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International Atomic and Molecular Code Centres Network: Database Services for Radiation Damage in Nuclear Materials

Summary Report of the 7th Biennial Technical Meeting of the Code Centres Network

IAEA Headquarters, Vienna, Austria
18 – 20 October 2021

Prepared by

C. Hill
International Atomic Energy Agency
Vienna, Austria

October 2021

IAEA Nuclear Data Section
Vienna International Centre, P.O. Box 100, 1400 Vienna, Austria

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ABSTRACT

The International Code Centres Network (CCN) is a group of experts developing codes and models for atomic, molecular and plasma-surface interaction data relevant to fusion applications. Variable subsets of the group are brought together by the IAEA Atomic and Molecular Data (AMD) Unit in order to discuss computational and scientific issues associated with code developments. At the 7th Technical Meeting described in this report, which was held virtually from 18 – 20 October 2021, 18 experts in the field of Density Functional Theory (DFT) and Molecular Dynamics (MD) simulations of radiation damage reviewed the status of and proposed developments to the DefectDB and CascadesDB databases. These services, which are hosted by the AMD Unit, provide a central repository for the results of computational simulations of the evolution of a material's structure following an impact by a high energy particle.

October 2021

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1. Introduction

The International Code Centres Network (CCN) is coordinated by the IAEA Atomic and Molecular Data (AMD) Unit in order to gather, compare, validate, and provide access to computational codes relevant for modellers in fusion and plasma sciences. Since 2005, the Unit has organized a series of meetings of code developers in the CCN to address code-related issues including the accessibility of physics codes.

Computational modelling of the response of materials to bombardment by energetic particles is a crucial part of research directed towards the both the realization of a viable nuclear fusion reactor and the understanding of the behaviour and properties of materials in conventional fission reactors. Whilst the basic approach of classical Molecular Dynamics (MD) modelling in solids is well-understood and much used, special numerical algorithms are required to deal with the high energies and short timescales involved in the cascade processes resulting from the interaction of atoms in a crystal lattice, with particles with keV or MeV energies.

The AMD Unit organized the 6th Technical Meeting on the International Code Centres Network (CCN5) at IAEA Headquarters from 16 – 18 October 2019. This meeting is described in detail in the International Nuclear Data Committee (INDC) report INDC(NDS)-0803 available at https://www-nds.iaea.org/publications/indc/indc-nds-0803/ and online at https://amdis.iaea.org/meetings/ccn-6/. Experts in Molecular Dynamics simulations discussed developments to CascadesDB, a database to bring together, in a structured and searchable way, the results of MD simulations of high-energy collision cascades in a variety of crystalline materials. At that time, they also proposed a new resource, DefectDB, to curate datasets of Density Functional Theory (DFT) calculations of the defect structures caused by radiation damage in such materials.

This report documents the 7th CCN meeting, which was held virtually, due to the ongoing COVID-19 pandemic at the time, from 18 – 20 October 2021 to review CascadesDB and DefectDB projects and to propose enhancements and extensions to the services. The following section contains the meeting proceedings and a summary of discussions. Appendices 1, 2 and 3 list the participants, the meeting agenda, and abstracts of the participants' presentations.

2. Proceedings

The 7th Code Centres Network Meeting was opened by Melissa Denecke, Director of the Division of Physical and Chemical Sciences and Arjan Koning, Head of the Nuclear Data Section. C. Hill, Head of the Atomic and Molecular Data (AMD) Unit, welcomed all the participants and the participants introduced themselves. After some administrative formalities, the general meeting objectives were outlined and the agenda adopted (Appendix 2).

C. Hill (AMD Unit, IAEA) provided a review of the current status of nuclear material radiation damage resources available from the AMD Unit, and summarized the current status of the CascadesDB database. CascadesDB, at the time of writing, contains 478 GB of data in 4087 simulations across 251 archives and is available at on the IAEA's website at https://cascadesdb.iaea.org. An introduction to the newer DefectDB database was also given.

