

# Materials Models and Simulations for Nuclear Fuels

5<sup>th</sup> Workshop in Nice, France, 1-2 June 2006

## AGENDA AS OF MAY 5<sup>th</sup>, 2006

### Thursday June 1<sup>st</sup>

13.30 *Welcome and introduction*

#### **Session 1: Fundamental modelling of fuel properties**

13.45 J. Durinck, M. Freyss (CEA Cadarache): *Atomistic modelling of point defects formation and migration in uranium dioxide*

14.05 M. Freyss, J. Durinck, G. Carlot, C. Sabathier, P. Martin, P. Garcia, M. Ripert, C. Valot, (CEA Cadarache): *Modelling of the behaviour of rare gases in uranium dioxide: ab initio approach and separate effect experiments*

14.25. P. Blanpain (AREVA), M. Lippens (BN), H. Schut (RID), A.V. Federov (RID), K. Bakker (NRG) : *Helium solubility in UO<sub>2</sub> : the HARLEM project*

14.45 K. Govers (SCK•CEN), M. Verwerft (SCK•CEN), M. Hou (ULB), S. E. Lemehov (SCK•CEN): *Evaluation of interatomic potentials for the UO<sub>2</sub> system : molecular dynamics study of point defects and thermodynamic properties*

15.05 D. Terentyev, K. Govers, and S. E. Lemehov (SCK•CEN): *Molecular dynamic studies of oxygen migration mechanisms in fast reactor type uranium-plutonium oxides*

15.25 *Coffee break*

15.50 E. A. Kotomin (ITU), N. J. Ashley(IC), R.W.Grimes (IC), P.Van Uffelen (ITU), Yu. Mastrikov (UL), Yu. Zhukovskii (UL), V.V. Rondinella (ITU): *First-principles modeling of nitride nuclear fuels*

16.10 K. Kurosaki (OU), M. Uno (UO), S. Yamanaka (UO), K. Minato (JAEA Tokai-Mura): *Molecular dynamics studies and property measurements of actinide nitrides*

16.30 S. Phillpot (UF), T. Watanabe (UF), P. Shukla (UF), S. Sinnott (UF), J. Nino (UF), J. Tulenko (UF), R. Grimes (IC): *Thermal transport in nuclear fuels by atomic-level simulation*

16.50 D.Staicu (ITU), J.P. Hiernaut (ITU), T. Wiss (ITU), V.V. Rondinella (ITU), C. Ronchi (ITU), E. Yakub (OSEU): *Impact of irradiation on the thermophysical properties of oxide nuclear reactor fuels*

17.10 **Preliminary discussion about session 1**

18.00 *End of day 1*

### Friday June 2<sup>nd</sup>

- 8.30 M.H. Kaye, C. Morrison, J.D. Higgs, F. Akbari, B.J. Lewis and W.T. Thompson (RMC):  
*Thermodynamic model of the phase equilibrium in the U-O System containing fission products*
- 8.50 M. Osaka (JAEA Ibaraki), S. Miwa (JAEA Ibaraki), I. Sato (JAEA Ibaraki), K. Tanaka (JAEA Ibaraki), K. Kurosaki (JAEA Ibaraki), M. Uno (OU), S. Yamanaka (OU):  
*Modeling of the oxygen potential of americium-containing oxide fuels*
- 9.10 C. Guéneau (CEA Saclay), S. Gossé (CEA Saclay), S. Chatain (CEA Saclay), J.-C. Dumas (CEA Cadarache), B. Sundman (KTH), N. Dupin (Calcul Thermo), R. Konings (ITU), H. Noel (CNRS Rennes):  
*FUELBASE : a tool for thermodynamic modelling of advanced fuels. Examples of U-O-C and Pu-O systems*
- 9.30 **Final discussion about session 1**

10.00 *Coffee break*

**Session 2 : Integral fuel performance codes and their validation**

- 10.20 R.Dubourg. (IRSN, Cadarache):  
*Mechanistic modeling of fission gas behavior in UO<sub>2</sub> irradiated fuel by the MFPR code*  
C V.Ozrin (IBRAE):  
*Mechanistic modeling of behavior of chemically active FP elements in UO<sub>2</sub> irradiated fuel by the MFPR code*
- 10.40 M.S. Veshchunov (IBRAE):  
*Models for defect structure evolution in fuel rods of the MFPR and SVECHA mechanistic codes*
- 11.10 M.J. Welland, W.T. Thompson and B.J. Lewis (RMC):  
*Melting Behaviour Model for UO<sub>2+x</sub>*
- 11.30 K. Mikityuk, P. Petkevich, P. Coddington, R. Chawla (PSI):  
*FRED transient fuel rod model: brief description and adaptation for GCFR analysis*
- 11.50 V. Blanc, B. Michel, J.-M. Ricaud (CEA Cadarache):  
*HTR fuel behaviour modelling : Thermo-mechanical characterization of a Representative Volume Element for a random heterogeneous material*
- 12.10 R. Calabrese (ENEA), F. Vettriano (ENEA), T. Tverberg (HRP): *Inert Matrix Fuels Modelling: TRANSURANUS Analysis of the Halden IFA-652 First Irradiation Cycle*
- 12.30 *Lunch break*
- 14.00 **Discussion about session 2**

### **Session 3: collaborations and integration of activities**

- 14.30 M. Stan, J. C. Ramirez, P. Cristea (LANL): *Materials models and fuel performance simulations*
- 14.50 J. Rachid (ANATECH): *Architecture for generalized fuel modeling code for advanced fuel cycle*
- 15.10 P. Van Uffelen, E. Kotomin, A.Ciriello, V.V.Rondinella, D.Staicu, T. Wiss, R. Konings, J.Somers (ITU): *The multi-time-scale approach for MX fuels at ITU*
- 15.30 J. Killeen (IAEA) to be confirmed
- 16.00 *General discussion*
- 17.00 *End of the workshop*

## Poster session

C. Deo (LANL), M. Okuniewski (UIUC), M. Weber (WSU), F. Selim (WSU),  
K. Lynn (WSU), S. Srivilliputhur (LANL), S. Maloy (LANL), M. Baskes (LANL),  
M. James (LANL), J. Stubbins (UIUC):

*The effects of helium on irradiation damage in iron and ferritic steels*

J.C. Ramirez , M. Stan, and P. Cristea (LANL):

*Simulations of heat and oxygen diffusion in UO<sub>2</sub> nuclear fuel rods*

B Michel (CEA Cadarache):

*3D fuel cracking modelling in pellet cladding mechanical interaction*

N. Dupin (Calcul Thermo), C. Gueneau (CEA Cadarache), S. Chatain (CEA Cadarache):

*Thermodynamic assessments of Cr-U and Pu-Si systems*

S.J. White, M.H. Kaye, B.J. Lewis and W.T. Thompson (RMC):

*Neutron diffraction study of the U-Dy-O system*

F.Gupta (IRSN), A. Pasturel (CNRS Grenoble), G.Brillant (IRSN):

*Ab initio calculations of caesium incorporation energy in UO<sub>2</sub>*

M. Barrachin (IRSN), P.-Y. Chevalier, B. Cheynet, E. Fischer (THERMODATA/INPG/CNRS):  
*NUCLEA, a thermodynamic database for nuclear applications : validation, recent  
developments and applications*