, a continuous layer of alumina was observed immediately above the metal substrate. However, it was not exclusive as precipitation of Ti and Ta/Nb rich oxides occurred within alumina layer. In addition, Al-rich and Cr-rich spinel formed above the alumina layer. Furthermore, the three layered oxidation scale along with TiO2+(Cr,Al)(Nb,Ta)O4 precipitates has already separated from the metal substrate upon cooling due to stress development from oxide growth and differences in CTE.

Based on the results of this study and information obtained from our other studies of different alloys, IN738 is not able to form exclusive alumina at 1050◦C.

Th13

Corrosion Performance of High Temperature Alloys in Molten Salt Mixtures for Next Generation Energy Systems

Isabella McDonald

McMaster University

Molten chloride salts have been proposed to be used as the primary coolant in molten salt reactors, and as the heat transfer fluid in concentrated solar power plants in next generation energy system design. The corrosive properties of molten chloride salts make it challenging to find appropriate structural materials for plant/system realization. In this work, two corrosion mitigation strategies are investigated to determine the relative corrosion performance of high temperature alloys in molten chloride salt mixtures: (1) chemical purification of salt mixture using a Mg sacrificial anode and (2) developing a protective oxide layer on the surface of high temperature alloys after pre-oxidation. Three commercial high temperature alloys (Incoloy 800H, Haynes 214, Noram SX) were exposed to molten salts (62.5 wt % KCl + 37.5 wt % MgCl2·6H2O) with 1.7 wt % Mg as a corrosion inhibitor for 100 h at 700°C under inert Ar atmosphere. XRD analysis was used to compare the phase composition of the as-received salt mixture to the salt mixture post-exposure, and SEM-EDS characterization was used to compare cross-sections of each alloy exposed to molten salt with and without Mg additions. To assess the second mitigation strategy Incoloy 800H, Haynes 214, and Noram SX were pre-oxidized to form protective chromia, alumina, and silica oxide layers respectively. The raw and pre-oxidized high temperature alloys were exposed to the same molten chloride

salts with and without chemical purification under the same conditions. SEM-EDS characterization was used to compare cross-sections of each alloy after exposure. The talk will present and discuss the progress made to date.

Th14

Decreasing the binder setting time in bioactive glass composites for bone tissue scaffolds

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University of Alberta

The healing capacity of bone is delayed or impaired by critically sized defects and open fractures. Although natural bone grafts are considered as the gold standard treatment, their immunological, structural and quantity limitations motivated the development of synthetic bone graft substitutes. Bone tissue engineering is a promising approach for bone regeneration, in which a scaffold acts as temporary skeleton to support the new bone growth. Bioactive glasses (BG), such as 45S5, have been extensively used in bone scaffolds due to their excellent biodegradability, ability to bond to bone and induce new bone formation. However, we found three main challenges in common techniques for processing them into bone scaffolds: (1) The need for heat treatment which adversely affects the glass bioactivity; (2) Lack of formability; (3) The need for 3D models and imaging.

Based on the reviewed challenges, this research seeks to develop a new processing route for fabricating BG bone scaffolds. The design concept builds on our recent proof-of-concept work aimed at creating a formable scaffold composite by mixing 45S4 BG powder and a sodium silicate binder solution which sets upon exposure to CO2 gas in air. Despite their sufficient porosity and strength, the time it takes for the composites to set in air is in the order of days, making them impractical for clinical applications. The main driver of this work is to reduce the setting time by exposing the scaffolds to high-purity CO2 gas. Preliminary experiments have shown that using high-purity gas can reduce the setting time from 10 days to around 2 minutes. The effect of gassing time, specimen's height and layer-by-layer gassing on the compression strength of composites have been investigated. Next step will be to study the effect of gas flow rate and kinetics of the setting reaction. Further development will involve in vitro and in vivo studies to eventually develop a prototype kit for use in an operating room.

Th15

Smart headband for rehabilitation following jaw reconstruction

Pradipika Natamai Vasudevan, Patricia I. Dolez, Hyun-Joong Chung, Daniel Aalto

University of Alberta

Head and neck cancer is a devastating disease resulting in difficulties in chewing and swallowing even after treatment. Jaw reconstruction together with oral prostheses can restore anatomical structures. However, the chewing efficacy and efficiency are reduced. Various technologies for biofeedback related to chewing have been studied over the previous years; they show that tactile stimulation can be an effective sensory surrogate for identifying texture. Piezoelectric devices have been known to show precise control in terms of their amplitude of vibration making them good candidates for delivering biofeedback. In our study, a method for providing feedback through a smart headband has been developed. The detailed acoustic output of the actuators was measured by scanning laser Doppler vibrometer (sLDV). The results showed that these piezoelectric discs can vibrate in accordance with the input signals provided to them. This was observed from the output signals recorded by the LDV. The amplitude of vibration measured from the surface of the piezoelectric devices increased nonlinearly as the applied voltage increased. The piezoelectric device studied thus offers the vibration amplitude/voltage characteristics appropriate for an application as biofeedback for tactile simulation of chewing as the precise control of amplitude/voltage combination can allow the delivery of rich information by a single actuator. The results of the skin stimulation tests showed that the user can differentiate the lower amplitudes from the higher ones. In addition, the piezoelectric discs can deliver to deliver different types of signals with different amplitudes while providing spatial differentiation. The smart headband is also extremely durable, stretchable, and conductive. It has the potential to be further developed into a product for patients who are not able to make a judgement of the force exerted and identify texture during chewing.

Th16

Cold embossing of laser written diffractive optical elements on metals

Xitong Xie, Arnaud Wenk

University of Ottawa

In recent years, laser surface texturing has been applied to a wide range of bulk metallic materials for functionalization. The technology is used to impart a given function to metal surfaces or modify their properties, such as wettability, biocompatibility, and colours to name a few. By creating gratings with periodic spacing at the microscale, the machined surfaces can diffract the incident white light and render colours at different angles. To increase manufacturing speeds, embossing can be used where structures can be replicated from a die to a substrate in a fast and cost-effective way. However, evidence of repeatable embossing of microscale features is scarce in literature.

The current research is focused on developing a technique to transfer, at high speed, laser machined microscale patterns to metallic substrates using cold embossing. Optimization of the laser machining and embossing procedures is carried out to improve the transfer quality and to prolong the die life. Different patterns were designed, machined, and successfully transferred onto pure metal substrates, including

silver, copper, and aluminum. Intense structural colours are observed on the embossed metal surfaces, and the transferred patterns are clear and precise. A method of creating covert security features based on the diffraction of visible light is also demonstrated. These security features were successfully transferred via cold embossing. This microscale transfer technology is expected to be valuable in the colour marking and minting industries for esthetic and anti-counterfeiting purposes.

Th17

Synthesis of Synthetic Rock Materials Using One-Step Methods

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University of Saskatchewan - Department of Chemistry

The nuclear industry produces radioactive nuclear waste (spent fuel), which can be accommodated into ordered compounds that are densely packed. One major purpose of these waste forms is to prevent leaching of fission products and actinide elements into the environment. One proposed nuclear waste form is SYNROC (synthetic rock), which is a multi-phase ceramic material and contains phases adopting the crystal structures of zirconolite, perovskite, hollandite and rutile. SYNROC can be a strong candidate for long-term immobilization of spent nuclear fuel. The goal of this project was to investigate if different synthesis methods affect the properties of SYNROC and its local structure. The objectives were to synthesize the individual phases of SYNROC, to understand the properties of each component and then to synthesize SYNROC in one-step.

The current synthesis method for SYNROC used at ANSTO-Australia is hot isostatic pressing. ANSTO prepares the phases of SYNROC separately which incorporate the waste elements in their structures and then the components are mixed and heated under pressure. However, the synthesis of SYNROC using a one-step method via the ceramic synthesis route or solution-based methods has not been studied in detail.

