

Materials Modelling and Simulation for Nuclear Fuels
Gatineau, QC – Oct. 3-4, 2017
Program (D1)

October 3, 2017

| | | |
|------|------|---------------------------|
| 8:00 | 8:30 | Registration |
| 8:30 | 9:00 | Welcome and Announcements |

Session A: Electronic Structure

Session Chair: TBD

| | | |
|-------|-------|--|
| 9:00 | 9:20 | Electronic structure calculations of structural, electronic properties and irradiation damage in the uranium-plutonium mixed oxide (U,Pu)O₂ I.C. Njifon (CEA), M. Freyss (CEA), R. Hayn (Aix-Marseille Université), M. Bertolus (CEA) |
| 9:20 | 9:40 | Diffusion of intrinsic and extrinsic defect in V₂C from density functional theory calculations B.J. Demaske (U. Florida), A. Chernatynskiy (U. Florida), S.R. Phillpot (U. Florida) |
| 9:40 | 10:00 | Xenon diffusion by vacancy clusters in UO₂ D. Andersson (LANL), C. Matthews (LANL), R. Perriot (LANL), M. Cooper (LANL), C. Stanek (LANL) |
| 10:00 | 10:20 | Discussion |
| 10:20 | 10:40 | Coffee Break |

Session B: Electronic and Atomic Structure

Session Chair: TBD

| | | |
|-------|-------|--|
| 10:40 | 11:00 | Advances in the modelling of U₃Si₂ - an accident tolerant fuel candidate S. Middleburgh (Westinghouse), A. Claisse (Westinghouse), P. Olsson (KTH), D.A. Lopes (KTH), D. Andersson (LANL), S. Mašková (Charles U.) |
| 11:00 | 11:20 | Kinetic properties of solute elements (Xe, Kr, C, O) in uranium nitride A. Claisse (Westinghouse), D.A. Lopes (KTH), T. Schuler (École des mines de Saint-Étienne), P. Olsson (KTH) |
| 11:20 | 11:40 | Atomistic simulation study of structure and phase transitions in pure uranium and U-Mo alloys S. Starikov (JIHTRAS), L. Kolotova (JIHTRAS), A. Kuksin (JIHTRAS), D. Smirnova (JIHTRAS), V. Tseplyaev (JIHTRAS) |
| 11:40 | 12:00 | Discussion |
| 12:00 | 13:30 | Lunch |

Session C: Atomic Structure Continued

Session Chair: TBD

| | | |
|-------|-------|--|
| 13:30 | 13:50 | Modelling isolated dislocations and dislocation substructures in deformed uranium dioxide single crystals A.V. Lunev (JIHTRAS), S.V. Starikov (JIHTRAS, MIPT), A.Y. Kuksin (JIHTRAS, MIPT) |
| 13:50 | 14:10 | Mechanical behaviour of UO₂ under irradiation: a molecular dynamics study L.V. Brutzel (CEA), A. Chartier (CEA) |
| 14:10 | 14:30 | Average structure and local configuration of excess oxygen in UO_{2+x} J. Wang (Louisiana State U.) |
| 14:30 | 14:50 | Discussion |
| 14:50 | 15:10 | Coffee Break |

Session D: Mesoscale

Session Chair: TBD

| | | |
|-------|-------|---|
| 15:10 | 15:30 | Utilization of phase-field simulation on UO₂/Zr interaction in temperature increasing conditions M. Kurata (JAEA), T. Ishikawa (Nagoya U.), N. Shirasu (JAEA), T. Koyama (Nagoya U.) |
| 15:30 | 15:50 | Integration of thermodynamic potentials into transport phenomena and phase-field models M.J. Welland (CNL), K. Birdee (CNL), S. Hibbins (CNL), M.H.A. Piro (CNL, UOIT), N. Wang (CNL) |
| 15:50 | 16:10 | Modelling grain boundary fission gas bubbles with a shell based phase-field model A.A. Prudil (CNL), E. Thomas (CNL, McMaster U.), M.J. Welland (CNL) |
| 16:10 | 16:30 | Discussion |
| 16:30 | 17:00 | Poster Flash Talk |
| 17:00 | 18:30 | Poster Session/Wine & Cheese |
| 18:30 | | Adjourn |

October 4, 2017

| | | |
|------|------|---------------|
| 8:30 | 9:00 | Registration |
| 9:00 | 9:15 | Announcements |

