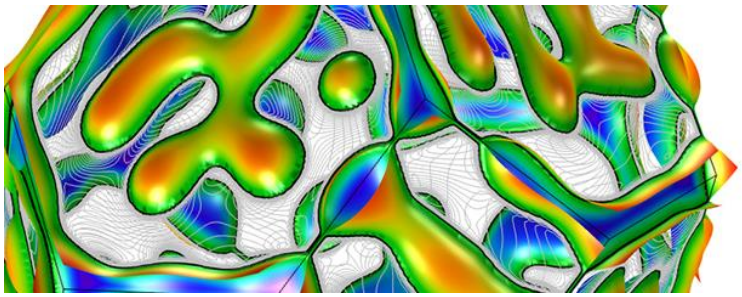

GATINEAU,QC, OCTOBER 2017
MATERIALS MODELLING & SIMULATION
FOR NUCLEAR FUELS

Materials Modeling and Simulation for Nuclear Fuels 2017

Abstracts

Gatineau, Quebec, Canada
October 3rd and 4th 2017

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Electronic Structure Calculations of Structural, Electronic Properties and Irradiation Damage in the Uranium-Plutonium Mixed Oxide $(U,Pu)O_2$

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Electronic structure calculations, and especially the density functional theory (DFT), are efficient methods to investigate point defect properties in nuclear materials [1–3]. These point defects are created under operating conditions, through collisions of high energy recoil particles with the atoms of the fuel. While the point defect properties have been investigated widely for UO_2 and to a certain extent for PuO_2, the uranium-plutonium mixed oxides (MOX), have been little studied although they are of great interest as the reference fuel for sodium-cooled fast reactors (GEN IV).

In this study, we use the DFT+U approach to model structural and electronic properties of MOX as a function of the Pu content and compare the results with experimental data. The distribution of cations in $(U,Pu)O_2$ is modelled in the approximation of an ideal solid solution for the actinide sublattice through the "special quasi-random structures" (SQS) [4,5]. We also investigate the oxygen and cation (U and Pu) point defect formation in various charged states and for various stoichiometry conditions. Furthermore, we calculate the migration barrier of oxygen through vacancy and interstitial mechanisms, thereby achieving a first step towards the determination of oxygen self-diffusion coefficients in uranium-plutonium mixed oxides.

[1] Andersson et al., Phys. Rev. B 79, 024110 (2009).
[2] Dorado et al., Phys. Rev. B 82, 035114 (2010).
[3] Vathonneet al., J. Phys. Condens. Matter 26, 325501 (2014)

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Advances in the Modelling of U_3Si_2 - An Accident Tolerant Fuel Candidate

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Accurate density functional theory modelling of U_3Si_2 has thus far proven to be difficult. A new treatment of the Hubbard correction for U_3Si_2 has been investigated by this team, treating the symmetrically distinct U sites with varying +U values. Both U-ramping and occupational matrix control has been used to verify the improved behaviour which, for the first time, predicts the U_3Si_2 symmetry correctly as well as the magnetic structure at low temperature. The method has been applied to the U_3Si_2+H_2 system to verify the experimentally observed formation of $U_3Si_2H_2$ and this hydrides differing magnetic structure. Accurate modelling of U_3Si_2 is required to enable further materials modelling advances in terms of material design and fuel performance modelling.

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Kinetic Properties of Solute Elements (Xe, Kr, C, O) in Uranium Nitride

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Uranium nitride is considered as an accident tolerant fuel candidate due to its high thermal conductivity and high melting temperature. Its very high uranium density is another advantage. Some of the issues with this fuel are coming from the lack of experimental data on properties such as the fission gas release or the oxidation behavior. For both, atomistic modelling can help, and this is the purpose of the presented work.
This study presents kinetic properties of Xe, Kr, C and O in UN. In the first step, DFT+U using the OMC scheme is used to compute the incorporation energy, corrected for the elastic interactions, to determine where these atoms stay in the host material. Then, the binding of these species with vacancies is investigated, and the migration energies of vacancies in the vicinity of the solute atoms are computed. These simulations have to cover many cases, due to the type I antiferromagnetic ordering of UN Đ for instance, 16 migration energy calculations were needed for each solute. The ab initio data are then used to compute diffusion coefficients and other transport properties such as the drag coefficient or the diffusion path using the SCMF method.

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Diffusion of Intrinsic and Extrinsic Defect in V2C from Density Functional Theory Calculations

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Vanadium Carbide has been identified as a potential coating to zirconium-based clad in which it is intended to act as diffusion barrier, thereby mitigating fuel-clad chemical interaction. The self-diffusion behavior of vanadium subcarbide (V2C) is investigated using density functional theory calculations. Three ordered V2C structures, two of which correspond to experimentally observed phases, are characterized in terms of their equilibrium structural, electronic and elastic properties. Our model for self-diffusion in V2C considers diffusion of carbon and vanadium to occur separately on each sublattice. Two sets of self-diffusion coefficients are calculated for each structure: one for vacancy-mediated diffusion of vanadium and the other for interstitial diffusion of carbon. Calculated activation energies and diffusion prefactors are compared to experimental data where available. The diffusion of relevant extrinsic defects such as U, Fe, Ni and Nd is also discussed.

