

Materials Modeling **AIX-EN-PROVENCE** and Simulation for Nuclear Fuels

September 26-28, 2011

Workshop program

F★BRIDGE

Basic Research for Innovative Fuel
Design for GEN IV systems



energie atomique • energies alternatives

IRSN

INSTITUT
DE RADIOPROTECTION
ET DE SÛRETÉ NUCLÉAIRE

Monday, September 26th, 2011

8.30 am: Registration

9.00 am: Welcome

M. Mazière, CEA, Nuclear Energy Division, Director of the Cadarache Center
M. Schwarz, IRSN, Scientific Director

9.15 am: Keynote introduction to Workshop

K. Pasamehmetoglu: INL, DOE, National Technical Director, Advanced Fuel Cycle Initiative

September 26th 9.30 am – 1.00 pm: Session 1 – Electronic structure methods

9.30 am O1: Charge states of point defects and defect clusters in uranium oxide
Jean-Paul Crocombette, CEA, DEN, Centre de Saclay, France

10.00 am O2: Simulations of U and Xe transport in $UO_{2\pm x}$: From density functional theory to continuum
David Andersson, Blas Uberuaga, Pankaj Nerikar, Michael Tonks, Paul Millet, Chris Stanek, Los Alamos National Laboratory, USA

10.30 am Break

11.00 am O3: First principles study on interplay of defect cluster and stability of xenon in uranium dioxide
Ying Chen, Hua Y. Geng, Yasunori Kaneta, Motoyasu Kinoshita, Shuichi Iwata, Tokohu Univ., Japan

11.30 am O4: UO_2 surface stability by means of DFT+U calculations: towards overstoichiometry
François Bottin, Grégory Geneste, Gérald Jomard, CEA, DAM, France

12.00 am O5: First-Principles DFT+U study of Uranium and Plutonium carbides, Michel Freyss, Emerson Vathonne, Boris Dorado, Marjorie Bertolus, CEA, DEN, Centre de Cadarache, France

12.30 pm O6: First principles study of point defect and Xe behavior in alpha-Uranium-Zirconium Alloys
Brian D. Wirth, Gui-Yang Huang, University of Tennessee, USA

1.00 pm Lunch

September 26th 2.00 – 5.00 pm: Session 2 – Empirical potential studies

2.00 pm O7: Bulk, surfaces and defect properties of UO_2 using a Tight-Binding Variable-Charge model
Gaël Sattonnay, Robert Tétot, Université Paris Sud, France

2.30 pm O8: Classical molecular dynamics study of primary defect production in uranium dioxide under irradiation, Guillaume Martin, Catherine Sabathier, Philippe Garcia, Laurent Van Brutzel, Serge Maillard, CEA, DEN, Centre de Cadarache, France

3.00 pm O9: Metadynamics simulations of diffusion processes in uranium dioxide
Matthias Krack, Paul Scherrer Institut, Switzerland

3.30 pm Break

4.00 pm O10: The assessment of the damaged UO_2 thermal conductivity by Molecular Dynamics
Sergii Nichenko, Dragos Staicu, JRC-ITU, European Commission

4.30 pm O11: Investigation of intragranular bubble impact on thermal conductivity
Mehdi Colbert, Fabienne Ribeiro, Roland J.M. Pellenq, Guy Tréglia, IRSN Cadarache, France

5.00 pm Discussion on sessions 1 and 2

September 26th 5.30 – 7.00 pm: Poster Session 1 and Welcome Aperitif

Tuesday, September 27th, 2011

September 27th 9.00 am – 10.30 pm: Session 3 – Experimental studies

- 9.00 am O12:** Positron Annihilation characteristics of vacancy defects induced in UO₂ by irradiation
Marie-France Barthe, Tayeb Belhabib, Stéphanie Leclerc, Laszlo Liskay, Hicham Labrim, Virginie Moineau, Pierre Desgardin, Gaëlle Carlot, Philippe Garcia, CNRS Orléans, France
- 9.30 am O13:** Experimental characterization and simulation of the melting of oxides and carbides
Dario Manara, Michael J. Welland, Robert Böhler, JRC-ITU, European Commission
- 10.00 am O14:** Separate effects testing of oxide fuels under the Fuel Cycle R&D program
Kenneth J. McClellan, Los Alamos National Laboratory, USA
- 10.30 am Break**