One focus of this study was to reduce the reaction time as well as lowering the reaction temperature when synthesizing SYNROC. XRD was employed to confirm the phase purity of the phases of SYNROC. The wt% of the individual phases in the SYNROC materials were determined and compared to the expected values. Ti K-edge XANES spectra were collected from the SYNROC samples and were fitted using the spectra from zirconolite, hollandite, perovskite and rutile to further analyze the composition. The Zr K-edge XANES spectra collected from the SYNROC materials resembled the spectrum from zirconolite as this is the only phase in SYNROC that contains Zr. This study has demonstrated that SYNROC can be synthesized using the ceramic method in one step.

Th18

Development of Ring Forgings of 11Cr-10Ni-2Mo-1Ti PH Martensitic Stainless Steel for Rocket Motor Application

Bhavanish Kumar Singh, A. Panikishore, K. Rajasekhar

Mishra Dhatu Nigam Limited (MIDHANI), India

A programme for indigenous manufacturing aircraft quality, 11Cr-10Ni-2Mo-1Ti Precipitation Hardening Martensitic Stainless Steel (PHMSS) forged rings was successfully completed at Mishra Dhatu Nigam Limited (MIDHANI), Hyderabad, for making components of aero application. This alloy gains advantage by its superior mechanical and stress corrosion resistance properties than 17-4PH and 15-5PH stainless steels. Components of this alloy can be air hardened with relatively less distortion. Balance between high strength and toughness has been a difficulty in this alloy in lieu of the effect of chemistry and heat treatment. Data analysis of earlier processed forged bars indicated that material is sensitive to chemical composition and processing gets hampered by presence of inclusions. Therefore close control of chemistry and processing conditions is a challenge in this alloy. To achieve the desired chemistry, this alloy was primary melted in Vacuum Induction melting (VIM) and secondary melted in Vacuum Arc Remelting (VAR). Combination of cogging, drawing and upset forging followed by punching and saddle forging was adopted to realize the rings. Solution annealing heat treatment was carried out at 965°C (calculated using JMAT software). Test coupons were cut from the solution annealed rings for further detailed microstructure and mechanical property evaluation. Tensile testing was carried out at 27°C, 200°C, 350°C and 450°C on age hardened samples. High strength and toughness could be achieved with calculated conception of Mo and Ti and a controlled balance of precipitate size and reverted austenite during age hardening. B and Zr were microalloyed to enhance grain refinement as well as to improve hardenability. The optimized age hardening cycle was 530°C, 4 hrs soaking and air cool to achieve desired mechanical properties. Optical and SEM/EDS techniques were used for microstructure and fractography analysis.

Solute Defect Interaction 2

June 2, 2021 Morning – Session 1

Solutes Everywhere: High Entropy Alloys

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The classical picture of "the solute" is a single foreign atom introduced into a lattice site of a host matrix material. The solute has many attributes such as a heat of solution, a misfit volume, a migration barrier. As a defect in the host lattice, the solute can interact with other defects such as dislocations and grain boundaries, leading to many complex phenomena and important effects on macroscopic material properties. "Solid solution alloys" have traditionally been alloys where a low concentration c<<1 of solute atoms are introduced into a host matrix leading to strengthening due to solute/dislocation interactions [1]. A primary example is the Al-5xxx Al-Mg alloys consisting of ~4-5% Mg in Al widely used in the automotive industry. Here, we discuss a more general notion of a solute in multicomponent, non-dilute random alloys that are now called High Entropy Alloys (HEAs). By introducing the notion of an effective homogenized alloy, which can be illustrated in atomistic computations [2], we show that all of the individual atom types in the alloy can be treated as solutes. An HEA alloy is then a "solute strengthened" alloy where the solute concentration is 100% [3], explaining the high strengthening observed in many HEAs. A general parameter-free theory for solute strengthening [3] is outlined and then applied to accurately predict the finite-temperature/finite-strain-rate yield strengths of various fcc and bcc alloys. With the analytic theory, we can then efficiently search across a vast composition space of possible multicomponent alloys and identify new HEA alloys with exceptional strength.

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Stacking fault energy in concentrated alloys

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We revisit the meaning of stacking fault energy (SFE) and the assumptions of equilibrium dissociation of lattice dislocations in concentrated alloys. Conventionally, the equilibrium distance between partial dislocations is determined by a balance between the repulsive elastic interaction between the partial dislocations and the SFE [1]. This assumption is used to determine SFE from experimental measurements of dislocation splitting distances in metals and alloys, often contradicting computational predictions. For example, density functional theory (DFT) calculations predict a negative average SFE for CoCrNi[2]. However, TEM observations reveal a finite dissociation distance, indicative of positive SFE[3].

The picture of equilibrium dissociation of lattice dislocations is based on elemental fcc metals, in which SFE is a unique value and an intrinsic material property. In addition, these metals typically have very small Peierls stresses. Therefore, in the absence of solutes and other obstacles, the only opposing force to motion of Shockley partials is the SFE, which can be thought of as a force/length acting on the dislocation. Alloys, particularly those beyond the dilute limit, deviate from this picture. The problem arises when the same assumptions are used in alloys without any modifications.

We use atomistic simulations in a model alloy to study the dislocation dissociation process in a range of compositions with various average SFE. We then examine the balance of forces on the partial dislocations, considering the local effects on SFE. In addition, following the framework proposed by Varvenne et al [4]., we estimate the potential energy barrier posed by solutes to the motion of partial dislocations. We show that in concentrated solid solutions, the interaction of dislocations with local solute environments leads to a major force acting on partial dislocations. The presence of a high solute/dislocation interaction, which is neglected in experimental measurements of SFE explains the discrepancy between experimental and computational predictions of SFE.

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Interaction between screw dislocations and carbon in tungsten from *ab initio* calculations

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Solutes such as carbon can considerably impact the plasticity of metals, especially at high temperatures when they become mobile. Recent TEM *in-situ* straining experiments carried out in tungsten containing 1 appm carbon [1] have shown a return of the Peierls glide mechanism above 1373K, with a straightening of gliding screw dislocations, a consequence of a high lattice friction opposing their motion. Since carbon is mobile at these temperatures, it can strongly interact with dislocations, possibly segregating on them, and modify their mobility. Therefore, we are interested in modelling the interaction of interstitial carbon atoms with screw dislocations having a Burgers vectors 1/2<111> in body centred cubic (BCC) tungsten using *ab initio* calculations.

Previous *ab initio* calculations performed in various BCC transition metals have shown that carbon induces a spontaneous reconstruction of the dislocation core toward a lower energy structure called hard core. This configuration is unstable in pure metals and stabilised by the segregation of a carbon atom at the dislocation centre [2]. Our calculations confirm this reconstruction, associated with a strong attraction between carbon and screw dislocations. We then determine the equilibrium carbon concentrations in the different possible segregation sites around the dislocation by developing an Ising model parametrised on *ab intio* calculations and using a mean-field approximation. This thermodynamic model shows that, even for low carbon nominal concentration and low dislocation density, screw dislocations remain fully saturated with carbon atoms and pinned in their hard core configuration up to about 2500 K [3], *i.e*. at temperatures high enough to activate C diffusion and allow for such a segregation.

We finally calculate the energy landscape controlling the mobility of a screw dislocation saturated by carbon atoms, by considering the formation and nucleation of a kink pair and the migration of kinks. This energy landscape of a screw dislocation gliding by nucleation and propagation of kink-pairs is used to obtain the dislocation velocity, first with kinetic Monte-Carlo simulations, then analytically with classical nucleation theory. Results between both approaches are in good agreement and describe variations of dislocation velocity with temperature, dislocation length and applied stress. The obtained mobility law allows to estimate the local stress existing in TEM *in-situ* straining experiments from the measured dislocation velocity, leading to values comparable with the ones known from macroscopic tensile tests [4].