Session E: Mesoscale and Classical Thermodynamics

Session Chair: TBD

| | | |
|-------|-------|--|
| 9:15 | 9:35 | Current progress in the US on the development of microstructure based materials models for fuel performance codes M.R. Tonks (U. Florida), D. Andersson (LANL), C. Stanek (LANL), Y. Zhang (INL) |
| 9:35 | 9:55 | Morphological analysis and synthesis in nuclear materials science M. Glazoff (INL) |
| 9:55 | 10:15 | Thermodynamic modeling of the U-Fe-Si system E.E. Moore (U. South Carolina), S.C. Middleburgh (Westinghouse), T.M. Besmann (U. South Carolina) |
| 10:15 | 10:35 | Discussion |
| 10:35 | 10:55 | Coffee Break |

Session F: Classical Thermodynamics

Session Chair: TBD

| | | |
|-------|-------|---|
| 10:55 | 11:15 | Demonstration of the application of the TAF-ID (Thermodynamics Advanced Fuels – International Database) C. Guéneau (CEA), N. Dupin (Calcul Thermodynamique), T.M. Besmann (U. South Carolina), M. Kurata (JAEA), S. Gossé (CEA), J.C. Dumas (CEA), E. Corcoran (RMCC), M. Piro (UOIT), M.J. Welland (CNL), T. Ogata (CRIEPI), A.L. Smith (Delft U.), B.O. Lee (KAERI), M. Bankhead (NNL), P.E.A. Turchi (LLNL), R. Kennedy (INL), S. Massara (OECD/NEA) |
| 11:15 | 11:35 | Modeling phase equilibria and thermodynamics of U-Si and U-Si-N based nuclear fuel T.M. Besmann (U. South Carolina), E.E. Moore (U. South Carolina), M.R. Bogala (U. South Carolina), T.L. Wilson (U. South Carolina), S. Middleburgh (Westinghouse) |
| 11:35 | 11:55 | Uncertainty of thermodynamic data: humans and machines M. Stan (ANL) |
| 11:55 | 12:15 | Discussion |
| 12:15 | 13:45 | Lunch |

Session G: Classical Thermodynamics and Continuum Scale

Session Chair: TBD

| | | |
|-------|-------|---|
| 13:45 | 14:05 | Modelling the radiolytic corrosion of spent fuel inside a failed nuclear waste container Z. Qin (U. Western Ontario), N. Liu (U. Western Ontario), L. Wu (U. Western Ontario), Z. Zhu (U. Western Ontario), D.W. Shoesmith (U. Western Ontario) |
| 14:05 | 14:25 | Fission product release modelling for application of fuel-failure monitoring and detection - an overview B.J. Lewis (RMCC), P.K. Chan (RMCC), A. El-Jaby (RMCC), F.C. Iglesias (Kinectrics Inc.), A. Fitchett (Kinectrics Inc.) |
| 14:25 | 14:45 | Modelling microstructural effects on the fuel element behavior with the release V2 of the ALCYONE fuel performance code R. Masson (CEA), I. Ramière (CEA), S. Bernaud (CEA), P. Goldbronn (CEA), B. Michel (CEA) |
| 14:45 | 15:05 | Discussion |
| 15:05 | 15:25 | Coffee Break |

Session H: Continuum Scale

Session Chair: TBD

| | | |
|-------|-------|--|
| 15:25 | 15:45 | Modeling axial relocation of fragmented fuel during loss of coolant conditions using the BISON fuel performance code K.A. Gamble (INL) |
| 15:45 | 16:05 | MOX irradiations in BISON using a new fuel-to-sheath heat transfer model E.T. Rand (CNL), A.A. Prudil (CNL), W. Richmond (CNL), A. Williams (CNL) |
| 16:05 | 16:25 | Simulations of power ramps with ALCYONE including fission products chemistry and oxygen thermo-diffusion J. Sercombe (CEA), C. Riglet-Martial (CEA), P. Konarski (CEA), B. Baurens (EDF) |
| 16:25 | 16:45 | Discussion |
| 16:45 | 17:00 | Closing Remarks |
| 17:00 | | Adjourn |