September 27th 11.00 am – 12.00 pm: Session 4 – Thermodynamics

- 11.00 am O15:** Modeling thermochemical behavior of oxide nuclear fuel with rare earth fission products
Theodore M. Besmann, Stewart L. Voit, Dongwon Shin, Evan P. Noon, Robert J. Austin, Oak Ridge National Laboratory, USA
- 11.30 am O16:** Survey of methods for modelling defects and composition variations in UO₂
Bo Sundman, CEA, DEN, Centre de Saclay, France

12.00 pm Discussion on sessions 3 and 4

12.30 pm Lunch

September 27th 1.30 – 5.30 pm: Visit of CEA Cadarache facilities

September 27th 5.30 – 7.00 pm: Poster Session 2

September 27th 7.30 pm: Workshop dinner “La Mado” in Aix en Provence

Wednesday, September 28th, 2011

September 28th 9.00 am – 12.00 pm: Session 5 – Mesoscale studies

- 9.00 am O17:** An improved model for evolution of oxygen potential in irradiated UO₂ fuel
Vladimir D. Ozrin, IBRAE/RAN, Russia
- 9.30 am O18:** Modelling the Fission Gas Bubble Distribution in UO₂
Richard Skorek, Serge Maillard, CEA, DEN, Centre de Cadarache, France
- 10.00 am O19:** Mesoscale Modeling of Fuel Restructuring
Rémi Dingreville, Tim J. Bartel, Sandia National Laboratories, USA
- 10.30 am Break**
- 11.00 am O20:** Microstructure Stability in Irradiated Fuels
Anter El-Azab, Florida State University, USA
- 11.30 am O21:** Two- and three-dimensional thermal analyses of uranium-molybdenum dispersion fuel microstructures
Jeffrey C. King, Brianna Rister, Gwendolyn Bahun, Pavel Medvedev, Colorado School of Mines, USA
- 12.00 pm Lunch**

September 28th 1.00 pm – 4.00 pm: Session 6 – Fuel performance codes

- 1.00 pm O22:** Assessment of COMSOL Multiphysics for the use of CANDU fuel bundle deformation modeling
John Stuart Bell, Brent J. Lewis, Royal Military College of Canada, Canada
- 1.30 pm O23:** Recent improvements of mechanical modelling in fuel performance code GERMINAL for SFR oxide fuel pins
Marc Lainet, CEA, DEN, Centre de Cadarache, France
- 2.00 pm O24:** 3-dimensional, high-resolution modeling of nuclear fuel performance: pellet clad interaction
Christopher R. Stanek, Derek Gaston, Jason Hales, Richard Martineau, Robert Montgomery, Yusef R. Rashid, Brian D. Wirth, Los Alamos National Laboratory, USA
- 2.30 pm Break**
- 3.00 pm O25:** Generalization of Mechanistic Code SFPR to Modelling UO₂ Fuel Rods Behaviour in Fast Reactors
Mikhail S. Veshchunov, Andrey V. Boldyrev, Vladimir D. Ozrin, Valery E. Shestak, Vladimir I. Tarasov, IBRAE/RAN, Russia
- 3.30 pm O26:** Heterogeneity of Nuclear Fuels
Marius Stan, Argonne National Laboratory, USA
- 4.00 pm O27:** An overview of the multi-scale modelling activities at ITU and their integration in the TRANSURANUS fuel performance code
Paul Van Uffelen, Michael J. Welland, Marco Klipfel, Valentino Di Marcello, Arndt Schubert, Jacques van de Laar, Giovanni Pastore, JRC-ITU, European Commission

4.30 pm Discussion on sessions 5 and 6 and conclusions of the meeting

September 28th 5.00 pm: End of workshop