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Parameterizing Solution Hardening Models by First Principles Calculations: BCC metals and complex concentrated alloys

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Solution hardening in simple BCC metals is well described by Suzuki's classical model of screw dislocation motion by kink nucleation and propagation [1]. One downside of the approach is that the required solute dislocation interaction energies are not readily available from experimental observation or from atomistic methods. Atomistic methods lack the chemical interactions required to produce accurate interaction energies and often (i.e. Embedded Atom Method) produce spurious dislocation core structures [2]. In chemically complex BCC alloys, Suzuki's approach can be modified to account for the rough dislocation glide path produced by the local variations in composition and provides robust predictions for solution hardening in refractory complex concentrated alloys (RCCA) over a range of temperatures [3,4,5]. Unfortunately, the lack of reliable solute-dislocation interaction energies in the RCCA's also limits the application of this and other emerging models. Here we review first principles methods for calculating solute-dislocation interaction energies in the dilute limit (simple metals) as well as for the complex chemistries (i.e. RCCA's). First principles methods typically model dislocations using dislocation dipoles or embedding methods such as the Lattice Greens Function (LGF) method [2]. We will review previous and current predictions for solute-dislocation interactions in Nb, Mo, Ta and W and the predicted yield stress with composition and temperature. We have recently advanced the LGF method to model dislocations in CCA's and applied the method to screw dislocations in three NbTiZr alloys [6]. In two of these alloys we observe chemically driven instabilities in the equilibrium core geometries consistent with kink nucleation. Originally observed in atomistic simulations [7], this defect is widely recognized as being a key strengthening mechanism in the chemically complex BCC alloys. Finally, we review progress in obtaining solute–dislocation energy distributions in refractory complex concentrated alloys for both random alloys as well as systems with chemical short range order consistent with conventional heat treatments.

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Solute-Defect Interaction to Improve Metal Processing and Material Properties

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The challenge to materials science and materials engineering disciplines is its integration into materials science engineering. An illustrative case with a large economic and metal processing consequence was the advent of interstitial-free steels. In early 1970, intensive research to develop steels of high R-value was advanced when recrystallization temperature was lowered by reducing the carbon content in the matrix. Since the lowest solubility for Fe-C was about 15 ppm, a gettering element such as Nb or Ti was added to reduce C to about 2-3 ppm. This process permitted recrystallization below 660°C whereby preferential grain growth of orientations with <111> normal to the sheet occurred. The rest is history but this renown success was accomplished, *by trial and error*, not by materials science design. The realization of this phenomenon led to my venture into elucidating the formation of cube texture in Al capacitor foils. In most Al alloys, solute Fe is 3 ppm with crystallization above 325 °C. Reduction of Fe to 0.2 ppm permitted recrystallization below 300 °C due to formation of Al_6Fe below 325°C and preferential nucleation of cube texture. Thus the solubility limit of Al_6Fe in Al correlated with the grain growth mechanisms as illustrated in Figure 1. The three sections correspond to the well known grain growth theories of Burke-Turnbull, Hillert-Sundman and Stuwe-Lucke. A second example is that of α-constituent in Al-alloys which is more desirable than the softer Al_6Mn without Si additon to reduce galling during metal processing. However, the metallographic evidence showed that its presence was greater than allowed by the chemical composition. Atomic probe of such particles showed that the Si migrated to the large particles forming islands on the precipitate interface during cooling from the hot mill and eventually completely coating the substrate particle. Thus its apparent volume fraction was magnified. These example illustrates that a catalog of solute-defect interaction for a given system will facilitate resolutions to thermo-mechanical processing problems because the process can be modelled becoming the basis of materials science engineering to be described.

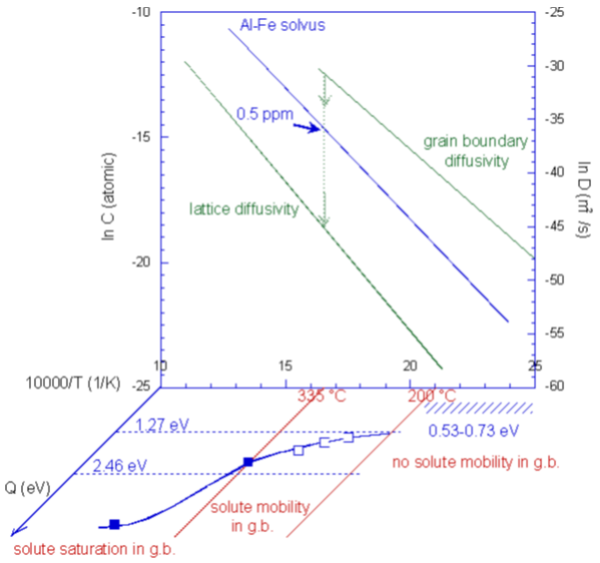

Fig.1. Combined solubility, diffusivity and measured activation energy versus 1/T plot for Fe solute in Al.

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A revision of Labusch's statistical theory of solid solution hardening

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Labusch (1970) provided a simplified mathematical model and a very complex, but still simplified, mathematical solution, for the statistical problem of estimating the critical resolved shear stress for a dislocation moving through a random array of solute-based pinning points. Labusch estimated that the contribution to the critical resolved shear stress from atoms in solid solution, scales with of the binding energy between a straight dislocation and a solute atom, in the power of 4/3, and with the concentration of solute atoms in the power of 2/3. This estimate is important and commonly used in multiscale simulations (Leyson and Curtin, 2013; Varvenne et al., 2017), where refined binding energies of straight dislocation segments can be estimated from atomistic simulations. A recent review on multiscale modelling of high-entropy alloys is given by LaRosa et al. (2019). More than ever, it is important that the scale-bridging relations, i.e. the Labusch theory, is correct.

In the current work, a precise numerical solution of Labusch's model is found, based on discrete dislocation dynamics simulations of a dislocation gliding through an array of elastic stress fields from a large number of randomly distributed solute atoms above/below the slip plane. The simplifying assumption that the dislocation line remains straight, is relaxed. Consequently, the elastic interaction energy is modified, e.g. the screw dislocation then has a non-zero effective interaction energy. As a result, a more complex scaling between the critical resolved shear stress and the solute concentration is reported.

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Does it Add Up? Dislocation Motion Through Aluminum Alloy Solute Fields at 78 K

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The starting point for precipitation of age-hardenable alloys is obtaining a super-saturated solid solution by rapidly cooling from a high temperature. The structure of the super-saturated solid solution at low temperature has long been understood to be a mixture of excess solute atoms and vacancy complexes determined by the alloy chemistry and its thermodynamics. Knowing where the solute atoms (and vacancies) are located in the average lattice are main topics of discussion, especially for multi-principal element materials [1]. For more dilute alloys, characteristic of age-hardening, the saturated state is important in determining the density and distribution of strengthening precipitates thermodynamically driven from solid solution. As stated at the outset, super-saturated solid solutions are usually obtained by thermal means, but there are thermodynamic and/or kinetic tricks available to the materials engineer to create seemingly metastable solid solutions in alloys, i.e. severe plastic deformation by continual shearing [2], or multi-principal element chemistries that promote high entropy [3]. Ultimately, dislocation-obstacle interactions determine the strength and plasticity of these systems. The dislocation-obstacle models used to predict strengthening consider random [4], simplified [5], or deviation from random [6] obstacle distributions describing the solid solution. The current models acknowledge the early formulations of Friedel [7] and Labusch [8]. Nonetheless, there is a genuine, though unintentional growing disconnect between the two topics: understanding the origin of mixing length-scale on phase stability with the literature currently focuses on "high entropy alloys"; and understanding strengthening of solid solutions in general. This talk sets out to connect these two-related, though rarely curated-together, topics [9], by asking what does a saturated solid solution in a multicomponent alloy look like to mobile dislocations? Plastic deformation measurements for a range of quaternary aluminum alloys made at 78 K are analyzed with a new interpretation of the Haasen plot [10, 11] to test additivity rules.

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Placing recent observations of solute strengthening, dynamic strain aging, and serrated flow in Mg alloys within a historical and theoretical context

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The current work analyzes recent cryogenic mechanical test results from the literature, including single crystal Mg–Zn, Mg–Y, and Mg–Dy as well as polycrystalline Mg–Sc and Mg–Y in light of the principle of "stress equivalence" proposed by Basinski et al. This analysis takes advantage of recent theoretical models of solid solution strengthening developed by Leyson and Curtin. For example, our analysis of polycrystalline samples accounts for the truly long-range strengthening effect of grain boundaries through established, temperature dependent Hall-Petch relationships but makes no other assumptions regarding an "athermal stress" that is frequently mentioned in the literature. In brief, the results emphasize the broad applicability of Basinski's principle of stress equivalence, highlighting the fact that the low temperature, thermally activated tensile response of textured, polycrystalline Mg alloys can be predicted once the flow stress at a single rate and temperature is known.

