Monday, Oct. 14, 2013

1:15-1:30  Welcome and announcements
T. Ewing (ANL, USA) and R. Rosner (UC, USA)

SESSION A:  ATOMISTIC MODELS AND SIMULATIONS
Session Chair: Mikhail Veshchunov (IBRAE, Russia)

1:30-1:50  First-principles DFT+U modeling of paramagnetic UO2 and (U,Pu) mixed oxides
Dorado, Boris (CEA, DAM, DIF, France), Garcia, Philippe (CEA, DEN, DEC, France)

1:50-2:10  Computational study of energetics and defect-ordering tendencies for rare earth elements in uranium dioxide
Solomon, Jonathan M. (UC Berkeley, USA), Alexandrov, Vitaly (UC Berkeley, UC Davis, USA), Sadigh, Babak (LLNL, USA), Navrotsky, Alexandra (UC Davis, USA), Asta, Mark (UC Berkeley, UC Davis, USA)

2:10-2:30  Defect structures induced by high-energy displacement cascades in $\gamma$ uranium
Miao, Yinbin (UIUC, USA), Beeler, Benjamin (GA Tech, USA), Deo, Chaitanya (GA Tech, USA), Baskes, Michael I. (LANL, UCSD, USA), Okuniewski, Maria (INL, USA), Stubbins, James F. (UIUC, USA)

2:30-2:50  Discussion

2:50-3:10  Coffee break

3:10-3:30  Thermodynamic Models of UO2 and UN
Stan, Marius (ANL, USA), Mei, Z.G. (ANL, USA), Thompson, A.E. (Northwestern U., USA), Wolverton, C.M. (Northwestern U., USA)

3:30-3:50  Fission product behaviour in UO2+/-x by classical molecular dynamics
Dubourg, Roland (IRSN, France), Ducher, Roland (IRSN, France)

3:50-4:10  Interatomic potentials accuracy: how do they bridge the scales? U-Mo fuel case
Stegailov, Vladimir (JIHT RAS, Russia), Smirnova, Daria (JIHT RAS, Russia), Kuksin, Alexey (JIHT RAS, Russia), Starikov, Sergey (JIHT RAS, Russia)

4:10-4:30  Discussion

4:30-5:30  Poster Session A (2-3 min introductions)

5:30  Adjourn
Tuesday, Oct. 15, 2013 – Morning

8:45-9:00  Announcements
T. Ewing (ANL, USA) and R. Rosner (UC, USA)

SESSION B:  CONTINUUM MODELS AND FUEL PERFORMANCE SIMULATIONS
Session Chair: Roland Dubourg (IRSN, France)

9:00-9:20  Continuum modelling of hydrogen transport by diffusion in materials
Toribio, Jesus (U. Salamanca, Spain), Kharin, Viktor (U. Salamanca, Spain)

9:20-9:40  Multiscale investigation of fission gas for the development of fuel performance materials models
Tonks, Michael R. (INL, USA), Millett, Paul (INL, USA), Andersson, David (LANL, USA), Pastore, Giovanni (INL, USA), Stanek, Chris (LANL, USA), Williamson, Richard (LANL, USA)

9:40-10:00  Recent advances on the nuclear fuel behaviour simulation
Masson, Renaud (CEA, DEN, DEC, France)

10:00-10:20  Discussion

10:20-10:40  Coffee break

10:40-11:00  The FAST fuel element model for NOC and transient conditions
Prudil, Andrew (RMCC, Canada), Chan, Paul (RMCC, Canada), Lewis, Brent (UOIT, Canada)

11:00-11:20  Thermo-chemo-mechanical couplings in the ALCYONE fuel code application to pellet cladding interaction
Baurens, Bertrand (CEA, DEN, DEC, France), Sercombe, J. (CEA, DEN, DEC, France), Riglet-Martial, C. (CEA, DEN, DEC, France)

11:20-11:40  Development of the mechanistic fuel performance and safety code SFPR using the multi-scale approach
Veshchunov, Mikhail (IBRAE, Russia), Boldyrev, A.V. (IBRAE, JIHT, Russia), Ozrin, V.D. (IBRAE, JIHT, Russia), Shestak, V.E. (IBRAE, JIHT, Russia), Tarasov, V.I. (IBRAE, JIHT, Russia), Norman, G.E. (IBRAE, JIHT, Russia), Kuksin, A.Yu. (IBRAE, JIHT, Russia), Pisarev, V.V. (IBRAE, JIHT, Russia), Smirnova, D.E. (IBRAE, JIHT, Russia), Starikov, S.V. (IBRAE, JIHT, Russia), Stegailov, V.V. (IBRAE, JIHT, Russia), Yanilkin, A.V. (IBRAE, JIHT, Russia)

