



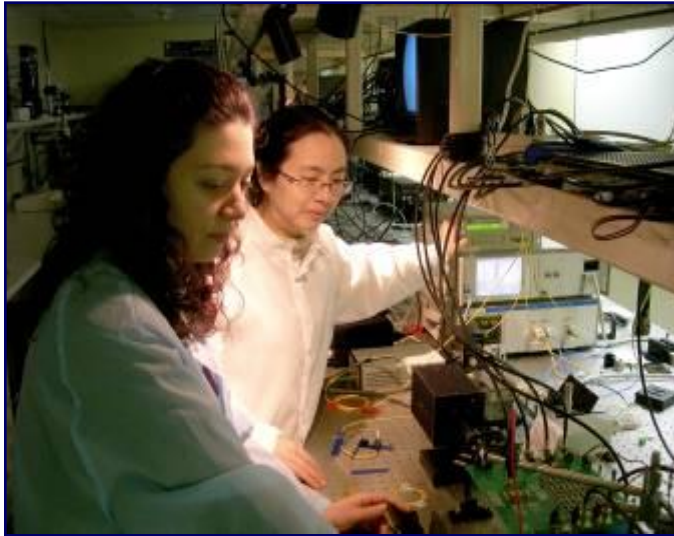
Computational materials modeling:

Fast-tracking materials design

Jun Song



- Associated with
 - **8 Nobel laureates**
 - **2 Canadian prime ministers**
 - **128 Rhodes Scholars**
- **Ranked 17th** in the *QS World Universities ranking*
- Named Canada's **top medical-doctoral** university in *Maclean's* magazine's 2011 University Rankings issue
- Students have the **high average** entering grades of any Canadian university at 88.9%.
- International students comprise 19% of McGill's student body, making it the **most diverse in Canada**.
- **Graduate students** make up 22% of McGill's 35,531 students, the highest proportion among Canada's top ten research universities.



Over 1000 Graduate Students

Photonic Systems Group

Departments

- Chemical Engineering
- Civil Engineering
- Electrical & Computer Engineering
- Mechanical Engineering
- Mining & Materials Engineering
- Bioengineering (*launched May 2012*)

Schools

- Architecture
- Urban Planning

Institutes

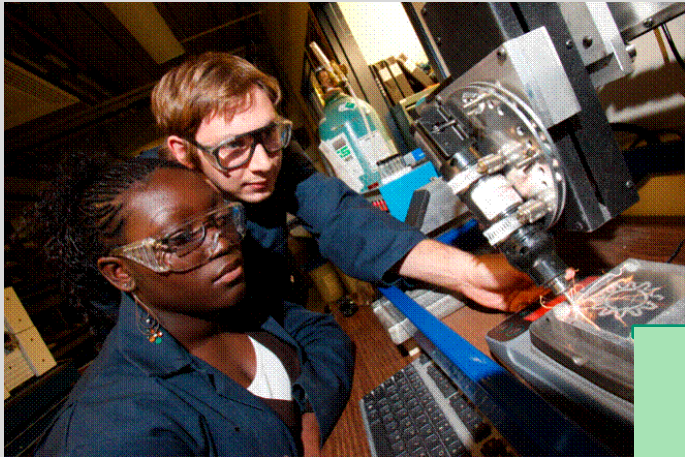
- McGill Institute for Advanced Materials
- McGill Institute for Aerospace Engr.
- Institute for Sustainability in Engr. & Design

■ WE ARE COMMITTED TO

- Producing self-reliant engineers who will become the leaders of tomorrow
- Defining the path of future discovery in engr. and technological research
- Making innovative, socially responsible contributions to the engr. community and society at large



Strategic research areas



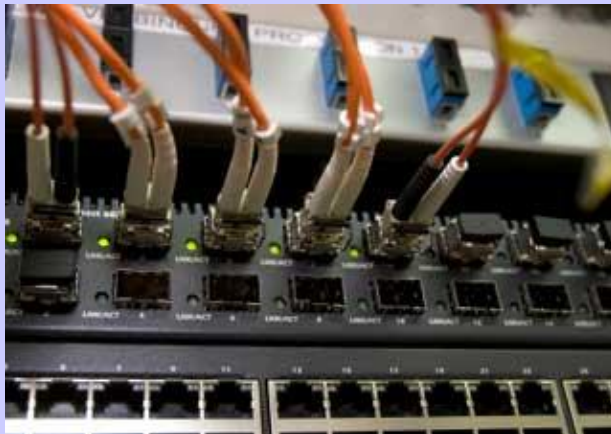
Advanced materials and nanotechnology



Aerospace Engineering



Bioengineering



Broadband Communications



Engineering and Design for Sustainability



Prof. Stephen Yue, Department chair
Director of McGill Institute for Aerospace Engr.