This work was supported by a DOE NEUP Award (DENE0000731).

Xenon Diffusion by Vacancy Clusters in UO_2

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Diffusion of Xe atoms in UO_2 nuclear fuel is important for fission gas retention and release. One of the main challenges in predicting Xe diffusion is linking the fuel conditions to the concentration of defects enabling diffusion and the interaction of defects with Xe atoms. Previous work has mainly focused on the role of small uranium and oxygen vacancy clusters ($XeUO_z$ and $XeUO_z$, z=0, 1, 2), however the solubility and mobility of larger clusters have not been considered. We have used atomistic calculations based on Density Functional Theory (DFT) and Empirical Potentials (EP) to investigate how Xe atoms interact with multiple U and O vacancies. The thermodynamic and kinetic properties determined from atomistic calculations are used in a continuum model to predict the effective Xe diffusivity as function of temperature and irradiation conditions. The MARMOT phase field code and the MOOSE framework are used for solving the continuum model.

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Modelling Isolated Dislocations and Dislocation Substructures in Deformed Uranium Dioxide Single Crystals

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We report recent data on the mobilities of edge and screw dislocations evaluated for uranium dioxide using classical molecular dynamics. In addition, we address the interaction of an edge dislocation with vacancy clusters and small pores. Finally, we discuss the development of our two-dimensional dislocation dynamics simulation software and present practical applications with respect to the mechanical behaviour of uranium dioxide and the formation and evolution of periodic sub-structures

Atomistic Simulation Study of Structure and Phase Transitions in Pure Uranium and U-Mo Alloys

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We studied structure and thermodynamic properties of cubic and tetragonal phases of pure uranium and U-Mo alloys using atomistic simulations: classical molecular dynamics and density functional theory. Mainly, attention was paid to the metastable gamma-0 phase, which may be seen in the experiments at low temperatures. The structure of gamma-0 phase is similar to the body-centered tetragonal (bct) lattice, but where the central atom of the unit cell is displaced in the [001] direction. At higher temperatures gamma 0 phase transforms to gamma-phase with a quasi body-centered cubic (q-bcc) lattice. The local positions of uranium atoms in gamma-phase correspond to gamma-0 phase, but orientations of the central atom displacements become disordered. Application of such concept for description of the uranium structure allows explanation of a number of unusual features found in the experiments for uranium and its alloys: anisotropy of lattice at low temperature; remarkably high self-diffusion mobility in gamma-phase; mechanical hysteresis; decreasing electrical resistivity at heating for some alloys. In addition, significant part of this work deals with the development (and testing) of a new interatomic potential for the U-Mo system. This potential takes into account atomistic description of the mentioned structures, and allows to study various uranium phases in details.

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Mechanical Behaviour of UO_2 Under Irradiation: A Molecular Dynamics Study

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Mechanical properties of nuclear fuel are a complex problem, involving many coupled mechanisms occurring at different length scales. Most of our knowledge regarding this mechanical behaviour is obtained by experiments on unirradiated fuel, or post-mortem analysis on spent fuel. Atomistic models can alternatively provide insight on the behaviour of the fuel in conditions inaccessible to current experiments, which are used as input parameter for models at larger length-scales. The present investigation considers recent studies on the evolution of the mechanical properties of UO_2 after irradiation damage by means of atomistic simulations with molecular dynamics method using empirical potentials.

Firstly, we will describe the mechanical behaviour under tensile and compressive load in pristine UO_2 single-crystal. Secondly, mechanical properties and crack propagation mode will be investigated in large UO_2 single-crystal including point defects distribution arising from irradiation events. The influence of the crystallographic orientations, temperature, and dose will be discussed. Finally, we will present the influence of gas fission nanobubble distribution in the UO_2 matrix on the mechanical properties.

Study of Defects Formation and Diffusion in UO_2

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We present results of the atomistic simulations of defects formation and diffusion in UO_2. We used molecular dynamics calculations to estimate diffusion coefficients of interstitials, vacancies, and vacancy complexes of oxygen and uranium in UO_2, as well as the coefficients of ion diffusion provided by these defects. The interatomic potentials have been chosen by comparing the defect formation energies with data of the DFT + U calculations. The results of the calculations have been compared with experimental data on the annealing of defects and the measurements of self-diffusion coefficients of ions. The limitations of the model of point defects for the description of the self-diffusion in nominally stoichiometric UO_2 have been discussed.

