



Materials Simulation & Engineering

Winter School

“ Modelling of Corrosion ”

INSTN CEA Saclay, December 10-14, 2012

- An introduction to Corrosion Mechanisms
 - Overview on Phase Diagrams
 - Atomistic Modelling of Diffusion
 - Molecular Modelling of Corrosion
 - Atomistic Simulation of Oxidation
 - DFT modeling of oxide surfaces
 - Modelling of Corrosion by Cellular Automata
 - Point Defect Model
 - DPCM Model
 - Modelling of a Passive Layer Growth

 - Passive Nanostructure and Localized Corrosion
 - Localized Corrosion
 - Stress Corrosion Cracking
 - Modelling of Oxides Layers
 - Atmospheric Corrosion
 - Multiscale Modelling of Materials
 - Multiscale Contribution on Corrosion Prediction
- P. MARCUS**, ENSCP Chime ParisTech
B. SUNDMAN, KTH, Sweden and CEA-INSTN, Saclay
J. D. GALE, Curtin University, Australia
C. TAYLOR, Los Alamos National Laboratory, USA
B. DIAWARA, ENSCP Chime ParisTech
B. DIAWARA & D.COSTA, ENSCP Chime ParisTech
D. DI CAPRIO, ENSCP Chime ParisTech
D. MACDONALD & M.URQUIDI, Penn State University, USA
C. BATAILLON, CEA-DEN, Saclay
K. LEISTNER & A. SEYEUX, ENSCP Chime ParisTech
C. TOULEMONDE, EDF
P. MARCUS, ENSCP Chime ParisTech
R. OLTRA, Université de Bourgogne
T. COUVANT, EDF
C. DESGRANGES, CEA-DEN, Saclay
S. PERRIN, CEA-DEN, Saclay
J.D. GALE, Curtin University, Australia
D. FERON, CEA-DEN, Saclay

Computer Sessions with Practical Training using relevant softwares:

- Phase Diagrams - Thermo-Calc
 - DFT and KMC modeling of oxidation
 - Localized Corrosion
 - Cellular Automata
 - EKINOX and DPCM Models.
 - Point Defect Model
- B. SUNDMAN, C. TOFFOLON & C. GUENEAU** CEA, Saclay
B. DIAWARA & D.COSTA, ENSCP Chime ParisTech
R. OLTRA Université de Bourgogne & **B.MALKI**, PHELMA
D. DI CAPRIO, ENSCP Chime ParisTech
C. DESGRANGES & C. BATAILLON, CEA-DEN, Saclay
D. MACDONALD & M. URQUIDI, Penn State University, USA

Organizers:

Damien FERON, CEA - DEN, Saclay, damien.feron@cea.fr
Constantin MEIS, CEA - INSTN, Saclay, constantin.meis@cea.fr
Philippe MARCUS, Chimie ParisTech philippe.marcus@chimie-paristech.fr
Julian GALE, Curtin University, Australia julian@ivec.org

Registration deadline: November 15, 2012

Registration and Information:

Martine MURY, martine.mury@cea.fr
Phone: +33 | 69 08 89 09 Fax: +33 | 69 08 57 53

www-instn.cea.fr (upcoming events / 2012)



Event n°354