At ambient temperatures, some Mg alloys exhibit evidence of dynamic strain aging (DSA), e.g., a negative slope in the Haasen plot which highlights a curious impact of strain hardening upon the activation volume, yet the strain rate sensitivity remains positive. At even higher temperatures, $T > 0.5T_m$, a number of Mg alloys exhibit serrated flow and negative strain rate sensitivity (i.e. the Portevin-Le Chatelier or PLC effect). It is curious that Mg alloys exhibit PLC at much higher temperatures than Al alloys, despite having similar melting points and similar solute diffusivities. Again, we explore whether recent efforts to theoretically model DSA can adequately describe the response of these Mg alloys. Hypotheses for the diverse observations will be suggested in terms of the diverse deformation mechanisms (basal and non-basal slip and twinning) known to operate in these alloys as well as the diverse microstructures (textures, grain sizes, and precipitates) present in the materials.

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Polytypes precipitates in Mg single crystals

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Hexagonal-close-packed (hcp) metals deform plastically by dislocation glide and twinning; under suitable conditions they undergo concurrent phase transition transforming their lattice to the other structure [1,2]. Geometrical considerations suggest that the activity of a/3⟨10-10⟩ Shockley dislocations on the basal planes may render the hcp lattice into the polytype structure [3]. Multicomponent Mg-Zn-based alloys containing long periodic stacking ordered phases (LPSOs) form many distinct polytypes [4, 5]. Recent findings suggest that polytype transformation in LPSO phases stems from the lattice distortion induced by the solute elements [6]. Here we present studies of the precipitate-like lattice imperfections, polytypes precipitates (PPs), formed in the microstructure of pure Mg single crystals during early compression. These three-dimensional defects emerge as co-products of lattice distortion developed in dislocations' tangles due to reactions and rearrangements of dislocations to the lower energy structures [4]. TEM observations indicate that entanglements containing an excess content of ⟨c⟩-component dislocations nucleate PPs. The distortion and rotation of the lattice induce the transition to the triclinic structure originating PPs. The overlapping strain fields from mutually interlocked dislocations and stacking faults promote local shears and shuffles that develop polytypes domains in PPs' structure. Ab initio and molecular statics simulations are used to understand the processes governing triclinic and polytypic transformations in Mg and the role of dislocations in PPs' self-assembly.

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Strain rate effect on hydrogen behavior in aluminum alloys during deformation

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Effect of strain rate on hydrogen evolution behavior during tensile deformation and fracture in T6-tempered 6061 and 7075 aluminum alloys was studied by means of a testing machine equipped with a quadrupole mass spectrometer installed in an ultra-high vacuum chamber [1)]. The evolution of hydrogen atoms in the deformed microstructure was also visualized with a hydrogen microprint technique. It is revealed that the hydrogen gas evolution rate during the tensile deformation changes according to the testing strain rate. The hydrogen gas evolution during deformation was decreased when the both alloys were tested at a strain rate above $2.5 \times 10^{-2}\ s^{-1}$. Similar tendency was also identified when the sinusoidal stress was applied. The amount of hydrogen evolved at the early stage of plastic deformation in the 7075 alloy was much higher than that in the 6061 alloys. This suggested that the hydrogen diffusion with the aid of hydrogen transportation by dislocations was retarded in the 6061 alloy because of the difference of the hydrogen trapping state in the microstructure, comparing with the 7075 alloy.

Besides, a novel analytical system was recently developed to monitor the environmental hydrogen embrittlement of aluminum alloys dynamically and quantitatively under atmospheric air pressure [2)]. The system involves gas chromatography using a SnO_2-based semiconductor hydrogen sensor, a digital image correlation step, and the use of a slow strain rate testing machine. Use of this system revealed that hydrogen atoms are generated during the plastic deformation of T6-tempered 7075 alloys caused by the chemical reaction between the water vapor in air and the alloy surface without oxide films. Digital image correlation also clarified that the generated hydrogen atoms caused numerous localized grain boundary cracks on the specimen surface, resulting in a localized grain boundary fracture.

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Revisit the work hardening mechanism of TWIP steels: carbon atoms vs. deformation twins

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Twinning-induced plasticity (TWIP) steels are promising structural materials for many engineering applications. Conventional views consider that deformation twinning is the decisive mechanism responsible for the excellent tensile properties of TWIP steels (*1, 2*). Nevertheless, our recent experiments showed that deformation twins only contribute about 10% of the ultimate tensile strength of a TWIP steel (*3*). In addition, it was found that a TWIP steel deformed at 473 and 298 K possessed comparable dislocation densities and tensile properties (*4*). But the deformation twins are largely inhibited at 473 K while intensive deformation twins are generated at 298 K (*4*). These new experimental evidence suggests that deformation twins may not be the main mechanism responsible for the high dislocation density and excellent tensile properties of TWIP steels(*4*). Furthermore, our recent experiments indicated that the carbon-dislocation interaction increases the dislocation generation rate and reduces the dynamic recovery rate, leading to a high dislocation density in TWIP steels. Therefore, carbon atoms play the most crucial role in enhancing the work hardening rate of TWIP steels (*5*). TWIP steels without carbon are just conventional face-centered cubic alloys similar to the 316L austenitic stainless steel.

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Inertial Contributions to Dislocation Drag in Alloys

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Dislocation motion is often described in a quasi-static or steady-state limit where behaviour is taken to be overdamped (see e.g. [1]). There are cases, however, where it is important to consider the actual dynamics of dislocation motion, including not only motion at constant velocity but also acceleration and deceleration, for example when dislocations interact with obstacles along the glide path. This is also of particular importance in situations of shock or high frequency, cyclical loading. Under such cases inertial effects may no longer be negligible [2].

Another situation where inertial effects can be important is when dislocation motion occurs in the presence of solute at finite temperatures and strain rates. The classical continuum theory for solute drag on dislocation motion originates from the seminal work of Cottrell, Louat, Fuentes-Samaniego and others [3-5], where dissipation at steady state leads to the classic over-damped prediction of a peak flow stress at a critical strain rate and temperature. This has been refined recently to consider the effects of extended dislocations [6-8] and atomistic effects involving fast cross-core diffusion [8]. In this limit, a second maximum in the flow stress – strain rate (temperature) relationship has been predicted [8] highlighting the importance of details only resolved at the atomistic scale.

The steady-state models described above implicitly consider only the pure dissipative contribution to dislocation motion in a solute field but does not consider the inertial contribution that arises under conditions of acceleration or deceleration when the dislocation moves relative to the solute distribution around it [9]. The extreme limit is the case of dislocation de-pinning from a static solute cloud that has segregated to it. While closed-form, approximate solutions to the continuum equations of motion for the dislocation and solute are not readily available (even for simple cases) [10], numerical methods that can account for finite solute concentrations, and the discrete, atomistic nature near the dislocation core should be well suited, so long as the appropriate length and timescales can be bridged. Here, results from the alloy diffusive molecular dynamics [11] model are presented showing the response of both straight edge and screw dislocations under finite strain rate and temperature for a model Al-Mg like alloy. Both the steady state flow stress and the full transient solute drag response are probed and used to illustrate some of the additional complexity that can arise when inertial contributions are accounted for.

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Is 3D and 4D characterization needed for studies of recrystallization?

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3D characterization of metal microstructures is not new, but fueled by novel possibilities at the large international Synchrotron X-ray facilities, a new wave aiming at developing more advanced 3D characterization tools emerged during the late 1990ies – early 2000ies. Today, these techniques are mature and user-friendly. They are used by many, both in academia and industries and a 3D Materials Science community has evolved. Is thus the right time for discussing what impact they have had and discuss the next "burning" scientific questions which may be addressed, see eg [1]. This is the aim of this presentation, where the focus is on recrystallization.