Average Structure and Local Configuration of Excess Oxygen in UO_{2+x}

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Determination of the local configuration of interacting defects in a crystalline, periodic solid is problematic because defects typically do not have a long-range periodicity. Uranium dioxide, the primary fuel for fission reactors, exists in hyperstoichiometric form, UO_{2+x}. Those excess oxygen atoms occur as interstitial defects, and these defects are not random but rather partially ordered. The widely-accepted model to date, the Willis cluster based on neutron diffraction, cannot be reconciled with the first-principles molecular dynamics simulations present here. We demonstrate that the Willis cluster is a fair representation of the numerical ratio of different interstitial O atoms; however, the model does not represent the actual local configuration. The simulations show that the average structure of UO_{2+x} involves a combination of defect structures including split di-interstitial, di-interstitial, mono-interstitial, and the Willis cluster, and the latter is a transition state that provides for the fast diffusion of the defect cluster. The results provide new insights in differentiating the average structure from the local configuration of defects in a solid and the transport properties of UO_{2+x}.

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Morphological Analysis and Synthesis in Nuclear Materials Science

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This presentation describes different applications of mathematical morphology in nuclear engineering and materials science. Examples include applications to surface metrology; reconstruction of 3D-images using 2D-images and SEM with tilting; quantitative decomposition of fracture surfaces into brittle and ductile fracture components; automated analysis of defects in nuclear fuel claddings; and other examples. The developed approach is based upon using simple geometric shapes for signal and image segmentation and filtering. It can be demonstrated that the so-called "tessellations" (e.g., Voronoi tessellation) in materials science represent just particular cases of morphological transforms. Also, it could be considered a geometry-based technique of modeling microstructure evolution that is supplementary to phase-field modeling.

Utilization of Phase-Field Simulation on UO_2/Zr Interaction in Temperature Increasing Conditions

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A multi-phase-field simulation model was developed for analyzing UO_2/Zr interaction in temperature increasing conditions in a severe accident. The chemical energy calculation was performed based on TAF-ID thermodynamic database. Phenomenology, a rapid increase in reaction rate on liquefaction, which was observed in various macro-scale simulation tests, was discussed using the calculation results. In the temperature regions lower than ~2250 K, hcp-Zr phase containing ~30 at% of oxygen is relatively more stable than liquid and consequently is able to act as a barrier to prevent liquefaction. In the higher temperature region, a miscibility gap was formed in liquid due to the sudden change in the composition of liquid. The composition of newly formed liquid is rather similar to hcp-Zr phase and potentially able to accelerate the liquefaction.

Integration of Thermodynamic Potentials into Transport Phenomena and Phase-Field Models

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There has been recent interest in the incorporation of CALPHAD-type thermodynamic potentials as driving forces for transport phenomena and phase evolution, an approach which can ensure thermodynamically self-consistency increase the accuracy and robustness of modelling techniques. This work describes a method of combining single phase thermodynamic potentials into a multiphase composite potential suitable for integration in temperature dependent, multicomponent phase-field models. Implicit interfacial energy contributions are avoided by starting from a grand potential formulation and approximating the Legendre transform between grand and Helmholtz potentials about a known equilibrium state. The resulting composite function is explicit, reproduces the equilibrium states exactly, approximates the non-equilibrium energy surface well, and is smooth such that it can be differentiated to provide the driving forces for coupled heat and mass transport and phase change in a thermodynamically self-consistent manner. Examples include simulation of a sequence of phase transformations for intermetallic growth in Al-Mg interdiffusion for advanced nuclear research reactor fuel and in transient heating experiments with phase change.

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Modeling Grain Growth and Investigating Grain Subdivision in Triuranium Disilicide

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U_3Si_2 has a higher thermal conductivity than UO_2, making it a potential fuel for light water reactors. Understanding its microstructure behavior is essential. While grain growth and grain subdivision have been investigated for UO_2, there is not enough data for U_3Si_2. The current work implements the U_3Si_2 grain boundary mobility and energy determined using MD simulations in the MARMOT mesoscale fuel performance code. Using this data, grain growth is modeled at typical temperatures in a U_3Si_2 fuel pellet.

Grain subdivision happens in UO_2 fuel pellets and results in the formation of a high burn-up structure represented by nano-sized grains at low temperature and high burn-up. The work also investigates the temperature and burn-up threshold for U_3Si_2 by comparing the free energy of large grains with high defects concentration to the free energy of nano-sized grains. We will present our grain growth and grain subdivision simulation approaches and current results.

Current Progress in the US on the Development of Microstructure Based Materials Models for Fuel Performance Codes

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Most materials models used in legacy fuel performance codes are empirical models that are fit to data and correlated to burnup. However, a new paradigm is currently being developed in which mechanistic materials models are that depend on microstructure rather than burnup are used in place of the traditional empirical models. The development of these new microstructure based models is accelerated by the use of modeling and simulation at the atomistic and mesoscales. In this talk we will provide an overview of the progress of the development of these new models in the US and their implementation in the US fuel performance code BISON. We will also provide an overview of the validation efforts underway for these models.

