

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

October 3, 2017

8:00	8:30	Registration Welcome and Announcements
8:30	9:00	Organizing Committee, K. McCarthy (CNL), A. Tokuhiko (UOIT)

Session A: Electronic Structure

Session Chair: S. Middleburgh (Westinghouse)

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 Structures

Session Chair: M. Freyss (CEA)

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 and Mesoscale

Session Chair: J. Pencer (CNL)

13:30 13:50 **Mechanical behaviour of UO₂ under irradiation: a molecular dynamics study**
L.Van Brutzel (CEA), A. Chartier (CEA)

13:50 14:10 **Average structure and local configuration of excess oxygen in UO_{2+x}**
J. Wang (Louisiana State U.)

14:10 14:30 **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)

14:30 14:50 Discussion

14:50 15:10 Coffee Break

Session D: Mesoscale

Session Chair: A. Jokisaari (ANL)

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: M. Kurata (JAEA)

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: E. Corcoran (RMCC)

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: M. Stan (ANL)

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: B.J. Lewis (RMCC Emeritus)

15:25	15:45	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)
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

Tour of the Chalk River Laboratories

Please meet in front of the Four Points Sheraton Hotel at 7:45. The bus will depart at 8:00. The drive is approximately 2 hours, and the bus will have a bathroom and limited wifi.

The bus will depart Chalk River at 16:00. The bus will stop off at The Ottawa International Airport before returning to the hotel *if a request is made to the bus driver in the morning.*

Poster Session

Study of defects formation and diffusion in UO₂

D. Smirnova (JIHTRAS), S. Starikov (JIHTRAS, MIPT), A. Kuksin (JIHTRAS, MIPT), M. Korneva (JIHTRAS, MIPT)

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)

The Influence of tungsten doping on sp³:sp² ratio in carbon co-deposits and the effectiveness of deuterium removal by thermo-oxidation in fusion devices

B.W.N. Fitzpatrick (UOIT), J.W. Davis (UOT), A.A. Haasz (UOT)

Thermodynamic modelling of thoria-urania and thoria-plutonia fuels: Description of the Th-U-Pu-O quaternary systems

A. Bergeron (CNL), E.C. Corcoran (RMCC), M.H.A. Piro (UOIT)

Multicomponent phase field model of intragranular pseudo-equilibrium fission gases

E. Tenuta (CNL, UOIT), M.J. Welland (CNL), A.A. Prudil (CNL), M.H.A. Piro (UOIT)

Modelling of dislocations in uranium dioxide

M. Krack (PSI), M. Kosa (PSI), R. Ngayam-Happy (PSI), S. Groh (U. Basel)

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)

Parameters for simulations of tri- and tetravalent lanthanides and actinides in polarizable SWM4-NDP water

C.I. Maxwell (CNL), J. Pencer (CNL)

First-principles calculations of the ground state properties of UO₂ and PuO₂

E. Torres (CNL), J. Pencer (CNL)

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)

Numerical experiments using the particle swarm optimization algorithm for nuclear fuel thermodynamic modelling

J. Siemons (U. Waterloo, UOIT), M.H.A. Piro (UOIT)

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)

Ab-initio calculation of oxygen diffusion coefficient in paramagnetic uranium dioxide UO₂

L. Andrea (CEA), B. Dorado (CEA)

UC_x 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)

Development of numerical simulation method to evaluate molten material behaviors in nuclear reactors

S. Yamashita (JAEA), Masaki Kurata (JAEA), Hiroyuki Yoshida (JAEA)

Extensive Deep Neural Networks for Multi-Scale Modelling of Complex Materials

I. Luchak (UBC), K. Mills (UOIT), K. Ryczko (U. Ottawa), A. Domurad (U. Waterloo), C. Beeler (UOIT), I. Tamblyn (NRC)

Development of a Synergistic Approach to Study Irradiated Materials Using Coupled Experiments and Simulation

C. Papesch-Adkins (INL), M. R. Tonks (U. Florida), A. Aitkaliyeva (U. Florida), D. Wachs (INL), J. Hirschorn (U. Florida)

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)