Well planned experiments on nucleation and grain boundary migration are reviewed with focus on novel information gained, which could not have been obtained by traditional 2D or destructive 3D methods [2]. Both controlled nucleation near a hardness indent [3], in an ideal tricrystal [4] and particle stimulated nucleation in an industrial aluminum alloy [5] is presented. The grain boundary migration experiments have reveal significant deviations for the expected equation

$$v = M\,F$$

where v is the boundary migration rate, F is the driving force provided by the stored energy in the deformed matrix material and M is the boundary mobility. The importance of interaction with defects are discussed [6,7].

It has also been found that the 3D/4D X-ray measurements sometimes happen to reveal phenomena, which were not expected and therefore not planned to investigate. Examples of this, related to an unexpected subdivision [8] and remaining residual strains [9] within recrystallizing grains are also discussed here. The implications of the new findings for advancing modelling of recrystallization are discussed with focus on phase field and molecular dynamics simulations [10,11], and vise-versa, how the simulations may be aid selecting key 3D/4D experiments for the future.

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Defect segregation in alloys: thermodynamics, kinetics and near atomic characterization

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Segregation or adsorption to crystalline defects like grain boundaries and dislocations has been widely associated with a wide variety of relevant phenomena for the design of new materials like medium manganese steels. Mobility and cohesion are two important properties of grain boundaries that are influenced by the local chemistry of the defect. Segregation plays a key role as well during the initial stages of diffusional nucleation and growth of a new phase from a supersaturated solid solution. Notwithstanding, these phenomena are often treated in a disconnected manner. The preferential nucleation (heterogeneous nucleation) of a phase at internal defects, such as grain boundaries and dislocations are usually attributed only to the reduction of the required interfacial energy. Nevertheless, nucleation often proceeds via multiple steps and pre-clustering is a common precursor pathway for nucleation (e.g. via formation of GP zones in the bulk of some Al-alloys). This talk renders a concise summary of our recent progress in approaches to better understand the thermodynamics and kinetics of defect segregation and its interplay with heterogeneous nucleation. It will cover (i) the characterization of solute segregation to internal defects in the bulk and first order transitions in the adsorption layers; (ii) the thermodynamics and kinetics of solute segregation; and (iii) the interplay of solute segregation and nucleation. Examples from diverse metallic alloy systems will be provided, placing emphasis on the Mn segregation and austenite reversion in martensitic Fe-Mn alloys, given the industrial relevance of this system.

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A Comparison of Solute Effects on Moving Grain Boundaries and Inter-Phase Interfaces

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The growth of proeutectoid ferrite from alloyed austenite is reviewed, with emphasis on the similarities with and distinctions from solute effects in grain growth in dilute and concentrated solid solutions. The problem of ferrite growth is fundamentally a multi-component one: substitutional alloying elements effects are overlaid on transformations in the binary iron-carbon system. In recent decades, an international initiative "AlEMI", aimed at elucidating these effects, has resulted in a measure of progress in the field. Some of the modelling and experimental advances are reviewed, and remaining issues are discussed.

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Grain boundary phase transitions probed by tracer diffusion measurements

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Grain boundary diffusion is strongly affected by interface structure and segregation of solute and residual impurity elements and represents, thus, an extremely sensitive tool to probe grain boundary phase transitions. Recently, the existence of temperature-induced transitions in the grain boundary structure were revealed by high-precision radiotracer diffusion measurements in low-sigma Cu bicrystals [1, 2]. An existence of critic temperatures, which corresponds simultaneously to specific "kinks" in the temperature dependences of the grain boundary diffusivity and the disappearance of the grain boundary diffusion anisotropy, was discovered and related to the temperature-induced phase transitions [3]. Solute elements diffusing along grain boundaries could provoke structure transitions, too.

Segregation-induced grain boundary phase transitions in the Cu-Bi system were investigated by the radiotracer measurements and explained in terms of a pre-wetting phase transition [4]. Measurements of Ag grain boundary diffusion in the same Cu-Bi alloys highlight an intrinsic heterogeneity of the grain boundary phase transitions when the pre-melted and almost segregation-free high-angle grain boundaries co-exist in the polycrystalline Cu-Bi alloy in a broad range of volume concentration of Bi.

Recent advances with respect to grain boundary transitions in multicomponent alloys will be presented, too [5,6].

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Grain Growth in Polycrystals

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Simulations can be used to measure the properties of interfaces in materials. The central role of quantitative phase field simulations in this effort is illustrated by a rapid throughput method to determine grain boundary properties. By comparing the evolution of experimentally determined three-dimensional grain structures to those derived from simulation, we measure the reduced mobilities of thousands of grain boundaries. Using a time step from the experiment as an initial condition in a phase-field simulation, the computed structure is compared to that measured experimentally at a later time. An optimization technique is then used to find the reduced grain boundary mobilities of over 1300 grain boundaries in iron that yield the best match to the simulated microstructure. We find that the grain boundary mobilities are largely independent of the five macroscopic degrees of freedom given by the misorientation of the grains and the inclination of the grain boundary.

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Solute segregation at precipitate-matrix interfaces in aluminium alloys

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Solid-state precipitates are key microstructural components of high-strength aluminium alloys [1]. Characterising the interaction of solute with precipitate-matrix interfaces is crucial to understanding the mechanisms of precipitate growth and thermal stability, particularly so for low-dimensional precipitates, because they share large interfacial areas with the matrix in which they are embedded. Such precipitates also tend to nucleate and grow in a solute-rich environment.

Here, we describe the atomic-scale structures associated with solute segregation at precipitate-matrix interfaces in several model aluminium alloy systems, including the Al-Cu and Al-Ag textbook systems. These alloy systems have been the subject of many studies on the mechanisms of solid-to-solid phase transformations [2-9]. We focus on rationally oriented, low-dimensional precipitate phases as well as voids. Voids can be regarded as vacancy precipitates, with the precipitate-matrix interface being the void surface. Interfacial structures were characterised experimentally by scanning / transmission electron microscopy (S/TEM) using a variety of imaging and diffraction techniques, exploiting recent advances in aberration-corrected S/TEM. Atomistic modelling was also performed, using first-principles and semi-empirical computational methods.

We found that solute segregated at almost all interfaces [10-18]. In some cases, this behaviour could be explained by the solute defect energy [10,15,16], with vacancies playing an important role in the order in which precipitation and solute segregation take place [12,17]. Solute segregation was observed to result in different atomic structures, some of which were complex and akin to interfacial phases [10-11,17]. Segregation at the surfaces of nanoscale voids was also observed, in the form of an atomically thin layer [18]. Such segregation has a strongly stabilising effect on the thermal stability of voids, when compared with uncoated voids [19]. Overall, our work paints a picture in which solute segregation at precipitate-matrix interfaces is the norm, with diverse types of interfacial structures as a result. These structures suggest atomic scale mechanisms for precipitate growth and thermal stability, but many details remain to be uncovered.

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Precipitation strengthening of Al alloys through room temperature cyclic deformation

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Conventionally, precipitation strengthening through ageing treatment is an important way to produce high strength aluminium alloys with relatively good ductility, during which the supersaturated solid solution decomposes and a high number density of precipitates form in the Al matrix. Normally, time required to achieve the peak aged state is between 7 to 24 hours. In the past 100 years, such ageing treatment has developed to be a widely used method in industrial applications. However, there exists two common issues always coming with ageing treatment, that is, the deterioration of mechanical and unticorrosion properties caused by precipitate free zones and high energy consumption. This research innovatively proposed a precipitation strengthening manner using dynamically formed precipitates during room temperature cyclic deformation, which successfully strengthens the Al alloys as strong as and even more ductile than conventional T6 condition, meanwhile suppresses the formation of precipitate free zones. In this new cyclic strengthening method, the load on the cyclic deformed sample progressively increases as the cyclic deformation proceeds with a certain frequency. The main strengthening mechanism is the continuously injected vacancies due to the cyclic motion of dislocation jogs mediates the dynamic precipitation of a very fine distribution of solute clusters, resulting in better material strength and elongation properties relative to traditional thermal treatments. The strengthening procedure is also much faster than ageing treatment. Therefore, it has a great potential to contribute to the green manufacturing and could be fitted to other alloy systems.