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Uncertainty of Thermodynamic Data: Humans and Machines

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Thermal transport and thermodynamic stability of multi-component nuclear fuels and reactor materials are important during normal reactor operation and critical during accidents. Many journal articles report thermodynamic data – especially phase equilibria – without uncertainty/confidence intervals. The main reason for the lack of uncertainty quantification is the complexity of the physics and chemistry of the multi-component materials. In addition, there are mathematical and computational challenges associated with quantifying uncertainty in a multi-dimensional parametric space. In this talk we discuss uncertainty evaluation of thermodynamic data with a focus on high-temperature phase equilibria and thermal conductivity. The scientific approach is based on a Bayesian method that simultaneously accounts for different types of data and its provenance and delivers uncertainty intervals. Data analysis is enhanced by machine learning methods such as Kernel Ridge Regression, Bayesian Networks, and Evolutionary Algorithms. The presentation ends with a discussion of the changing role of computation in science and engineering.

Modelling the Radiolytic Corrosion of Spent Fuel Inside a Failed Nuclear Waste Container

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Diffusion-reaction models have been developed to determine the influence of redox conditions within the failed container on the fuel corrosion under nuclear waste repository conditions. These models take into account water radiolysis, the reaction of radiolytic H_2O_2 with the fuel both directly and via galvanic coupling to fission product phases in the fuel, the reaction with H2 catalyzed on the fuel surface, the scavenging of radiolytic H_2O_2 by reaction with Fe^{2+}, and diffusion of species.

The model has been adapted to simulate the corrosion rates measured on a wide range of alpha-doped UO_2 and spent fuel specimens. The good agreement between the model simulation and experimental results gives us confidence that our models can be applied to simulate the consequences of various failure scenarios. Model simulations show the critical hydrogen concentration, the minimum concentration of hydrogen produced from steel corrosion that is required to completely suppress fuel corrosion, changes with the dimensions of fractures in the fuel and is bounded by an upper limiting value, suggesting that, if the corrosion of the carbon steel canister can produce a $[H_2]$ higher than this value, the corrosion of spent fuel should not occur.

Modeling Phase Equilibria and Thermodynamics of U-Si and U-Si-N Based Nuclear Fuel

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Advanced Technology Fuel (ATF) systems are being explored that hold significant promise for improved performance and potential increased robustness in the face of over-temperature accidents. The fuels include uranium silicide (e.g., U_3Si_2) and composite uranium nitride-silicide (e.g., UN-U_3Si_2) which have higher uranium density and increased thermal conductivity over UO_2. To fully utilize such alternative fuels it is necessary to understand their phase equilibria and thermodynamics so as to predict behavior during operation and off-normal conditions. Available information together with experimental measurements and first principles calculations are being used to develop a CALPHAD assessment of the systems. The results are being used in fuel performance codes such as BISON.

This research is being performed using funding received from the DOE Office of Nuclear Energy's Nuclear Energy University Programs.

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Demonstration of the Application of the TAF-ID (Thermodynamics Advanced Fuels – International Database)

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[8] Canadian Nuclear Laboratories, Chalk River, ON, Canada
[9] Central Research Institute of Electric Power Industry, Tokyo, Japan
[10] Delft University of Technology, Delft, The Netherlands
[11] Korean Atomic Energy Research Institute, Deajeon, Korea
[12] Nuclear National Laboratories, Warrington, United Kingdom
[13] Lawrence Livermore National Laboratory, Livermore, CA, USA
[14] Idaho National Laboratory, Idaho Falls, ID, USA
[15] Organisation for Economic Co-operative Development Nuclear Energy Agency, Paris, France

The thermodynamic database TAF-ID (Thermodynamics of Advanced Fuels- International Database) has been under development since 2013 under the NEA/OECD [1]. The aim is to provide a computational tool to perform thermodynamic calculations on advanced nuclear fuels (mainly, oxide and metallic fuels) for Generation 2, 3 & 4 reactors. The database contains 41 elements and assessments for 204 binary and 66 ternary systems. The current content of the database allows calculations on complex compositions such as irradiated oxide fuels containing a large number of fission products and/or corium compositions, containing fuel and structural materials forming during a severe accident. The database will be described and examples of such application calculations will be presented.

[1] www.oecd-nea.org/science/taf-id/

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Thermodynamic Modeling of the U-Fe-Si System

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Uranium silicides are being considered to replace the current UO_2 nuclear fuel as an Advanced Technology Fuel (ATF) candidate. U_3Si_2 has the advantages of a high U-density and increased thermal conductivity compared to current oxide systems. Fe-Cr-Al-Y alloys are seen as an advanced cladding material for possible use with silicide fuel as it provides increased corrosion resistance and lower heat generation under steam oxidation during an accident. While investigating the thermodynamic compatibility of the U_3Si_2-FeCrAl(Y) multi-component system, a need to further investigate the U-Fe-Si ternary was established. To date there is no assessed CALPHAD (CALculation of PHAse Diagrams) model in the literature. While limited experimental data exists, this work aims to establish realistic physical relations, coupled with density functional theory calculations of formation enthalpies, to result in a self-consistent model. Such a model will aid in understanding complex phase formation across the compositional and temperature ranges for prospective ATF's.

