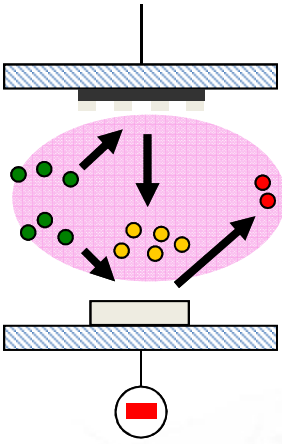
# WORKSHOP

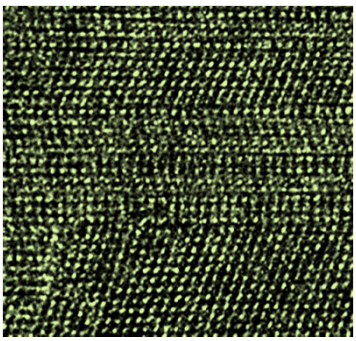
June 7th 2013

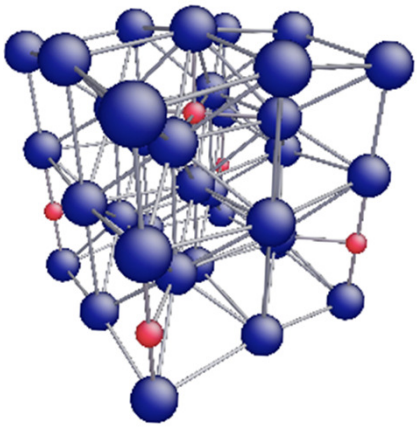
University of Ottawa, Desmarais Bld., Lounge 140-E
55 Laurier Avenue East, Ottawa, ON, K1N 6N5

## Designing Non-equilibrium and Non-Homogeneous Materials for Structural Applications:

## Fabrication - Characterization - Modelling








**Organized by:**

Arnaud Weck (University of Ottawa)
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# Scope of the Workshop

Conventional materials for structural applications have been designed so as to be close to equilibrium and relatively uniform at the micro, meso and macro-scales. This approach leads to materials whose structure-property relationships are well established and defines and envelope of available structure-property relationships. The use of novel processing strategies can allow for new opportunities to explore both non-equilibrium and non-homogeneous materials as routes to expand the range of available properties. This workshop will aim to discuss the potential of such materials from the perspective of their fabrication, characterization and modelling, particularly in metallic materials targeted towards structural applications. Challenges related to the fabrication of these materials, their stability, and the tools needed to extract and predict microstructural and mechanical property information will be addressed. The potential for designing non-equilibrium and/or non-homogeneous materials to open new property-structure relationships will be discussed.

# WORKSHOP PROGRAM

## *9:30 Coffee*

## *10:00 Introduction - Arnaud Weck*

## *10:15 Fabrication - Session Chair: Chad Sinclair*

1 *Elisa Cantergiani, Ben Lawrence, Chad Sinclair, Arnaud Weck*
Carbon gradient inside interstitial free steel

2 *Glenn Hibbard*
Designing composite cellular materials

3 *Vladimir V. Pankov*
Free-form fabrication of non-homogeneous structural materials and components using electron beam physical vapor deposition method

4 *Bertrand Jodoin*
Consolidation of Reactive Materials through Cold Spray

## *12:00 Lunch*

## *13:00 Modelling - Session Chair: Michel Perez*

5 *Ben Lawrence, Chad Sinclair, Michel Perez*
Stability and diffusion of carbon in highly carbon supersaturated BCC($alpha$) iron by atomistic simulation

6 *Nikolas Provatas, Nana Ofori-Opoku, Michael Greenwood*
Multi-scale modeling of microstructure in engineering alloys: from atomic to continuum methods

7 *Kuiying Chen*
Materials modeling for industry and defence :from fundamental issues to practical applications

8 *Kevin Boyle*
The influence of material property gradients on sheet metal formability