11:40-12:00  Discussion

12:00-1:30  Lunch
Tuesday, Oct. 15, 2013 – Afternoon

SESSION C: EXPERIMENTAL VALIDATION AND HIGH PERFORMANCE COMPUTING
Session Chair: Masaki Kurata (JAEA, Japan)

1:30-1:50 Mechanical degradation of tungsten alloys at extreme temperatures in vacuum and oxidation atmospheres
García, Teresa Palacios (UPM, Spain), Martin, Antonia (DCM, UPM, E.T.S.I. Caminos, Canales y Puertos, C/ Profesor Aranguren s/n, Spain), Muñoz, Angel (DF, UC3M, Spain) Pastor, Jose Ygnacio (DCM, UPM, E.T.S.I. Caminos, Canales y Puertos, C/ Profesor Aranguren s/n, Spain)

1:50-2:10 Synthesis of uranium carbides doped with metal oxides using ICHTJ methods for modeling carbide fuels doped with minor actinides
Brykala, Marcin (INCT, Poland), Deptula, Andrzej; Rogowski, Marcin; Smolinski, Tomasz; Olczak, Tadeusz; Lada, Wieslawa; Wawszczak, Danuta

2:10-2:30 The Extreme Materials Beam Line for the accelerated study of radiation damage: XMAT
Pellin, Michael J. (ANL, USA), Yacout, Latif (ANL, USA), Nolen, Jerry (ANL, USA), Li, Meimei (ANL, USA), Stan, Marius (ANL, USA), Yun, Di (ANL, USA), Almer, John (ANL, USA), Ewing, Tom (ANL, USA)

2:30-2:50 Discussion

2:50-3:10 Coffee break

3:10-3:30 NEAMS
Bradley, Keith (ANL, USA), Hayes, Steve (INL, USA), Pointer, W. David (ORNL, USA)

3:30-3:50 The consortium for advanced simulation of light water reactors: A U.S. Department of Energy (DOE) energy innovation hub
Kothe, Douglas B. (ORNL, USA), Turinsky, Paul (NSCU, USA), Burns, Douglas E. (INL, USA)

3:50-4:10 Computational science at the Argonne Leadership Computing Facility
Messina, Paul (ANL, USA), Riley, Katherine (ANL, USA), Romero, Nichols (ANL, USA)

4:10-4:30 Discussion

4:30-5:30 Poster Session B (2-3 min introductions)

5:30 Adjourn

7:00-9:00 Reception at Riva Crab House, Navy Pier
Wednesday, Oct. 16, 2013 – Morning

8:45-9:00  Announcements  
  T. Ewing (ANL, USA) and R. Rosner (UC, USA)

SESSION D:  THERMOCHEMICAL TRANSPORT AND DATABASES  
  Session Chair: Marcin Brykala (INCT, Poland)

9:00-9:20  Thermochemical modeling of nuclear fuels: complex actinide and lanthanide oxides  
  Besmann, Theodore M. (ORNL, USA), McMurray, Jacob W. (ORNL, USA), Voit, Stewart L. (ORNL, USA)

9:20-9:40  The influence of oxygen activity upon the behaviour of nuclear oxide fuels  
  Garcia, Phillippe (CEA, DEN, DEC, France), Martin, G. (CEA, DEN, DEC, France), Freyss, M. (CEA, DEN, DEC, France), Bertolus, M. (CEA, DEN, DEC, France), Carlot, G. (CEA, DEN, DEC, France), Sabathier, C. (CEA, DEN, DEC, France), Crocombette, J-P. (CEA, DEN, DMN, France), Siméone, D. (CEA, DEN, DMN, France), Dorado, B. (DAM, DIF, France), Andersson, D. (LANL, USA), Stanek, C. (LANL, USA)

9:40-10:00  Monte Carlo simulation of phonon transport in UO2 crystals with defects  
  El-Azab, Anter (Purdue, USA), Deskins, Ryan (Purdue, USA)

10:00-10:20  Discussion

10:20-10:40  Coffee break

10:40-11:00  High temperature thermochemical and isotopic simulations of high burnup UO2 fuel  
  Piro, Markus Hans Alexander (CRL, Canada), Banfield, James (UTK, USA), Clarno, Kevin (ORNL, USA), Simunovic, Srdjan (ORNL, USA), Besmann, Theodore (ORNL, USA)