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Fission Product Release Modelling for Application of Fuel-Failure Monitoring and Detection - An Overview

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A review of fission product release theory is presented in support of fuel-failure monitoring analysis for the characterization and location of defective fuel. This work is used to describe: (i) the development of the steady-state Visual_DETECT code for coolant activity analysis to characterize failures in the core and the amount of tramp uranium; (ii) a generalization of this model in the STAR code for prediction of the time-dependent release of iodine and noble gas fission products to the coolant during reactor start-up, steady-state, shutdown, and bundle-shifting manoeuvres; (iii) an extension of the model to account for the release of fission products that are delayed-neutron precursors for assessment of fuel-failure location; and (iv) a simplification of the steady-state model to assess the methodology proposed by WANO for a fuel reliability indicator for water-cooled reactors.

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Modelling Microstructural Effects on the Fuel Element Behavior with the Release V2 of the ALCYONE Fuel Performance Code

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The fuel performance code ALCYONE (PLEIADES software environment) simulates fuel rod evolutions during irradiation in pressurized water reactors. Among the new features of the latest release (V2) of ALCYONE, we focus here on the simulation of the effects of fuel heterogeneities on its in-pile behavior. The mechanical effect of these heterogeneities are usually modeled by "mean-field" homogenization techniques which are able to deliver the time-evolution of the macroscopic strain-stress experienced by the fuel. To compute the evolution of the mechanical fields at microscopic scale during the irradiation, a multi-level finite element approach has been integrated in ALCYONE V2. We propose a hybrid version of the Finite Element square (FE2) method that enables the use of such a time consuming methodology in an industrial context. This hybrid approach consists in using the FE2 multilevel approach in a limited (but relevant) number of integration points while the constitutive law derived by homogenization is used in the remaining domain. This hybrid approach naturally takes advantage of the parallelization offered by the new version of the PLEIADES platform. Numerical simulations of fuel pins show the interest of the proposed multilevel approach.

MOX Irradiations in BISON Using a New Fuel-to-Sheath Heat Transfer Model

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The BISON fuel performance code uses finite element methods, implemented through the MOOSE framework, to solve the coupled non-linear partial differential equations associated with nuclear fuel behaviour. The BISON code includes a variety of models used to calculate physical parameters such as grain growth, sheath strain, etc. To date, BISON employs a modified form of the Ross and Stoute's fuel-to-sheath heat transfer model, which is widely used for thick non-collapsible clad used in pressurized water reactor fuel. When comparing to validated codes used in Canada, it has been found that this model underestimates the heat transfer coefficient for collapsible clad used in pressurized heavy-water reactor fuel. In this work, we incorporated the Campbell et al. modified fuel-to-sheath heat transfer model into BISON and simulated a number of mixed oxide irradiations. Preliminary results comparing the two fuel-to-sheath heat transfer models, including a comparison to post irradiation experimental results, will be presented.

Simulations of Power Ramps with ALCYONE Including Fission Products Chemistry and Oxygen Thermo-Diffusion

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In this presentation, we will describe the latest developments regarding the CEA multi-dimensional fuel performance code ALCYONE (PLEIADES computational system). In recent years, a thermo-chemical solver (called ANGE) has been introduced in ALCYONE and used to estimate the chemical equilibria at hand in the fuel pellet during power ramp irradiations. Work is now on-going concerning the modeling of chromia-doped UO2 fuel thermo-chemistry. To this end, a solubility model for chromium in UO2 has been incorporated in the thermodynamic database of ANGE. Evidence of oxygen redistribution during power ramps on chromia-doped fuels has led to the introduction of an oxygen thermo-diffusion model in ALCYONE. With respect to previous work on oxygen thermo-diffusion, the purpose of our latter development is to study the impact of radial oxygen redistribution on fission products thermochemistry and on corrosive fission gas release. ALCYONE simulation results are compared to experimental measures of iodine, tellurium, cesium and chromium radial profiles (SIMS and EPMA).

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Parameters for Simulations of Tri- and Tetravalent Lanthanides and Actinides in Polarizable SWM4-NDP Water

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A parameter set for the trivalent and tetravalent lanthanide and actinide ions based on the Drude polarizable SWM4-NDP water model is derived. The resulting parameter set is designed to reproduce experimental parameters including hydration coordination numbers, hydration free energies and ion-oxygen distances. Simulations using the derived parameters reproduce hydration free energies and ion-oxygen distances with average relative errors of 2.8% and 1.8%, respectively. The accuracy in structural properties required a compromise in the accuracy of dynamic properties; the rate of water exchange between the first and second coordination spheres is overestimated. The reported results demonstrate the possible use in the modelling of ion-ligand interactions in applications such as aqueous fuel reprocessing, chelation, or environmental speciation, subject to additional tests of transferability.

First-Principles Calculations of the Ground State Properties of UO_2 and PuO_2

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We have performed calculations of nuclear fuels using the Hubbard corrected density functional theory (DFU+U). The spin-polarized generalized gradient approximation (GGA) approach correctly predicts the insulating electronic structure with antiferromagnetic ordering. Direct control of the occupation matrix was necessary to determine the correct electronic ground state. The structural properties, such as lattice parameter and bulk modulus, and bandgap obtained from the DFT+U calculations are in good agreement with the available experimental results and previous calculations. We have calculated the elastic constants, phonon dispersion curves and density of states. The results are compared to available experimental data.