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Ultra-high strengthening of A2024 alloy by grain refinement and grain boundary segregation

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It is widely known that additional strengthening is feasible for aluminum alloys by reducing the grain size to submicron level [1]. In this study, the method of high-pressure torsion (HPT) [2] was applied for grain refinement to an age-hardenable A2024 (Al-Cu-Mg) alloy. Disk samples with 10mm diameter were processed by HPT under an applied pressure of 6 GPa for 10 turns. Tensile tests showed that the ultimate tensile strength (UTS) reached 910 MPa immediately after 10 turns. It is noteworthy that extremely high strengthening was successfully achieved by further conducting the subsequent aging, leading to the UTS of 1 GPa. The microstructures were analysed by transmission electron microscopy and atom probe tomography. According to TEM analysis, the ultra-fine grained structure with the average grain size of 160 nm was retained after aging treatment. Atom probe tomography revealed that both Cu and Mg are segregated on the grain boundary even before aging treatment, and it becomes remarkably after aging. The mechanism for the high strength was clarified in terms of solid-solution hardening, cluster hardening, work hardening, dispersion hardening and grain boundary hardening. It is shown that the segregation of solute atoms at grain boundaries including subgrain boundaries plays a significant role for the enhancement of the tensile strength [3].

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Lattice point defect-mediated semi-coherent precipitation in irradiated alloys

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Nuclear reactor pressure vessel steels undergo embrittlement under neutron irradiation, due to the formation of nanometric point defect and solute (Cu, Ni, Si, Mn etc.) clusters [1]. To understand the effect of Ni on the microstructure, a bcc Fe-3%at.Ni ferritic alloy has been irradiated with 27 MeV Fe^{9+} ions at 673 K at a damage rate of 10^{-6} dpa.s^{-1}, up to a displacement damage of 1.2 dpa, within the Jannus Saclay facility. Using high-resolution transmission electron microscopy and atom probe tomography, the formation of an out-of-equilibrium fcc phase in the irradiated bcc matrix has been demonstrated [2]. In this presentation, the characterization of radiation-induced precipitates will be detailed. A combined crystallographic-thermodynamic approach of semi-coherent precipitation was developed to make the connection between lattice, phases and defects, thereby uncovering the prominent role of excess point defects in unforeseen phase transformations [3].

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Early-stage solute clustering in the phase-field crystal model

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Solute clusters often act as precursors to precipitation in age-hardenable alloys. In this talk we discuss results on the use of a diffusive atomistic modelling formalism, the phase-field crystal model, to demonstrate the early stages of solute clustering. We investigate the dislocation-mediated nucleation and growth mechanisms of these solute clusters. Our results are compared with high resolution TEM to determine the persistence of dislocation defects in association with solute clusters and orientation selection of 3D clusters.

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The solid solution hardening in design of aluminum alloy for application at elevated temperatures

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Solid solution hardening is one of the critical strengthening mechanisms for aluminum alloys, but it is usually confined within the ambient temperature range. In the present work, the solid solution hardening from Mg and the associated grain boundary hardening in aluminum from room temperature up to 345°C were investigated. It has been found that there exists a transition temperature around 200°C. Below the transition point the frictional stress, solid solution hardening and grain boundary hardening are little affected by temperature, due to the enhanced solute pinning on dislocations by Cottrell clouds or other extensive segregation of solutes to dislocations. Above the transition point, the solid solution hardening is controlled by the temperature-dependent shear modulus, which decreases linearly with increasing temperature up to ~300°C, so both the frictional stress and the solution hardening from Mg decrease linearly with increasing temperature above ~200°C. Meanwhile, the grain boundary hardening obeys the Hall-Petch equation over the whole temperature range. Below the transition point the Petch slope is mainly controlled by the solute Mg, while above the point it is dependent on both the solute Mg level and temperature. Consequently, semi-empirical expressions for the yield strength at 25-345°C were derived including both the solid solution and the grain boundary effects. Based on this discovery, a high strength aluminum alloy has been developed successfully for the high performance automotive heat exchangers, especially the ones may serve at elevated temperatures above 150°C.

References: The chapters regarding (1) solid solution hardening or solute-dislocation interaction and (2) the strengthening mechanisms in metals, in any physical metallurgy textbooks.

Solutes partitioning at crystal defects in crept Ni-based superalloys: towards a better understanding for enhanced materials properties

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Characterizing, quantifying and understanding the solutes segregation at crystal defects during high-temperature deformation of Ni-based superalloy is of great interest, in order to develop a deeper knowledge of the materials behavior during service and prevent unpredictable fracture of safety-critical components. Some studies have shown that solutes, such as Co and Cr, are prone to segregate at dislocations modifying the local composition and leading ultimately to an alteration of the microstructure such as the undesirable dissolution of the strengthening γ' precipitates, the formation of TCP phases or of inverted structures [1–4]. In contrast, solutes partitioning onto stacking faults has been shown to possibly be, in some cases, beneficial for the mechanical properties by promoting desirable local phase transformations [5]. Segregation of a few at.% can thus have dramatic consequences, and achieving a better understanding of the diffusion-controlled dynamic phenomena is critical for alloy design of next-generation alloys [6,7].

Evidencing such segregation at near-atomic scale is challenging, often requires state-of-the-art equipment, such as atom probe tomography, that can be used to provide quantitative compositional information. In the present talk, the interactions between solutes and crystal features in Ni-based superalloys will be exemplified through two case-studies, showing ultimately how these interactions may modify the mechanical properties of the alloys. The first case-study explores the segregation behavior of solutes at stacking faults leading to enhanced creep performance by promoting a local phase transformation along stacking faults [8]. The second case-study is focused on the microstructural evolution of grain boundary borides during creep, where planar compositional fluctuations and segregation at dislocations are evidenced [9]. These are believed to be correlated to the coarsening of these particles during creep, and bring new insights on the role of these precipitates on the mechanical performance of superalloys.

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Industrial Consequences of Solute Defect Interactions related to Nickel and Titanium Alloy Production and Application.

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In my experience, industrial metallurgical conundrums occur when the limits of conventional alloys are pushed to meet a new requirement. Often this results in unexplained results that producers do not have the interest, or resources to investigate in a scientific manner due to the commercial uncertainty of the opportunity. In many of the cases it is likely that an underlying metallurgical phenomenon is at work below the resolution of typical industrial laboratory. In this talk, I will review developmental projects where I suspected that solute defect interactions were controlling the behavior of the product. Examples in titanium include cold workability of a CP grade and strengthening on a new near ß grade. In nickel, embrittlement of precipitation hardened alloys is a constant concern in the oil and gas industry and remains a source of contention as to the precipitation reactions occurring at grain boundaries. Nickel superalloys now going through the ASME BPVC process to determine stress allowable are being hampered by the instability of the precipitating phases that occur at operating temperatures. In each of these cases, a combination of chemistry adjustment or heat treat parameters made a significant change to the response of the alloy. This talk will provide the background and industrial results in each of these examples. Connecting these macro results to the underlying solute-defect interaction is best left to the participants of this conference.

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APPENDIX A - Four Readings for Purdy and Zurob abstract from the Alemi network

READING 1

Contact conditions for gamma to alpha Transformation in Ternary Fe-C-X, Part I: Thermodynamic Models

In the study of alloying effects on transformations in steels, one can trace the evolution of these concepts to the realization that the austenite decomposition reactions, although clearly influenced by the presence of substitutional alloying elements, often proceed at rates determined essentially by the diffusion of carbon. The diffusion coefficients of typical alloying elements (X=Mn,Ni,Cr,Mo…) in austenite are many orders of magnitude less than those of interstitial solutes (C, N).

Hultgren [1] coined the term “paraequilibrium” (PE) to describe the hypothetical case where the alloying element is essentially bypassed by the transformation interface; the situation then becomes quasi-binary, the substitutional solution behaving, in the thinking of many researchers, as a single “element”. In an internal report of the Swedish Institute for Metals, Hillert [2] developed this concept quantitatively, showing that corresponding interfacial constrained equilibria for carbon would always lie inside the true equilibrium boundaries on a ternary isotherm. Since the PE tie-lines are required to connect compositions of equal Fe/X ratio, they correspond to component rays, each passing through the carbon corner of the Gibbs triangle. Hillert also employed isoactivity lines and their extrapolations into the two phase region to show how the PE boundaries could be generated.