October 5, 2017

Trip to Canadian Nuclear Laboratories

Poster Session

- P1 **Development of a tight-binding Ising model to describe Zircaloy cladding hydriding**
P. Eymeoud (IRSN), A. Dufresne (Marseille Université), G. Tréglia (Marseille Université),
F. Ribeiro (IRSN)
- P2 **Study of defects formation and diffusion in UO₂**
D. Smirnova (JIHTRAS), S. Starikov (JIHTRAS, MIPT), A. Kuksin (JIHTRAS, MIPT),
M. Korneva (JIHTRAS, MIPT)
- P3 **Theoretical study of xenon adsorption on UO₂ surfaces**
J. Arayro (IRSN), G. Tréglia (Marseille Université), F. Ribeiro (IRSN)
- P4 **Modeling grain growth and investigating grain subdivision in triuranium disilicide**
A. Cheniour (Penn. State), M.R. Tonks (U. Florida), J. Lian (RPI), Y. Zhang (INL)
- P5 **Fuel relocation recovery implementation in BISON**
M. Zahoor (INL), A. Casagrande (INL)
- P6 **Non-local model for diffusion-mediated dislocation climb and cavity growth**
I. Rovelli (Imperial College), S.L. Dudarev (UK-AEA), A.P. Sutton (Imperial College)
- P7 **Review of hydrogen uptake mechanisms in Zircaloy-2 – the role of Ni and environmental conditions**
V.I. Arimescu (Areva)
- P8 **Status of metallic fuel irradiation testing for PGSFR**
B.G. Kim (KAERI), J. Kim (KAERI), J.H. Kim (KAERI), B. Lee (KAERI), J. Cheon
(KAERI)
- P9 **IM3D: A full-3D, MPI-parallelized Monte Carlo simulation code for ion radiation in matters**
Y. Yang (MIT), Y. Li (MIT), M.P. Short (MIT), C. Kim (MIT), K.K. Berggren (MIT),
J. Li (MIT)
- P10 **Multicomponent phase field model of intragranular pseudo-equilibrium fission gases**
M.J. Welland (CNL), E. Tenuta (CNL, McMaster), A.A. Prudil (CNL), M.H.A. Piro
(UOIT)
- P11 **Database of modelling software codes for nuclear materials applications**
S. Massara (OECD/NEA), M. Bankhead (NNL)
- P12 **Modelling of dislocations in uranium dioxide**
M. Krack (PSI), M. Kosa (PSI), R. Ngayam-Happy (PSI), S. Groh (U. Basel)
- P13 **First-principles study of the effect of americium content in mixed oxide fuels**
M.S.T. Noutack (CEA), M. Freyss (CEA), G. Jomard (CEA), G. Geneste (CEA)

- P14 **Parameters for simulations of tri- and tetravalent lanthanides and actinides in polarizable SWM4-NDP water**
C.I. Maxwell (CNL), J. Pencer (CNL)
- P15 **Atomistic simulation study of helium bubbles in nickel**
E. Torres (CNL), J. Pencer (CNL)
- P16 **Effects of alpha-decay on advanced heavy water reactor fuels during long term storage**
J. Pencer (CNL), M.H. McDonald (CNL), D. Roubtsov (CNL), G.W.R. Edwards (CNL)
- P17 **Equilibrium molecular dynamics calculations of thermal conductivity: a “how to” for the uninitiated**
J. Alexander (CNL), C. Maxwell (CNL), J. Pencer (CNL)
- P18 **Numerical experiments using the particle swarm optimization algorithm for nuclear fuel thermodynamic modelling**
J. Siemons (U. Waterloo, UOIT), M.H.A. Piro (UOIT)
- P19 **Multiscale MOX modelling at the Canadian Nuclear Laboratories**
M.J. Welland (CNL), K. Birdee (CNL), Y. Ding (CNL), C. Maxwell (CNL), E. Torres (CNL), J. Pencer (CNL), M.H.A. Piro (CNL, UOIT), A.A. Prudil (CNL), E.T. Rand (CNL), W. Richmond (CNL), E. Thomas (CNL), A. Williams (CNL)
- P20 **Performance prediction of enhanced thermal conductivity composite fuels for accident tolerant nuclear power generation**
W.Z. Zhou (City U. Hong Kong), W. Zhou (City U. Hong Kong), R. Liu (South China U. Tech.)
- P21 **Ab-initio calculation of oxygen diffusion coefficient in paramagnetic uranium dioxide UO_2**
L. Andrea (CEA), B. Dorado (CEA)
- P22 **UCx as target material for isotope production at TRIUMF**
L. Egoriti (TRIUMF), A. Gottberg (TRIUMF), P. Kunz (TRIUMF), P. Bricault (TRIUMF), J. Wong (TRIUMF, U. British Columbia), M. Cervantes (TRIUMF, U. Victoria)