## *14:40 Coffee*

### *15:00 Characterization - Session Chair: Xavier Sauvage*



### *16:40 Conclusion - Arnaud Weck*

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# CARBON GRADIENT INSIDE INTERSTITIAL FREE STEEL

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**ABSTRACT**

Steel companies are interested in cheaper ways to strengthen interstitial free (IF) steel used in packaging applications. This is currently done using carburization where a carbon rich atmosphere is in contact with the sample at high temperature (above 800°C). The goal of the GraCos research project is the creation of carbon gradients inside IF steel in order to increase its strength using temperatures that are lower than the ones used during conventional carburizing treatments. Samples of interstitial free steel are first coated on both sides with an amorphous carbon-containing film using a physical vapour deposition (PVD) process. After deposition of the film, tensile coupons are annealed at different temperatures (lower than 730°C) to diffuse carbon from the film to the base material. Once annealed, tensile coupons were tested in tension and showed an increase in yield strength and ultimate tensile strength. A Lüder's plateau was also observed on the stress-strain curves whose characteristics depend on the amount of carbon diffusion in the sample. Scanning electron microscopy analyses of the fracture surface were performed to verify if the increase in strength is compromising the ductility of the graded materials. Further tests have been carried out on samples with different coating thicknesses which showed that carbon diffusion takes place only if the film thickness is at least 100 nm.

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# DESIGNING COMPOSITE CELLULAR MATERIALS

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**ABSTRACT**

Microtruss cellular materials can be used as structurally efficient cores in light-weight sandwich panels. Because of their internal strut connectivity, these structures are stretch-dominated, as opposed to the bending-dominated behaviour of conventional foams, enabling them to achieve greater weight-specific strengths and stiffnesses. For most practical microtruss strut slenderness ratios, inelastic buckling is often seen as the strength-limiting failure mechanism during compression and three-point bending. When inelastic buckling occurs, the load-bearing capacity is reduced and the governing strength equations depend on the tangent modulus of the struts material and the struts second moment of area. Since the surface area of microtruss architectures is high and the cross-sectional dimensions of microtruss struts are small, it is possible to take advantage of what would otherwise be considered a surface treatment in order to strengthen these cellular materials. This talk will outline the effectiveness of various surface treatments that can be used to strengthen the outer surface of the struts, discussing the relevant design parameters in creating these new composite cellular materials.

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# FREE-FORM FABRICATION OF NON-HOMOGENEOUS STRUCTURAL MATERIALS AND COMPONENTS USING ELECTRON BEAM PHYSICAL VAPOR DEPOSITION METHOD

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**ABSTRACT**

Aerospace and other industries may benefit from artificially engineered non-homogenous materials due to their unique physical properties. Recently, it was shown that these materials can be synthesized in the form of structural components by various free-form fabrication (F3) techniques. High-rate Electron Beam Physical Vapor Deposition (EBPVD) is a well known method for fabricating thick coatings. In our presentation, we demonstrate the possibility of using high-rate EBPVD as a method for F3 of shell-shaped aerospace components with non-homogenous structures. We review various technical approaches for fabricating compositionally graded and laminated materials by this particular method, present several practical examples, and discuss the associated technological challenges.

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# CONSOLIDATION OF REACTIVE MATERIALS THROUGH COLD SPRAY

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**ABSTRACT**

The present study focused on the use of cold gas dynamic spraying for manufacturing nano and micro-scale energetic materials with high reactivity, limited porosity, structural integrity and arbitrary shape. The experiments have focused on gasless inter-metallic system, such as Ni-Al, as well as thermite reaction with the Al-CuO system. To increase the gasless system reactivity, initial mechanical activation was achieved through interrupted ball milling. The consolidation of the materials used the cold gas dynamic spray technique, in which the particles are accelerated to high speeds and consolidated via plastic deformation upon impact, forming activated nano and micro-composites with close to zero porosity. This technique permits retaining the feedstock powder microstructure and minimizes reactions during the consolidation phase. Reactivity of mixtures has been investigated through flame propagation analysis on cold sprayed consolidated samples and compacted powder mixture. Deflagration tests showed the influence of porosity on the reactivity, which modifies the deflagration rate by up to two orders of magnitude, depending of the reaction type.