Aaronson and Domian [3] independently proposed a closely-related type of partial equilibrium, called “no-partition equilibrium”, which differed only in minor aspects from PE, and presented a series of ternary isotherms calculated on this basis.

There is another way in which the transformation can proceed rapidly with negligible alloying element partition: this was also anticipated by Hillert [2], and termed “quasi-paraequilibrium”. The situation requires that the interfacial contact conditions conform to a true local equilibrium tie-line, but one that corresponds to a product phase substitutional composition very close to the bulk austenite composition, so that a thin alloying element “spike” exists in the parent austenite at the interface. Kirkaldy [4], studied the full multicomponent diffusion problem, including cross-terms in the diffusion matrix, and found solutions that corresponded to local equilibrium unpartitioned growth. Subsequently, Purdy et al [5] showed that the requirement of simultaneous mass balances for the two solutes generated a regime on the ternary isotherm within which such solutions could exist, and called its limit the “envelope of zero partition”. Coates [6] explored the consequences of differences between the diffusivities of two solutes, and obtained this same envelope as a limiting case for very large ratios DC/DX. More recently, this condition and its limit have been termed local equilibrium with negligible partition LE-NP [7].

For a simple ternary steel containing an austenite-stabilizing alloying element, such as Fe-C-Ni, the isothermal section then divides into three regions: LE-NP, where both PE and LE-NP are thermodynamically possible; a larger region where the only paraequilibrium contact conditions will lead to an unpartitioned product, and an even larger region (full equilibrium) where, on this basis, only partitioned product (ferrite in this case) can form.

These arguments are entirely thermodynamic; they do not explicitly contain kinetic information, nor do they account for departures from local equilibrium contact conditions. They were initially based implicitly

on the concept of an infinitely thin interface; it was only somewhat later that the concepts of interfaces with separate thermodynamic (e.g. segregation, anisotropy of energy) and kinetic (transport, mobility) properties were overlaid on the earlier constructs.

The increasing widespread availability of assessed thermodynamic databases and computational thermodynamic methods has led to the quantitative evaluation of the LE-NP and PE limits for ternary and higher-order systems. In addition, thanks largely to Aaronson and his colleagues [8,9,10], the kinetics of grain boundary ferrite precipitation in high purity homogenized ternary and quaternary steels has been investigated: in many cases, the agreement between the models (often using the PE interfacial condition) and observed rates of ferrite growth is not encouraging. It is not at all clear that the PE interfacial condition, even if established, will persist throughout the precipitation event. Different researchers have attributed observed deviations from the predictions of the PE model to solute drag [11,12], cross-interface atomic transport [13] and interfacial structural inhibition [10].

The study of controlled decarburization has proven informative, in part because the structural influences are absent; the interface, once established, is essentially "incoherent". A planar ferrite layer develops from the surface of an initially austenitic specimen, and grows at a rate determined by carbon diffusion in both ferrite and austenite. With a knowledge of the carbon diffusion coefficients in ferrite and austenite, this allows the deduction of the interfacial contact conditions. For Fe-C-Ni [14], for all compositions and temperatures investigated, the growth of ferrite was accurately parabolic in time, implying semi-infinite boundary conditions and constant interfacial compositions, and consistent with LE-NP, rather than PE conditions. For Fe-C-Mn alloys [15,16], in contrast, one finds LE-NP conditions at lower temperatures, and a surprising gradual transition to PE conditions at the highest temperatures. This behavior has been modeled on the basis of multiple discrete atomic jumps to and from a solute-enriched interfacial energy well [16].

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READING 2

Kinetic models for austenite to ferrite transformation in Fe-C-X

Introduction

There are at least three kinds of models of moving interfaces. The simplest one is the sharp interface model and it is very widely used for the treatment of diffusion controlled phase transformations. Basically, it simply assumes that there is full chemical equilibrium between the two phases locally at the interface. That will give the boundary conditions for diffusion inside the volumes of the phases in the system. In reality, there may be important cases where there is an appreciable deviation from local equilibrium at the moving interfaces in phase transformations. It may be described as an effect of some friction in the interface acting against the motion, which is usually assumed to be proportional to the rate of motion. It may be visualized as a difficulty of the atoms to rearrange themselves into the structure of the new lattice. Another kind of model is based on a description of the interface as a layer of appreciable thickness, which makes it possible to consider the composition profile inside the interface. It is then possible to describe the friction as a requirement of driving force for the diffusion inside the interface. This is closely related to the phenomenon of solute drag occurring in grain growth in single phase materials. A third kind of model is based on assuming that there is a diffuse region of gradual transition of the properties from one phase to the other. The first approach (1) was one-dimensional and was made on the atomic level but has now developed into the very powerful Phase Field Method where one considers mesh points in a three-dimensional network. It will be treated in another section.

Sharp interface models

a) *Modelling of friction term*. One may accept that there is some friction acting against the motion of the phase interface and requiring some driving force. It is usually assumed that the velocity should be proportional to the driving force and the constant of proportionality is regarded as the mobility. Its value under various circumstances is not well established but a new attempt has recently been made to evaluate the mobility of “random” ferrite/austenite interfaces by analyzing experimental data on the massive transformation from the literature (2).

The driving force for overcoming the friction has to come from some deviation from local equilibrium at the moving interface. Thus, one must evaluate the deviation and that gives the necessary boundary conditions at the interface and, in turn, that makes it possible to treat the diffusion inside the volumes of the phases. It is thus necessary to analyze the relation between the fluxes across the interface and the fluxes in the two phases simultaneously. This has now been attempted in a special case (3).

b) *Modelling of diffusion across interface.* Another method of predicting the rate of motion is to assume that the atoms cross the interface by individual jumps and to evaluate the net flux of atoms. That process will dissipate Gibbs energy, i.e., consume driving force. The effect could be experienced as a friction although it originates from a different physical process. The rate of motion of the interface would depend on the individual diffusivities of the components across the interface. The diffusion equation for this process must take into account that there is a considerable difference in composition between the two sides of the interface, which is not allowed by the ordinary diffusion equation. Such an equation has now been found and it could be derived using an absolute reaction rate approach (4).

c) *Finding the proper tie-line for a moving interface*. The conditions at the phase interface, which will be used as boundary conditions for diffusion within the phases, are directly obtainable by calculation from a thermodynamic database if one can assume local equilibrium and if one works with binary systems. In ternary systems there is a twophase field with a series of tie-lines and it is not self-evident how to find the operating tie-line and that tie-line will normally change during diffusional phase transformations. The problem increases with each increase of the number of components in the alloy. Advanced programs for

simulating diffusional transformations must be provided with an automatic procedure for finding the "relevant tie-line". It seems that such a procedure may turn very time-consuming for higher-order systems and may even have difficulties converging. A new approach has now been attempted where those boundary conditions are not required but the local conditions at the interface are made to approach the relevant tie-line gradually during the ordinary iteration procedure for diffusion by considering the diffusion across the interface and inside the phases simultaneously. Since local equilibrium between the two phases is not used as a prerequisite but will be the result of the process itself, it seems possible to apply the method also to cases where there is some deviation from local equilibrium (5).

d) *Modelling trapping and diffusionless growth.* The equation mentioned above cannot describe the phenomenon of trapping and even less the diffusionless growth of the new phase that may happen in a massive transformation, i.e., a partitionless transformation where there is not even a pile-up of solutes in front of the moving interface. To handle such cases work has started to include cooperative transfer of groups of atoms across the interface. Experimental study of the critical solute content, above which massive transformation cannot occur, has been performed on the Fe-Ni (6) system and a first version of the revised equation has been applied to analyze the new information (7). A method that has been used before is based on adding cross terms to the diffusion equations of individual alloy elements (8).