M. Serrano (Centro de Investigaciones Energeticas, Medioambientales y Tecnologicas, Spain) gave an account of the status of the ENTENTE database project; this EU-funded project intends to design a European database for radiation embrittlement experimental and modelling data, where data produced in previous EU-funded projects and within ENTENTE will be collected, cured and stored. The ENTENTE project interfaces with CascadesDB, which provides primary damage configurations that are propagated through subsequent multi-scale simulations.

A. Sand (Aalto University) gave an account of her group's latest work on electronic energy losses during a collisional cascade; two coupling regimes capture the cascade dynamics: electronic stopping in the early phase of the cascade and electron-phonon coupling in the later phase.

F. Gao (University of Michigan, USA) discussed progress in simulating radiation damage and microstructural evolution in multicomponent equiatomic alloys, including medium- and high-entropy alloys (MEAs and HEAs). Compared with pure nickel (Ni), the HEA NiCoCrFe displays delayed defect accumulation and enhanced defect suppression.

W. Setyawan (Pacific Northwest National Laboratory, USA) detailed molecular dynamics simulations of collision cascades in a Ni-30at.%Fe fcc solid solution, using primary knock-on atom (PKA) energies up to 70 keV. DFT calculations were also employed to study the interaction between helium (He) and the various component atoms of 14-YWT nano-structured ferritic alloy; the interactions are found to potentially promote He bubble nucleation; the formation of such bubbles is predicted to be exacerbated by hydrogen.

H. Deng (Hunan University, China) described calculations of interatomic potentials and collision cascade simulations for tungsten (W) and tungsten-based alloys, particularly those involving the transmutation elements rhenium (Re) and tantalum (Ta). Among other findings. it was reported that the presence of Re or Ta atoms does not significantly affect the number of surviving defects.

C. Domain (EDF R&D Lab Les Renardières, France) spoke about the statistical analysis of collision cascades in iron, tungsten and nickel.

U. Bhardwaj described the CSaransh software that has been developed at the Bhabha Atomic Research Centre, India, to visualize and provide a statistical summary of defects in the CascadesDB MD simulation data sets. A demonstration was given and the utility of CSaransh for detecting anomalies and errors in the data sets discussed.

M. J. Caturla, from the University of Alicante, Spain, spoke about the latest calculations from her research group of Cu and Fe irradiation in the presence of edge dislocations. In such face-centred cubic (fcc) metals, the presence of such dislocations has an important effect on the evolution of defects, including a change in orientation of self-interstitial clusters and preferential formation of stacking-fault tetrahedra defects.

A. Goryaeva (CEA; Université Paris-Saclay, France) outlined the development of a software package, MiLaDy (Machine Learning Dynamics) to determine practical force fields for complex defects in damaged materials and efficiently explore the atomistic free energy landscape of these defects in metals with *ab initio* accuracy.

J. Tian (Peking University, China) introduced recent computational studies on high-dose irradiation damage in hcp zirconium (Zr), a widely-used material for fuel tubes in nuclear reactors. Extreme radiation damage is simulated by an alternative and more efficient method to molecular dynamics, that of Frenkel pair accumulation (FPA).

D. Mason (UK Atomic Energy Authority, UK) described modelling activities carried out at UKAEA on highly-damaged materials at the "high-dose limit" where saturation of damage is often observed (> 0.1 displacements per atom); the results are used to predict the deuterium retention capacity of tungsten as a function of radiation exposure, with a good match to experimental data.

The remainder of the meeting was spent in discussion sessions involving all participants:

- Prospects for improvement and expansion of CascadesDB and DefectDB: data exists but the time and expertise required to put it into the correct format for upload may prohibit large-scale adoption. New functionality should be added to the websites to facilitate upload by users.
- Further practical aspects: data availability, validation, provenance and licensing; CascadesDB should continue to be maintained and available at the IAEA website, though the CSaransh software cannot be operated at this location for security reasons. Therefore, the existing service at https://cascadesdb.org should also continue to be maintained as a mirror service. CascadesDB data is freely available and licensed under either the Apache 2.0 or Creative Commons 4.0 Public License.
- Formulation of future plans and roadmap: several participants expressed an interest in high-dose damage simulations and in adding functionality for curating such data sets, which typically rely on computational techniques other than molecular dynamics for reasons of efficiency. This can be explored when data is made available.