Effects of Alpha-Decay on Advanced Heavy Water Reactor Fuels During Long Term Storage

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The decay of actinides such as ^{238}Pu, results in recoil damage and helium production in spent nuclear fuels. The extent of the damage depends on storage time and spent fuel composition, and has implications for the integrity of the fuels. Some advanced nuclear fuels intended for use in heavy water pressure tube reactors have high initial plutonium content and are anticipated to exhibit swelling and embrittlement. They are also expected to accumulate helium bubbles over storage times as short as hundreds of years. Calculations are performed to provide estimates of helium production and fuel swelling associated with alpha decay as a function of storage time. Significant differences are predicted between predicted aging characteristics of natural uranium and the advanced fuels, including increased helium concentrations and accelerated fuel swelling in the latter. Implications of these predicted for long term storage of advanced fuels are discussed.

First-Principles Study of the Effect of Americium Content in Mixed Oxide Fuels

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The objective of this study is to contribute to a better understanding of the properties of the mixed actinide oxide fuel $(U,Pu)O_2$ containing americium in low concentrations, and in particular to determine the effect of the americium content on the fuel behavior. $(U,Pu)O_2$ is the reference nuclear fuel for the future 4th generation fast reactors in France. It will be fabricated from spent fuel coming out of the current pressurized water reactors and will, as a consequence, contain a few percent of americium.

We use first-principles electronic structure calculations, based on the DFT+U approach, to investigate the influence of americium on the properties of oxide fuels. As a first step, bulk properties of the pure oxide AmO_2 are calculated as a function of the U and J parameters of the DFT+U method, using the occupation matrix control (OMC) scheme to avoid convergence of the calculations to metastable states. We show that the use of OMC is essential for AmO_2. We then study the influence of Am in the mixed oxides $(U,Am)O_2$. Bulk properties, valence of cations, formation energies of oxygen point defects are determined for various content of Am and compared to those obtained in UO_2.

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Numerical Experiments Using the Particle Swarm Optimization Algorithm for Nuclear Fuel Thermodynamic Modelling

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Significant efforts are underway in developing comprehensive thermodynamic treatments of irradiated nuclear fuel, such as the Thermodynamics of Advanced Fuels – International Database (TAF-ID), which is being developed under the auspices of the Organization for Economic Co-operation and Development (OECD) Nuclear Energy Agency (NEA). A great numerical challenge associated with the calculation of equilibrium conditions of a large thermodynamic system, such as TAF-ID, is ensuring that the integral Gibbs energy is a global minimum. This work describes progress in performing a series of numerical experiments using multiple variations of the Particle Swarm Optimization (PSO) algorithm for 10 thermodynamic systems. Variations in the implementation of PSO include the number of particles released for a given system, initial locations of particles, constraints imposed on particle trajectories, etc. The overall goal of the work is to quantify both reliability and performance of these variations of PSO with regards to a statistically relevant number of evaluations.

Modelling of Dislocations in Uranium Dioxide

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The nuclear fuel material uranium dioxide (UO_2) undergoes severe microstructural changes along its fuel cycle, forming extended defects like dislocations. Experimental evaluation of structural deformations in UO_2 is difficult due to safety and cost, and therefore computer simulations could bridge this gap. Density Functional Theory (DFT) is employed to study dislocations in UO_2. The dislocations are studied in the framework of the Peierls-Nabarro model by computing the Generalized Stacking Fault energies, or at 2D the gamma-surfaces. The gamma-surfaces computed at DFT level are used for the validation of empirical potentials.

Multiscale MOX Modelling at the Canadian Nuclear Laboratories

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Within the multiscale paradigm, a range of phenomena in MOX fuels are being investigated at the Canadian Nuclear Laboratories with the goal of improving the robustness and accuracy of fuel performance models to improve manufacturing, operating efficiency, and nuclear safety. The diffusivity of Xe and Kr within the fuel lattice is being investigated by electronic structure calculations scaled up to molecular dynamics simulations. The thermal conductivity of stoichiometric and hyperstoichiometric fuels are examined using charge-scaled molecular dynamics. Thermodynamic potentials are employed as driving forces for transport phenomena and phase-change in phase-field models which capture over pressurized, intragranular bubble evolution. Long-range intergranular bubble networks are being simulated using a novel shell porosity technique, which efficiently captures the 3D system in a 2D computation. A rapid-prototyping platform for fuel performance models has been developed 0061nd applied to international benchmarking activities. Finally, predictions of full-scale fuel performance codes are compared to post-irradiation examination data of fuel samples irradiated at Canadian Nuclear Laboratories.

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

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We present a procedure for training and evaluating a deep neural network which can efficiently infer extensive parameters of arbitrarily large systems, doing so with O(N) complexity. We use a form of domain decomposition for training and inference, where each sub-domain (tile) is comprised of a non-overlapping focus region surrounded by an overlapping context region. The relative sizes of focus and context are physically motivated and depend on the locality length scale of the problem. Extensive deep neural networks (EDNN) are a formulation of convolutional neural networks which provide a flexible and general approach, based on physical constraints, to describe multi-scale interactions. They are well suited to massively parallel inference, as no inter-thread communication is necessary during evaluation. Example uses for learning simple spin models, Laplacian (derivative) operator, and approximating many-body quantum mechanical operators (within the density functional theory approach) are demonstrated.