Wide interface model

The simplest version this model was applied to an interface of fixed width and uniform properties and an analytical expression was used to describe the composition profile inside the interface. The dissipation of Gibbs energy due to the diffusion was treated as a friction (9). In the next version (10) the properties were allowed to vary across the interface and the diffusion process was solved numerically. Then one can describe a composition profile within the interface and work with some special thermodynamic model for a solution phase within the interface. It was then possible to simulate the transition from diffusion controlled to diffusionless solidification (11).

Solute drag

If that model is made to attract the solute atoms to the central part of the interface, they tend to diffuse with the interface if it moves. That causes a dissipation of Gibbs energy which has to be subtracted from the driving force for the motion. This is related to the phenomenon called solute drag which was modelled in a similar way for grain boundaries in homogeneous, single-phase systems (12). It got its name because the treatment was not based on the dissipation of Gibbs energy but considered the actual attraction between the solute atoms and the centre of the interface. It turned out that when the solute drag treatment was applied to a phase transformation in an alloy, it did not give the same result as the treatment based on the dissipation of Gibbs energy. Finally a unified treatment was found (13).

Today the term 'solute drag' is commonly applied to both grain growth and phase transformations. The application of the mathematically formulated treatments are few but it is common to propose that various discrepancies from expected results are caused by solute drag or even by a 'solute drag like effect'. It is interesting that it was found (12) that the same treatment does not always give a drag but a driving force. That is always the case when applied to the phenomenon called CIGM (Chemically Induced Grain boundary Migration) (14), a name that was later changed to DIGM (Diffusion induced grain boundary Migration) when it was incorrectly proposed that it was the diffusion process itself that caused the phenomenon (15).

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READING 3

Models for diffusion control of migrating phase interfaces

a) *Sharp Interface Model*. There are at least three kinds of models of migrating interfaces. The simplest one is the sharp interface model and it is very widely used for the treatment of diffusion controlled phase transformations. Basically, it simply assumes that there is full chemical equilibrium between the two phases locally at the interface. In addition, one may accept that there is some friction acting against the migration, which is usually assumed to be proportional to the rate of migration. That migration will then require some driving force that has to come from some deviation from local equilibrium at the interface. In order to evaluate that driving force it is necessary to analyze the relation between the fluxes across the interface the fluxes in the two phases. This has now been analyzed in detail (1). An attempt has also been made to evaluate the mobility of "random" ferrite/austenite interfaces by analyzing experimental data on the massive transformation from the literature (2).

Another method of predicting the rate of migration is to assume that the atoms cross the interface by individual jumps. The rate will then depend on the individual diffusivities of the components across the interface. The diffusion equation for this process must take into account that there is a considerable difference in composition between the two sides of the interface. Such an equation has now been derived using an absolute reaction rate approach (3).

This equation cannot describe the phenomenon of trapping and even less the diffusionless growth of the new phase in a massive transformation. To handle such cases work has started to include cooperative transfer of groups of atoms across the interface. Experimental study of the critical solute content above which massive transformation cannot occur has been performed on the Fe-Ni (4) systems and a first version of the revised equation has been applied to analyze the new information (5).

As an attempt to improve the sharp interface model further we have tried to make it find the correct boundary conditions for diffusion in a phase at the interface to an adjacent phase automatically. They are directly obtainable by calculation from a thermodynamic database if one can assume local equilibrium and if one works with binary systems. In ternary systems there is a two-phase field with a series of tie-line and it is not self evident how to find the operating tie-line and that tie-line will normally change during diffusional phase transformation. Advanced programs for simulating diffusional transformations must be

provided with automatic procedures but they may turn very time-consuming for higher order systems and may even have difficulties converging. A completely new approach (6) is now attempted where those boundary conditions are not required but the local conditions are made to gradually approach the relevant "tie-line" during the ordinary iteration procedure for diffusion. Since local equilibrium between the two phases is not used as a prerequisite but will be the result of the process itself, it should be possible to apply the method also to cases where there is some deviation from local equilibrium.

b) *Wide interface model.* In the simplest version this model is applied to an interface of fixed width. Then one can describe a composition profile within the interface and work with some special thermodynamic model for a solution phase within the interface. If that model is made to attract the solute atoms to the central part of the interface, they tend to diffuse with the interface if it migrates. That causes a dissipation of Gibbs energy which has to be subtracted from the driving force for the migration. This is called solute drag and was first modelled for grain boundaries in homogeneous, single-phase systems. Another model was developed for phase transformations and there seemed to be a conflict between the two approaches. That conflict has now been resolved by a treatment that applies to both cases (7).

c) *Interface with undefined width*. This case will be discussed under the heading "Phase-Field Model".

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READING 4

Chemistry of ferrite/austenite boundaries

In the workshops the influence of alloying element segregation on the migration of ferrite/austenite boundaries was the subject of primary concern and thus, measurements of chemical composition of ferrite/austenite boundaries and correlation with the structure of the boundary in binary Fe-X and ternary Fe-C-X alloys were proposed. Fletcher et al [1], Humphrey et al [2] and Enomoto et al [3] employed a STEM technique all to measure the Mo segregation at ferrite/austenite boundaries in Fe-C-Mo alloys, and the latter two reported an increase in the Mo concentration with transformation time [2, 4]. The enrichment of Mo atoms at ferrite/austenite boundaries was also revealed by atom-probe in an Fe-C-Mo alloy [5]. Hackenberg and Shiflet [6] conducted an EDS microanalysis of the chemistry of the reaction front at the bay in a Fe-C-Mo alloy to observe small amounts of Mo enrichment and diffusion into austenite. They also noted alloy partitioning between ferrite and carbide and proposed tha this was responsible for the slow kinetics in the alloy around the bay temperature.

The mechanism for the segregation at moving boundaries was discussed. It can be different from segregation at static boundaries, and is called accumulation [2]. It is thought that the accumulation of impurity or solute atoms several times the bulk concentration can be readily achieved during the migration of the interface.

Guo et al [7] conducted a STEM analysis of Mn segregation at ferrite/austenite boundaries in a low carbon Fe-C-Mn-Si alloy. The height and width of Mn concentration peaks increased with holding time. Coupled with the observed kinetic features of the transformation they concluded that three growth stages existed

in this alloy which are characterized by the initial rapid growth involving no partition or interfacial accumulation of Mn and presumably Si also, enrichment of Mn at the ferrite/austenite boundaries and partitioning of Mn between ferrite and austenite. The co-segregation of Si was expected, but was not observed consistently. Both the interfacial segregation and the diffusion pile-up could contribute to the enrichment of alloying element in the boundary region.

It is probable that the segregation of Mo or Mn at ferrite/austenite boundaries is increased by carbon. The effects of substitutional alloying elements which presumably co-segregate with interstitial solute, the diffusion of which primarily is rate-controlling, and enhance the amount of free energy dissipation at the boundaries, are termed coupled-solute drag effects (C-SDE) [8, 9]. Further studies are needed which are concerned with the correlation of alloying element segregation with boundary structure. For example, the segregation at ledge risers would play a crucial role in the boundary migration and morphological development.

A series of experiments of migration of ferrite/austenite boundaries were conducted under controlled decarburization conditions in ternary Fe-C-X alloys. In this experiment the influence of boundary structure and crystallography on the migration is likely to be minimal. Another advantage of this method is that the boundary migration can be studied at such a high temperature (or low undercooling) that ferrite precipitation is suppressed due to nucleation barrier. In Fe-C-Ni alloys the migration rate tends to follow LE-NP growth at lower temperatures, rather than growth under paraequilibrium [10].

Hutchinson et al [11] employed this method to measure the influence of Mo segregation at moving ferrite/austenite boundaries in an Fe-C-Mo alloy. They chose an alloy composition such that the uncertainty of the local interfacial condition, i.e. paraequilibrium or LE-NP, and the influence of carbide precipitation were eliminated. They observed a significant retardation of boundary migration and attributed it to the interfacial segregation (or accumulation) of Mo at ferrite/austenite boundaries.

In contrast to usual expectation a transition from LE-NP to paraequilibrium kinetics was observed in an Fe-C-Mn alloy as the temperature was raised in the (α+γ) two-phase region. This was discussed in relation to possible segregation of Mn to the moving interface [12].

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