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# STABILITY AND DIFFUSION OF CARBON IN HIGHLY CARBON SUPERSATURATED BCC(T) IRON BY ATOMISTIC SIMULATION

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**ABSTRACT**

The diffusion of carbon in supersaturated BCC(T) iron is important in the tempering of martensite, the dissolution of carbon in heavily deformed steels, crystallization of high-carbon iron films, and in the long-range movement of carbon in the PVD coated steel sheet developed in the GraCoS project. Due to the extremely low equilibrium solubility of carbon in BCC iron it is difficult to directly measure the effect of carbon concentration on the carbon diffusivity in this system. Furthermore, various forms of ordering of carbon within these systems have been reported, and this ordering is thought to directly impact the diffusivity of carbon. Using monte carlo simulations, with a recently developed empirical iron-carbon potential, the stability of carbon ordering within BCC(T) iron has been determined over a range of temperatures and carbon contents. It has been shown that carbon is stable when ordering as stoichiometric $Fe_{16}C_2$, directionally ordered BCT iron, and fully disordered BCC iron, depending on temperature and carbon content. The transition between these phases has been determined in temperature and carbon content. Starting from these stable supersaturated phases we have evaluated carbon diffusivity by molecular dynamics over a wide range of temperatures. It was found that in disordered BCC iron, carbon diffusivity decreases slightly with increasing carbon content. Within ordered BCT iron a much larger decrease in carbon diffusivity was observed, which is accompanied by a systematic increase in the activation energy of diffusion. The dependence of measured activation energy on carbon content was found to be similar to predictions made Zener/Hillert based on the global strain energy of martensite.

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# MULTI-SCALE MODELING OF MICROSTRUCTURE IN ENGINEERING ALLOYS: FROM ATOMIC TO CONTINUUM METHODS

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**ABSTRACT**

We review recent mathematical and numerical innovations in quantitative multi-scale modelling of microstructure evolution in multi-component metal alloys. We begin with a brief review of the phase field methodology and the role it has played in predicting solidification microstructure evolution under industrially relevant casting conditions. Diving down to the atomic scale, we then review a new hybrid phase field/atomistic methodology, coined the phase field crystal (PFC) method. The PFC approach has emerged in recent years as an efficient yet fundamental alternative to molecular dynamics for incorporating atomic-scale effects on diffusional times scales that govern most phase transformation. These effects include, elasticity, dislocation interaction and flow and polycrystalline boundaries. We present the latest developments of an N-component alloy PFC model capable of a robust range of structural transformations. We highlight applications of the model to grain growth under forced driving, solute clustering, defect stability, solute trapping and second phase formation. We conclude with a vision for connecting microstructure models to meso-scale phase field and sharp-interface engineering models.

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# MATERIALS MODELING FOR INDUSTRY AND DEFENCE: FROM FUNDAMENTAL ISSUES TO PRACTICAL APPLICATIONS