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Development of Numerical Simulation Method to Evaluate Molten Material Behaviors in Nuclear Reactors

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In the accident at the Fukushima Daiichi Nuclear Power Plant, the core was melted and then melt relocation occurred, however the current status of the plant still has not been clarified. To consider the fuel debris distribution and characteristics, understanding the relocation process of the molten materials is very important. In order to simulate the melt relocation in a reactor core phenomenologically without any assumption, a numerical simulation code that can phenomenologically evaluate the melting phenomena is required. Therefore, a phenomenologically-based numerical simulation code for predicting the melting core and its accumulation behavior, including solidification and melting based on the computational fluid dynamics, has been developed in JAEA. In addition, the code also has a capability of massively parallel computing based on the high performance computational algorithms. In this presentation, results of some validation works, implementation of fuel or CR melting model, and some preliminary results will be shown.

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

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In carbon-walled nuclear fusion devices, the erosion of carbon from the wall and re-deposition with the deuterium and tritium fuels creates films on the wall known as "co-deposits". In the event that tungsten is employed as an additional wall material, eroded tungsten will unavoidably contribute to the co-deposit matrix. One technique for removing the hydrogen isotopes from the co-deposit (or destroying the co-deposit itself) is thermo-oxidation, where wall tile surfaces are heated and oxygen is admitted into the vessel (sometimes with an inert gas such as He). Thermo-oxidation has been demonstrated as safe and effective both in ex-situ studies [1] and in-situ, in the DIII-D tokamak [2].

The concentration of tungsten in the film was correlated with a reduction in the effectiveness of thermo-oxidation (lower fraction deuterium removed). We present evidence for a mechanism. X-ray photoelectron spectroscopy shows lower sp3:sp2 ratios in the carbon bonds of films with higher tungsten concentrations. This suggests that the tungsten has effected a change in structure during the deposition process. The sp3 bonds are shown to be preferentially eroded during thermo-oxidation. A similar proposal has been made for boron [3], which also inhibits oxidation.

[1] J.W. Davis, A.A. Haasz, J. Nucl. Mater. 390 (391) (2009) 532.
[2] J.W. Davis, et. al. Nuclear Fusion 53 (2013) 073008.
[3] Schenk, A., et. al. J Appl Phys, 77(11) (1995) 6006–6014.

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UCx as Target Material for Isotope Production at TRIUMF

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As the only high-power ISOL (Isotope Separation OnLine) facility worldwide, ISAC-TRIUMF is routinely operating carbide targets fission and spallation under proton irradiation in the high-power regime to produce a variety of radioisotopes through nuclear reactions between the incoming beam and the target material. These products diffuse out of the target material and undergo an effusion path to the ionizer where are extracted in the form of radioactive ion beams. At TRIUMF, a variety of target materials which include UC2 and UO2 have been developed in order to withstand not only high-temperature environments (up to 1500 C – 2000 C) but also to allow fast transport processes which ultimately boost the RIB yields.

This contribution focuses on the description of the uranium carbide (UCx) targets usually operated at TRIUMF in the ISAC facility, and its ongoing development strategies. These include the optimization of the target production procedure and performance, the setup of an experimental procedure for quantifying transport phenomena in some target materials, and the development of models and new ideas for describing particle transport in ISOL targets.

Ab-initio Calculation of Oxygen Diffusion Coefficient in Paramagnetic Uranium Dioxide UO_2

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Uranium dioxide is the most widely used nuclear fuel worldwide and its atomic transport properties are relevant to practically all engineering aspects of the material. Although transport properties have already been studied in UO_2 with antiferromagnetic ordering by means of first-principles calculations, the ab-initio determination of defects diffusion coefficients in paramagnetic order has never been done because of the computational cost.

The present work reports our results related to the ab-initio calculation of the oxygen diffusion mechanisms in paramagnetic UO_2. We first determine the ground state of paramagnetic UO_2 using special quasirandom structures method, followed by harmonic phonon calculations using density functional perturbation theory. In order to compute the diffusion coefficient, we studied the oxygen diffusion properties using the nudged elastic band method. We were able to show that previous studies were underestimating migration barriers. We then determine the electronic contribution to the Gibbs free energies of formation. The results are compared to the available data obtained experimentally.

Multicomponent Phase Field Model of Intragranular Pseudo-Equilibrium Fission Gases

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The work describes a phase-field model for isothermal multi-component, multi-phase system which avoids implicit interfacial energy contributions by starting from a Grand potential formulation. A method is developed for incorporating arbitrary forms of the equilibrium thermodynamic potentials in all phases to determine an explicit relationship between chemical potentials and species concentrations. The model has the ability to define and account for variations in adjacent phases, simulate defect migration, and display the dependence of internal pressure on object shape, dimension and orientation ranging from the macro- to nano-scale. Demonstrative simulations of an overpressurized nano-scopic intragranular bubble in nuclear fuel migrating to a grain boundary and Ostwald Ripening under kinetically limited vacancy diffusion are shown.