11:00-11:20  OECD-NEA thermodynamics of advanced fuels international database (TAF-ID) project  
  Guéneau, Christine (CEA, DEN, DPC, SCCME, LM2T, France), Dupin, N. (Calcul Thermodynamique, France), Barber, D.H. (AECL, Canada), Besmann, T. (ORNL, USA), Corcoran, E.C. (RMCC, Canada), Dumas, J.-C. (CEA, DEN, DEC, SESC, France), Hania, R. (NRG, Netherlands), de Haas, G.-J. (NRG, Netherlands), Kim, J.-H. (KAERI, South Korea), Kurata, M. (JAEA, Japan), Lee, B.O. (KAERI, South Korea), Ogata, T. (CRIEPI, Japan), Turchi, P. (LLNL, USA), Massara, S. (OECD, NEA, France)

11:30-11:40  Development of dedicated modeling and database for elucidating fuel degradation mechanism -METI project in Japan-  

11:40-12:00  Discussion

12:00  End of Workshop

2:00  Chicago River and Lakefront boat tour  
  Harbor near Gleacher Center
PA1  Defect interaction with grain boundaries in molybdenum
    Yanilkin, Alexey (VNIIA, Russia), Kuksin, Alexey; Novoselov, Ivan

PA2  Defect disorder and electrochemical effects of voids in UO2
    Hassan, Abdel-Rahman (Purdue, USA), Allen, Todd (Purdue, USA), El-Azab, Anter (Purdue, USA)

PA3  Multi-scale model of radiation defects in Mo: atomistic calculation of defect diffusion coefficients, surface sink strength and dislocation loops growth rates
    Insepov, Zeke (Purdue, USA), Yanilkin, A. (VNIIA, Russia), Rest, J. (ANL, USA), Stegailov, V. (JIHT, Russia), Kuksin, A. (JIHT, Russia), Norman, G. (JIHT, Russia)

PA4  Atomistic simulation of radiation damage of metallic and oxide fuels by swift heavy ion irradiation
    Starikov, Sergey (JIHT RAS, Russia), Pisarev, Vasily (JIHT RAS, Russia), Kuksin, Alexey (JIHT RAS, Russia), Stegailov, Vladimir (JIHT RAS, Russia)

PA5  Density functional theory for fission products transport in UO2
    Ducher, Roland (IRSN, France), Dubourg, Roland (IRSN, France)

PA6  First-principles study for effects of Pb on oxide films on Ni(110) surface
    Kim, Jong Jin (UNIST, South Korea), Kim, Ji Hyun

PA7  Kinetic Monte Carlo study of oxygen defect migration in urania fuel
    Hoffman III, Richard T. (GA Tech, USA), Bahera, Rakesh (GA Tech, USA), Deo, Chaitanya S. (GA Tech, USA)

PA9  Electronic structure calculations in uranium dioxide: strong electronic correlations and migration of krypton
    Vathonne, Emerson (CEA, DEN, DEC, France), Freyss, M. (CEA, DEN, DEC, France), Amadon, B. (CEA, DAM, DIF, DPTA, France), Bertolus, M. (CEA, DEN, DEC, France)

PA10  KMC modeling of helium-vacancy diffusion and clustering in iron
    Oaks, Aaron (UIUC, USA), Stubbins, James F. (UIUC, USA)

PA11  Ab initio calculations of the U-Zr-Np: DFT vs. DFT+U
    Xie, Wei (U. Wisconsin, USA), Xiong, Wei (U. Wisconsin, USA), Shen, Chao (U. Wisconsin, USA), Marianetti, Chris (U. Columbia, USA), Chang, Y. Austin (U. Wisconsin, USA), Morgan, Dane (U. Wisconsin, USA)

PA12  Pressure-induced phase transitions in UN: a density functional theory study
    Mei, Zhi-Gang (ANL, USA), Stan, Marius (ANL, USA)

PA13  Thermophysical properties of urania-based mixed oxide fuels using atomic level simulations
    Behera, Rakesh K. (GA Tech, USA), Zavala, Martin (GA Tech, USA), Hoffman III, Richard T. (GA Tech, USA), Deo, Chaitanya S. (GA Tech, USA)
Non-destructive studies of fuel pellets and their cladding by spatially resolved neutron transmission spectroscopy at pulsed neutron sources
Tremsin, Anton S. (UC Berkeley, USA), Vogel, S.C. (LANL, USA), Mocko, M. (LANL, USA), Bourke, M.A.M (LANL, USA), Yuan, V. (LANL, USA), Nelson, R.O. (LANL, USA), Brown, D.W. (LANL, USA), Feller, W.B. (NOVA Scientific, Inc., USA)

Stabilities of actinyl ion complexes in aqueous phase
Tiwari, Surya Prakash (ND, USA), Maginn, Edward J. (ND, USA)

Effects of grain boundary on hydrogen isotope diffusion in erbium oxide for tritium permeation barrier
Mao, Wei (U. Tokyo); Chikada, Takumi; Suzuki, Akihiro; Terai, Takayuki; Yamaguchi, Kenji