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**ABSTRACT**

Research activities on multiple-scale materials modeling will be briefly summarized. Particular interest, however, will be given on modeling high-temperature gas turbine protective coatings. The sequential coupling methods were developed and implemented in each individual modeling scenarios. Three technical topics that relate to fundamental issues and practical applications will be presented briefly in this workshop: (1). Adhesive behavior of NiAl/$Al_2O_3$ interface in thermal barrier coatings was studied using the newly developed dislocation-based fracture toughness model at micromechanics level hierarchically linked to first-principles density functional theory (DFT) calculations. The effect of impurity sulphur, reactive elements (RE) and Platinum on the interface was evaluated in terms of electronic structures. In addition, Pt on sulphurs diffusivity in $\beta$-NiAl was also examined to investigate Pts mitigation of sulphurs detrimental effect. (2). Multilayer thin-film thermocouple sensors fabricated directly on the surface of gas turbine engine components have been used by major aerospace OEMs for real-time temperature monitoring of these components. Experimentally, it was revealed that Pt/$Al_2O_3$ and PtRh/$Al_2O_3$ interfaces in these multilayer thermal couple sensors represent weak structural points affecting durability and long term stability of the sensors. DFT calculations combined with fracture mechanics were applied to identify possible mechanisms causing interface degradation by examining effects of impurity doping, moisture and point defects such as vacancy and microvoids. (3). Erosion, oxidation, and more significantly, their interplays at elevated temperatures are the major degradation modes that could lead to failure of gas turbine components. To understand such degradation, a physics-based erosion model that incorporates parabolic oxide growth formulation was applied to evaluate high-temperature erosion-oxidation behavior of oxidation resistant coatings. The erosion- oxidation degradation depends on temperature, impacting particle velocity, incident angle, size and flux rate. The synergistic effect of these parameters on coating degradation was also analyzed. Based on the identified erosion-oxidation regimes, an attempt was made to construct a material selection map where the materials properties could be optimized to reduce the erosion degradation for oxidation resistant coatings.

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# THE INFLUENCE OF MATERIAL PROPERTY GRADIENTS ON SHEET METAL FORMABILITY

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**ABSTRACT**

TBA

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# CRYSTALLIZATION BEHAVIOUR OF SPUTTERED AMORPHOUS $FE_{1-X}C_X$

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**ABSTRACT**

Amorphous $Fe_{1-x}C_x$ alloys have been obtained at room temperature, by reactive magnetron sputtering, in a wide C content range ($0<x<0.4$). Formation of such highly supersaturated iron films remains poorly understood and their crystallization often leads to the formation of new metastable phases like unconventional carbides (in comparison to the reported carbides). X-ray diffraction, mssbauer spectroscopy, transmission electron microscopy (TEM) and atom probe tomography (APT) have been used to study their sputtered form and their crystallization behaviour upon heating. The purpose of this first part of the study is to identify the crystallization temperatures and the products of thermal decomposition which remain strongly dependent of the C level initially present in amorphous $Fe_{1-x}C_x$ films. By isothermal ageing near the crystallization temperature, a single-stage or a two-stage decomposition process occurs, depending on the C concentration of the as-sputtered amorphous alloys. The appearance of complex and variable set of co-existing metastable crystallization products, such as solvent-rich precipitate nanoparticules enclosed in a highly-faulted and twinning solute-rich structure is reported. The second part of this work was devoted to the deposition of thin layers of amorphous $Fe_{1-x}C_x$ on interstitial-free steel sheets, to act as C reservoirs, and to produce compositionally graded bulk microstructures during low-temperature diffusion annealing. C diffusion out of the film into the ferritic sheet has been monitored and microstructural changes of the film and substrate have been studied. High-resolution and analytical TEM was performed to characterize the gradient of microstructure from the surface to the bulk (phases identification and distribution) and revealed the existence of an O-rich layer at the film/substrate interface. APT analysis have been attempted to provide 3D imaging and chemical composition measurements at the atomic scale (distribution of the C atoms, composition of carbides, morphology, size, spatial distribution, volume fraction). Of particular interest in this more complex system is the role of the interface on the crystallization process.