Materials Engineering

- In conjunction with Mining Engineering
- The **oldest** Materials Engineering department in Canada

Traditional strength in materials processing

Classical Metallurgy: one of the very few in North America



Undergraduate Program

- International reputation in Materials Engineering, particularly in *materials processing*
- **Laboratory 'intensive'** education
- Materials **Co-op program** (1yr industrial experience)
 - ❖ *Mandatory, integrated into curriculum, allows students to acquire valuable work experience through 3 semesters of industrial training (6 credits)*
 - ❖ *The program design includes one 4-month (January - April) and one 8-month (May - December) work term in industrial field work.*

Graduate Program

- 100 graduate students
- Graduate programs leading to M.Eng., M.Sc. and Ph.D. research





Research in Materials Engineering:

- Mineral Processing
- Hydrometallurgy and Pyrometallurgy
- Metal Processing and Process Engineering
- Texture and Microstructure
- Electron Microscopy
- Automotive and Aerospace Materials
- Thermodynamic and materials Modelling
- Nanomaterials
- Biomaterials



Relevance to Today's Research and Education

- Increasing capacity of computational modeling
 - Cost and time efficient
 - Complement experimental approaches
- *Necessity in curriculum***

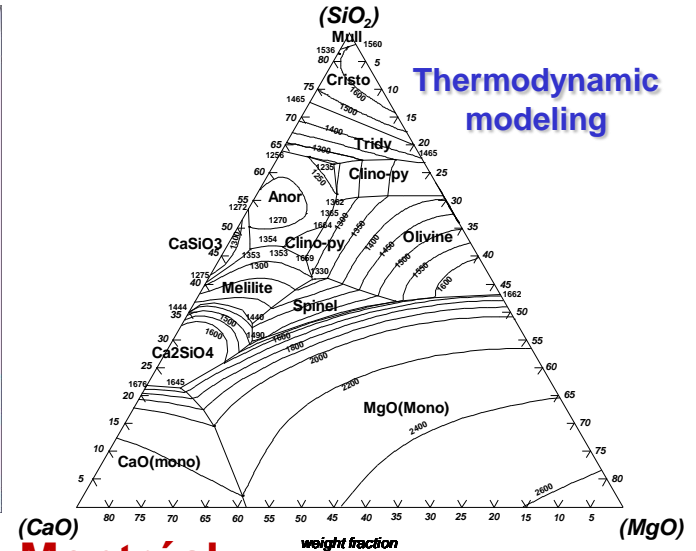


Computational Expertise in Materials Engr. at McGill

- Computational thermodynamic modeling – Prof. In-Ho Jung
- Electronic Materials Modeling (DFT) – Prof. Kirk Bevan
- Atomistics based multi-scale modeling – Prof. Jun Song

Current courses with computational components

- Undergraduate level
 - *Mathematical Applications*
- Graduate level
 - *Computational Thermodynamics*



In-Ho Jung, PhD (2003) École Polytechnique de Montréal
Assistant Professor, Hatch Faculty Fellow

Close collaboration with industry for process optimization and new materials design

□ Thermodynamic modeling

- Oxides (ferrous/non-ferrous extractive); light alloys (Mg, Al);
- Recycling of RE magnet

□ Phase diagram measurement

□ Process simulations

□ Development of FactSage software



Assistant Professor

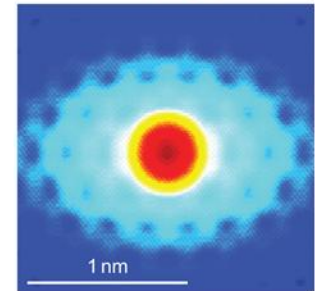
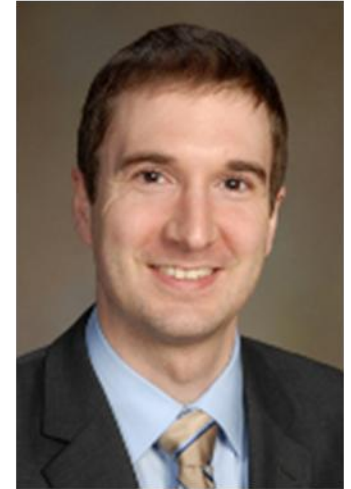
- Division of Materials Engineering,
Dept. Mining and Materials Engineering,
McGill University

Education

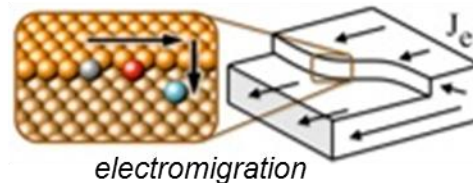
- Ph.D. 2008, EE, Purdue Univ.
- Visiting Research Scientist, 2008-2011, ORNL