Uranyl(VI) and plutonyl(VI) coordination and dynamics in a task-specific ionic liquid
Maerzke, Katie A. (ND, USA), Schneider, William F. (ND, USA), Maginn, Edward J. (ND, USA)

The experimental reactor facility for test application of high fuel rod structural elements

POSTER SESSION B
Tuesday, October 15, 4:30 – 5:30 pm

PB1 DART-THERMAL analysis of irradiation behavior of U-Mo/Al dispersion fuels
Ye, Bei (ANL, USA), Rest, Jeff (ANL, USA), Kim, Yeon Soo (ANL, USA), Hofman, Gerard (ANL, USA)

PB2 Numerical considerations in phase field models
Anitescu, Mihai (ANL, USA)

PB3 Simulation of fission-induced creep of U-Mo/Al dispersion fuel
Kim, Yeon Soo (ANL, USA), Hofman, G.L. (ANL, USA), Mohamed, W. (ANL, USA)

PB4 Modeling elasticity at the mesoscale
Heinonen, Olle (ANL, USA), Karpeev, Dmitry (ANL, USA), Gu, Shiyuan (ANL, USA), Nakhmanson, Serge (UCONN, USA)

PB5 Investigation of U-10Mo monolithic plate post irradiation failure: a finite element method approach
Mohamed, Walid (ANL, USA), Kim, Yeon Soo (ANL, USA), Hofman, G.L. (ANL, USA), Yacout, Abdellatif M. (ANL, USA), Cheon, Jin Sik (KAERI, South Korea)

PB6 Impact of thermal conductivity and oxygen diffusion models on the coupling of heat transport, oxygen diffusion and deformation in UO2 and (U,Pu)O2 nuclear fuel elements
Mihaila, Bogdan (NSF, USA), Stan, Marius (ANL, USA), Crapps, Justin (LANL, USA), Yun, Di (ANL, USA)

PB7 Heterogeneity and thermal transport in UO2
Stan, Marius (ANL, USA), Mei, Zhi-Gang (ANL, USA), Yun, Di (ANL, USA), Mihaila, Bogdan (NSF, USA), Hu, Shenyang (PNNL, USA), Cristea, Petrica (U. Bucharest, Romania)

PB8 Thermodynamic treatment of the thorium-uranium-oxygen system
Bergeron, Andrew (AECL, Canada), Piro, Markus (AECL, Canada), Corcoran, Emily (RMCC, Canada)
PB9  Finite element simulations of Zr and Mo based metallic fuels: thermo-mechanical model validations  
Yun, Di (ANL, USA), Mohamed, Walid (ANL, USA), Yacout, Abdellatif M. (ANL, USA)

PB10 Activation energy consideration in computer model for tritium release in lithium titanate pebbles for fusion reactor  
Chandra LAL, Himanshu (BIT, India), Sinha, S.K. (BIT, India), Raole, P.M. (IPR, India)

PB11 Advanced finite element modeling of a horizontal nuclear fuel element using a multiphysics object-oriented simulation environment  
Gamble, Kyle (RMCC, Canada), Williams, Anthony (AECL, Canada), Chan, Paul K. (RMCC, Canada)

PB13 Phase field modelling of grain growth in porous ceria and uranium dioxide  
Ahmed, Karim (Purdue, USA), Pakarinen, Janne; Allen, Todd; El-Azab, Anter

PB14 Continuum theory of defects and materials response to irradiation  
El-Azab, Anter (Purdue, USA)

PB15 Interactions between platinoid fission products (Pd-Rh-Ru) and chalcogen elements (Se-Te)  
Gossé, Stéphane (DEN, DANS, DPC, SCCME, LM2T, France), Gossé, S. (DEN, DANS, DPC, SCCME, LM2T, France), Bordier, S. (DEN, DANS, DPC, SCCME, LM2T, France), Guéneau, C. (DEN, DANS, DPC, SSME, LM2T, France), Dupin, N. (Calcul Thermodynamique, France)

PB16 Development of ENGINE - A 3D Computational Tool for Modeling and Simulation of Nuclear Fuels and Materials  
Karahan, Aydin (ANL, USA)

PB17 Fuel Performance Modeling of Traveling Wave Reactor Fuel Elements  
Miller, Samuel S. (TerraPower, USA), Latta, Ryan (TerraPower, USA)

PB18 Conjugate Heat Transfer Simulations of Advanced Nuclear Reactor Fuel  
Piro, Markus Hans Alexander (CRL, Canada), Leitch, B.W. (CRL, Canada) and Wang, N. (CRL, Canada)

PB19 Phase-field Simulation for Laser Flash Melting of Nuclear Fuels  
Welland, M.J. (JRC-ITE, Germany), Böhler, R. (JRC-ITE, Germany) and Manara, D. (JRC-ITE, Germany)