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# QUENCH NANO-VOIDS AS A MODEL SYSTEM FOR VOID NUCLEATION PROBLEMS

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**ABSTRACT**

The equilibrium temperature dependence of the vacancy concentration in aluminium is well described by the work of Simmons and Balluffi [1]. Under special conditions rapid quenching from higher temperatures can stabilize a non-equilibrium concentration of mono- and di-vacancies, loops, or three-dimensional nano-void structures [2]. This work presents results from the thermal quenching of 99.988 and 99.995 at.% aluminium and the detection of nano-voids by synchrotron small angle x-ray scattering (SAXS). Absolute intensity calibration using a glassy carbon standard is used to extract the weak SAXS signature from the nanovoids. SAXS analysis methods, including Guinier, Porod and Indirect Transform, are used to obtain values for the void size, number distribution and volume fraction, as well as measures of the void-metal matrix interface structure in quenched aluminum samples. The fraction of nano-voids is consistently less than expected from the available vacancy concentration at the quench (originating) temperature, and indicates a non-equlibrium structure. The experiments have identified a residual impurity effect on nanovoid formation, and have been used to characterize trends in nano-void size, number distribution, and interface structure as a function of aging time at elevated temperatures (artificial aging). This level of information will be useful in developing phenomenological models of void nucleation and growth during deformation capable of linking atomic scale phenomena to macroscopic material properties. As an example, quench voids were created in an Al alloy, which was then deformed in tension at 195K. Measurement of the thermally activated portion of the flow stress show that nano-voids act as very strong obstacles to dislocation motion. After deformation, nano-voids were observed in the necked region by both SAXS and TEM to be larger than the as-quenched state, indicating that they also may act as sinks for deformation vacancies.

[1] R.O. Simmons and R.W. Balluffi, Phys. Rev., 117 (1960) p.52.

[2] M. Kiritani, J. Phys. Soc. Japan, 19 (1964) p.618.

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# NITRIDE PRECIPITATION IN COMPOSITIONALLY HETEROGENEOUS ALLOYS : A NON CONVENTIONAL PHASE TRANSFORMATION PATH

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**ABSTRACT**

The attractive properties of microalloyed steels combined with the presence of nitride-forming elements make them excellent candidate materials for nitriding applications in the aeronautic and automotive industries. During nitriding, nitrogen atoms can diffuse from surface to the bulk and interact with iron and/or alloying elements to form very fine nitride precipitates. As a consequence, precipitation occurs in compositionally heterogeneous alloys and a huge driving force for nitride precipitation is continuously available. In such a situation, the precipitation states are strongly influenced and differ radically from classical precipitation in a single phase where the driving force for precipitation is consumed. In particular, coarsening is strongly delayed, some non-equilibrium phenomena can be observed and the strain field around particles play a key role in the microstructural evolution. In this paper, the atypical and non-intuitive behaviors are discussed in order to improve our understanding about precipitation in compositionally heterogeneous ferrous alloys.

