Understanding Atomic Scale Structure in Four Dimensions to Design and Control Corrosion Resistant Alloys

Location, University of Virginia, Department of Materials Science and Engineering

Thursday, June 30, 2016, 8:00 AM to 5:15 PM (EDT)
Mechanical Engineering Building, Room 205

Friday, July 1, 2016, 8:00 AM to 12:20 PM (EDT)
Mechanical Engineering Building, Room 205

PROGRAM

Thursday, June 30th, Mechanical Engineering Building, Room 205

8:00 Registration

8:45 Overview of MURI Program, L. D. Marks, Northwestern University

9:15 Oxidation resistant Mo-Si-B and Ni-Cr-Al Alloys-Phase Structures and Evolution, J. Perepezko, University of Wisconsin-Madison

10:00 Exploring the Electrochemical Passivation of Ni-Cr Compared to Ni-Cr-Mo Alloys: Interfaces between Corrosion Science, Surface Science and First Principles Based Modelling, J. Scully, University of Virginia

10:45 Coffee

11:00 Towards an Integrated Multiscale Model of Oxidation, P. W. Voorhees, Northwestern University

11:30 Imaging Pre-Transient Oxidation L. D. Marks, Northwestern University

12:00 Lunch in Wilsdorf café

1:00 Accurate Thermodynamics and Electrochemistry from First Principles, J. M. Rondinelli, Northwestern University

1:40 Nanoscale Modeling of Ni-Cr-Al and Mo-Si Oxidation and Interfacial Properties, H. Heinz, University of Colorado, Boulder
2:20  Investigating the Early Stages of Corrosion with Scanning Probe Microscopy and Spectroscopy, P. Reinke, University of Virginia

3:00  Coffee & Poster Session in Wilsdorf Hall atrium & café

5:00  Adjourn

6:00  Dinner at Vivace Restaurant and Lounge, 2244 Ivy Road

Friday, July 1st, Mechanical Engineering Building, Room 205

8:00  Coffee and Breakfast

8:30  Transient Oxidation, J. Perepezko, University of Wisconsin-Madison

9:10  3D Characterization of Oxidized Mo-Si-B, Ni-Cr and Ni-Cr-Mo Systems with Elemental Specificity, J. Miao, UCLA

9:50  Homogeneity and Inhomogeneity in Pre-Transient Oxidation, L. D. Marks, Northwestern University

10:30  Coffee Break

10:45  Mesoscale Modeling of Oxide Growth, P. W. Voorhees, Northwestern University

11:25  Revisiting the Passivation of Ni-Cr and Ni-Cr-Mo Alloys – New Understandings Facilitated by Combined Operando Spectro-Electrochemistry, Atomic Scale Measurements and Computational Modeling J. Scully, University of Virginia

12:05  Summary, L. D. Marks, Northwestern University

12:20  Adjourn

Posters

Tribocorrosion of 2507 Super Duplex Stainless Steel
J. Michael Shockley, Derek Horton, and Kathy Wahl
Chemistry Division, Naval Research Laboratory

3D Tomographic Imaging of the Oxidized A15 Phase in the Mo-Si-B System with Elemental Specificity
J, Zhou
Early and Transient Oxidation Stages of Cu and Cu alloys
J. Wang
University of Pittsburgh

Oxidation of MoSi$_2$ observed at the Nanoscale
C. Volders and P. Reinke
University of Virginia

Atomic and Mesoscale Insights into the Oxidation of NiCr and NiCrMo Alloys – A Scanning Tunneling Microscopy & Spectroscopy Study
G. Ramalingam, E. Monazami and P. Reinke
University of Virginia

Predicting and Controlling the Role of Minor Elements in the Passivation and Local Dissolution of Ni-Cr-based Alloys
K. Lutton, K. Gusieva and J. R. Scully
University of Virginia

Connection between Atomic Scale Characterization and Electrochemical Behavior During Passivation of Single Crystals on Ni-Cr and Ni-Cr-Mo Alloys
K. Gusieva and J. R. Scully
University of Virginia

Experimental Investigation of the Nickel Pourbaix Diagram through Electrochemical and Spectroscopic Techniques
M. Hutchison, R. J. Santucci and J. R. Scully
University of Virginia

The Effect of Crystallographic Orientation on the Corrosion of Commercially Pure Mg
L. G. Bland, K. Gusieva and J. R. Scully
University of Virginia

A Phase Field Model for Thin Film Oxide Growth
Q. Sherman, P. Reinke, L.D. Marks, J.M. Rondinelli and P.W. Voorhees
Northwestern University and University of Virginia

The Growth of Oxide Islands During Oxidation
R. Ramanathan, J.H. Perepezo, P. Reinke and P.W. Voorhees
Northwestern University, University of Wisconsin-Madison and University of Virginia

Accurate and Efficient First-Principles Calculations of the Thermodynamics and Electrochemistry of Solids
L-F Huang and J. M. Rondinelli
Northwestern University

Energetics of Ni-Al Intermetallic Alloys Point Defects and Strained NiO Vacancies
E. Tennessen and J. M. Rondinelli
Northwestern University

Incommensurate Structures in A15 Mo3Si
Northwestern University and University of Wisconsin-Madison

Cabrera-Mott Oxidation: Interfaces, Chemistry and More
X. Yu, L. Huang, J. M. Rondinelli and L. D. Marks
Northwestern University

Sample Design for Early Stage Oxidation Experiments
A. Gulec, X. Yu and L. D. Marks
Northwestern University

Evolution of Oxides with Time and Thickness in MoSiB
Northwestern University and University of Wisconsin-Madison

Imaging the Development of Aqueous Corrosion
X. Yu, A. Gulec, J. Scully and L. D. Marks
Northwestern University and University of Virginia

Oxidation/reduction behavior of the metal-oxide in the Environmental TEM
A. Yoon and J.M. Zuo
University of Illinois at Urbana-Champaign

Reactive Modeling of Mo3Si Oxidation and Resulting Silica Morphology
C. Dharmawardhana, J. Perepezko, J. Miao, and H Heinz
University of Colorado, University of Wisconsin, and University of Virginia

MoSi2 Oxidation: Mechanism and Silica Growth
C. Dharmawardhana, H. Heinz and P. Reinke
University of Colorado and University of Virginia

Surface Diffusion of Oxygen Species on Ni, Al, and NiCr Alloy Surfaces
K. Kanhaiya, N. Mehio, H. Heinz, R. Ramanathan, Q. Sherman and P. W. Voorhees
University of Colorado and Northwestern University

Electronically Refined Force Fields for BCC and HCP Metals
C. Dharmawardhana, S. Deshmukh and H. Heinz
University of Colorado

*Electronegativity Concepts and Atomic Charge Differences in Alloys to Understand Alloy Formation and Defect Energies*
N. Saikia, E. Tennessen, J. M. Rondinelli and H. Heinz
University of Colorado and Northwestern University