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Modeling Grain Boundary Fission Gas Bubbles with a Shell Based Phase-Field Model

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The production and time-evolution of fission gas bubbles on grain boundaries contributes significantly to the macroscopic performance of oxide fuels. Gas atoms diffusing from the fuel grains may be retained in the grain boundary porosity. This increases the pressure, thereby attracting vacancies, causing the bubbles to grow, and resulting in macroscopic swelling of the fuel. The morphology of the grain boundary bubbles evolves to minimize the combined interfacial energy, internal energy of the gas, and elastic energy in the matrix. With sufficient time and irradiation, the bubbles interlink forming tunnels, which can terminate at cracks or the fuel surface. This allows the release of the gas inventory to the fuel-clad gap, which results in the subsequent collapse of the tunnels. A novel parameterized surface approach is used to model the evolution of the phase interfaces on, the grain boundary. The method captures the 3D the interfacial effects using 2D surfaces imbedded in 3D, drastically reducing the computational cost compared to traditional 3D phase-field techniques, and allowing larger scale simulations.

IM3D: A Full-3D, MPI-parallelized Monte Carlo Simulation Code for Ion Radiation in Matters

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Recently, ion implantation on nanostructured materials has generated broad interest. For example, small-scale mechanical testing of ion-irradiated materials is often performed to study the radiation-induced effects on mechanical properties. For these applications, an accurate estimation of defects distributions/concentrations are significant to bridge the results of nano-scale and micro-scale. As such, Monte Carlo (MC) simulations that can model ion exchange/leakage at target boundaries/interfaces become necessary.

Here we introduce a full three-dimension (3D) MC simulation code for ion radiation in matters, named IM3D. It is equipped with constructive solid geometry (CSG) method and finite element triangle mesh (FETM) method, thus it can handle arbitrary complicated 3D shapes and microstructures conveniently. Also, its MPI-parallelized engine offers satisfactory computation efficiency. IM3D is based on the stopping power database of SRIM (The Stopping and Range of Ions in Matter), but it can replicate SRIM's results in a homogeneous target with much faster speed. Using IM3D, we quantified the target size effect for several classical applications of nano-scale ion beam implantation. It is found that full-3D simulations should be performed if the target size is below five times the SRIM longitudinal ion range. We also discovered some new phenomena with IM3D, such as the effect of surface roughness on sputtering yield.

Status of Metallic Fuel Irradiation Testing for PGSFR

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The prototype generation-IV sodium-cooled fast reactor (PGSFR) will be built by 2028 in Korea. Metallic fuel, U-10wt%Zr fuel, is being developed for the initial core of the PGSFR, and U-transuranics (TRU)-Zr fuel will gradually replace U-10wt%Zr fuel through its qualification in the PGSFR. In order to validate KAERI's SFR fuel design and fabrication technologies, the first irradiation testing, SMIRP-1, up to the maximum burnup of ~3 at% for 182 EFPD in HANARO and PIE were successfully performed. In addition, the second irradiation testing, SMIRP-2, has been prepared, and will be then carried out up to the maximum burnup of ~6 at% in HANARO form the year 2018. Also, irradiation testing of U-10 wt%Zr fuel has been conducted in a fast research reactor, BOR-60, in Russia since the year 2016. Therefore, status of metallic fuel irradiation testing including some PIE's result for SMIRP-1 for PGSFR will be presented.

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Thermodynamic Modelling of Thoria-Urania and Thoria-Plutonia Fuels: Description of the Th-U-Pu-O Quaternary Systems

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A thermodynamic treatment for $(Th,U)O_2$ and $(Th,Pu)O_2$ fuels has been developed using the CALPHAD method to describe phase diagram and thermodynamic data of the phases in the Th-U-Pu-O oxide systems. The thermodynamic and phase diagram properties calculated by the models are in good agreement with the available data for the binary and ternary subsystems. This treatment is useful to predict the behaviour of ThO_2-based fuels at various temperatures and compositions.

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

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This project is working to provide an established procedure for coupling experiments with modeling and simulation to investigate critical material behavior in nuclear fuel. Such a coupled approach has the potential to provide detailed and quantitative understanding of atomic scale in-reactor degradation behavior of nuclear fuels. The first task is developing experimental procedures to obtain the specific pre- and post-irradiation characterization data required for validation and uncertainty quantification of MARMOT models. The second task is demonstrating a phase field model of a coupled experimental and simulation using critical thermal properties in a material of broad interest (the U-Pu-Zr system and its component binary systems). Finally, by conducting irradiation experiments in the Transient REActor Test (TREAT) facility we will use our model to understand the evolution of microstructure under transient irradiation conditions and its impact on thermophyscial properties. Pre-irradiation characterization and phase-field models of constituent redistribution and thermal conductivity will be presented.