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# NEUTRON SCATTERING METHODS FOR MATERIALS CHARACTERIZATION

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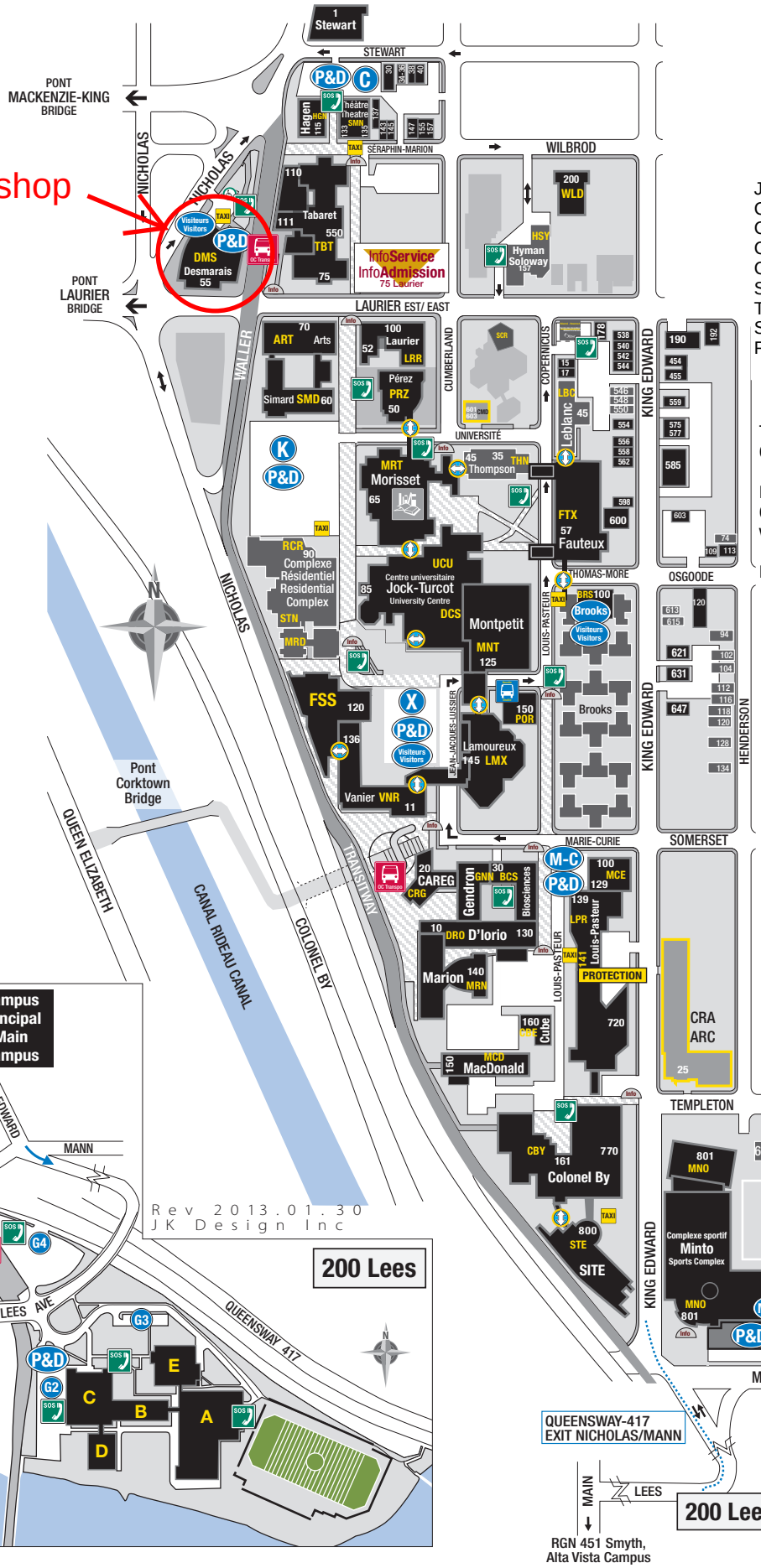
**ABSTRACT**

The mechanical properties of steels depend on the distribution and scale of precipitating phases, on the grain orientation distribution (texture), on the distribution and scale of flaws, and on the presence and distribution of residual stresses. Neutron scattering methods can provide quantitative data on the crystal structures and volume fractions of phases that form during thermomechanical treatments, on the kinetics of solid state reactions, on the distribution of grain orientations, and on the stresses that develop during processing. Due to their high penetrating power, neutrons can pass through the walls of specialized environment chambers (furnaces, corrosion cells, controlled-humidity cells) and thus are routinely used to study materials under processing or field conditions (load, temperature, controlled atmosphere). They can also be used to map residual stress fields in bulk materials. In this presentation, we discuss several examples of neutron scattering studies, including bulk and near-surface residual strain mapping, in-situ loading experiments, texture analysis, and powder diffraction.

# List of Authors

# WORKSHOP
# Designing Non-equilibrium and Non-Homogeneous Materials for Structural Applications

## Main Campus Map




## Where to eat?

Jazzy Restaurant - University Centre (UCU) - Level 1
Cafe Ecolo - Lamoureux Hall (LMX) - Level 1
Cafe Esculape - Roger Guindon (RGN)
Cafe Lees - Lees - Level 0
Cafe Plus - Tabaret Hall (TBT) - Level 0
Starbucks Coffee - Desmarais Hall (DMS) - Main Level
Tim Hortons - SITE Building - Level 1
Second Cup - Morisset Hall (MRT) - Level 1
Première Moisson - Faculty of Social Sciences (FSS) - Level 0

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