Research Interests

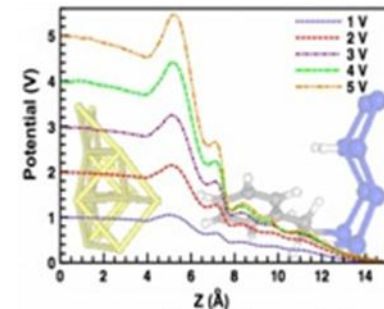
- Electronic device modeling: operation and reliability
- Electronic materials modeling
- Surface chemistry
- Solid state electrochemistry



graphene oxidation



electromigration



negative differential
resistance¹¹



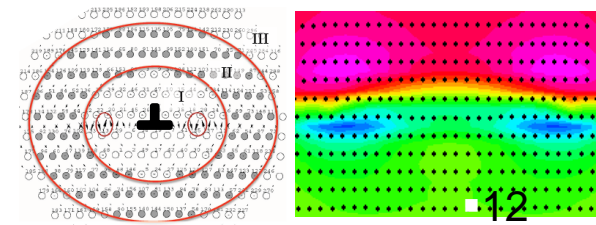
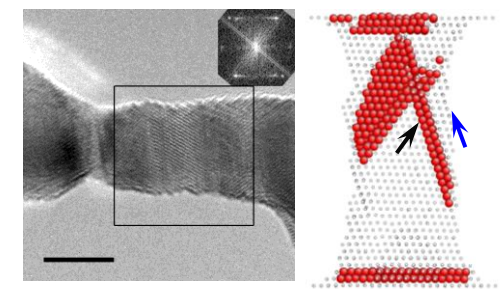
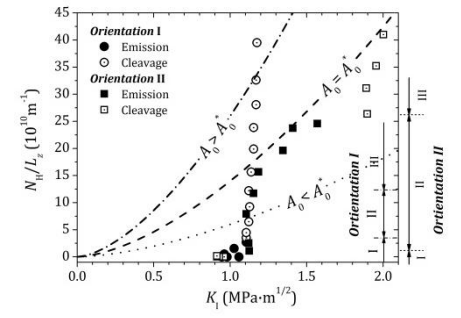
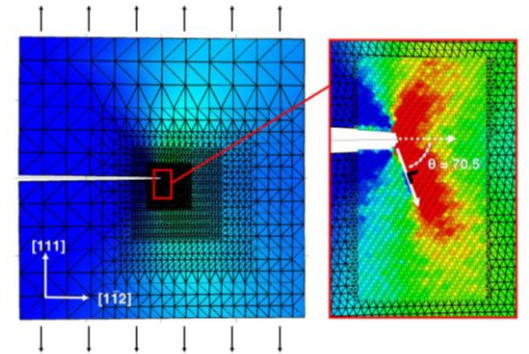
Atomistics based Multi-scale Modeling



Assistant Professor at McGill since 2011
PhD (2008) Princeton University
Post-doc (2008-11) Brown University

Research interests

- Multi-scale modeling of embrittlement in metals
- Nanoscale adhesion/contact mechanics
- Dynamics and mechanics of dislocations
- Strengthening and failure mechanisms in metals & alloys





New undergraduate course

■ Title: *Computational materials modeling*

- Starting on fall 2012
- In the process of being integrated as a **core course** in undergraduate curriculum (expected on fall 2013)

■ Objective*

- Convey the fundamental methods and concepts applicable to materials modeling and computational materials design
- Help students be familiar with various simulation tools and “*bottom-up*” computational design approach

*The course is intended for materials engineering students with no background in numerical methods.



New undergraduate course

■ Syllabus

- ***Introduction (3 weeks)***
 - Basics of quantum mechanics and solid-state physics
 - Bonding and structure in materials
 - Concepts of different modeling techniques in materials engineering and examples of applications
- ***Density functional theory (4 weeks)***
- ***Midterm review + exam (1 week)***



New undergraduate course

■ Syllabus (continued)

- *Molecular dynamics (4 weeks)*
- *Brief intro to phase field method (1-2 weeks)*
- *Computational thermodynamics (2 weeks)*
- *Term project (2 weeks)*

■ Notes

- Minimized coding/programming requirements
- Implement small simulation modules
- Projects
 - individual projects + term project



High-level courses for senior UG and graduates

■ Existed course

Computational Thermodynamics by In-Ho Jung

■ Courses coming soon

Computer simulations of defects in solids by Jun Song

Density functional theory and electronic structure by Kirk Bevan

Other relevant courses

Numerical methods in materials modeling (expected 2013)



Questions?