The abstracts of the participants' presentations are given in Appendix 3 and are available on the AMD Unit's website at https://amdis.iaea.org/meetings/ccn-7/.

Appendix 1: Meeting Participants

Utkarsh BHARDWAJ, PEB-3, Computational Analysis Division, Bhabha Atomic Research Centre, Gandivanipalem, Dossuru Panchayat, Atchuthapuram Mandal, VISAKHAPATNAM, Andhra Pradesh 531011, INDIA

Max BOLEININGER, Culham Centre for Fusion Energy, ABINGDON, Oxfordshire, OX14 3DB, UNITED KINGDOM

María J. CATURLA, Universidad de Alicante, Dept. Física Aplicada, Facultad de Ciencias, Fase II, E-03690 ALICANTE, SPAIN

Huiqiu DENG, Hunan University, School of Physics and Electronics, CHANGSHA, CHINA

Christophe DOMAIN, EDF R&D, Lab Les Renardières, Dpt MMC, F-77250 MORET SUR LOING, FRANCE

Sergei DUDAREV, Culham Centre for Fusion Energy, ABINGDON, Oxfordshire, OX14 3DB, UNITED KINGDOM

Fei GAO, University of Michigan, Department of Nuclear Engineering and Radiological Science, 2355 Bonisteel Blvd, MI 48109-2014 ANN ARBOR, USA

Sehila GONZÁLEZ DE VICENTE, IAEA Division of Physical and Chemical Sciences, Nuclear Data Section, Vienna International Centre, A-1400 VIENNA, AUSTRIA

Alexandra GORYAEVA, Bat. 520, CEA Saclay, 91191 GIF SUR YVETTE, FRANCE

Fredric GRANBERG, Department of Physical Sciences Accelerator Laboratory, University of Helsinki, Pietrari Kalmin katu 2, P.O. Box 43, 14 HELSINKI, FINLAND

Kalle HEINOLA, IAEA Division of Physical and Chemical Sciences, Nuclear Data Section, Vienna International Centre, A-1400 VIENNA, AUSTRIA

Christian HILL, IAEA Division of Physical and Chemical Sciences, Nuclear Data Section, Vienna International Centre, A-1400 VIENNA, AUSTRIA

Byeongchan LEE, Kyung Hee University, 1732 Deogyeong-daero, YONGIN, Gyeonggi 17104, REPUBLIC OF KOREA

Daniel MASON, Culham Centre for Fusion Energy, ABINGDON, Oxfordshire, OX14 3DB, UNITED KINGDOM

Kai NORDLUND, Department of Physics, University of Helsinki, P.O. Box 43, Pietari Kalmin katu 2, 00014 HELSINKI, FINLAND

Andrea SAND, Aalto University, Otakaari 5, FI-02150 ESPOO, FINLAND

Marta SERRANO, Centro de INvestigaciones Energeticas Medioambientales y Technologicas (CIEMAT), Avenida Complutense, MADRID, SPAIN

Wahyu SETYAWAN, Pacific Northwest National Laboratory, Bldg 3410, Rm 2207, PO Box 999, MSIN J4-55, 99352 RICHLAND WA, USA

Jiting TIAN, Department of Physics, Peking University, BEIJIN, CHINA

Manoj Kumar WARRIER, PEB-3, Computational Analysis Division, Bhabha Atomic Research Centre, Gandivanipalem, Dossuru Panchayat, Atchuthapuram Mandal, VISAKHAPATNAM, Andhra Pradesh 531011, INDIA

Appendix 2: Meeting Agenda

Monday, 18 October 2021

14:00 – 14:30	Melissa DENECKE (DIR-NAPC), Arjan KONING (SH-NDS), Christian HILL (UH, AMD Unit): Welcome, introduction of the participants, adoption of the agenda
14:30 – 15:00	**Marta SERRANO**, *Centro de Investigaciones Energeticas, Medioambientales y Tecnologicas, Spain* Status of the ENTENTE database, Sept 2020 – Oct 2021
15:00 – 15:30	**Andrea SAND**, *Aalto University, Finland* Electronic energy losses in collision cascade simulations
15:30 – 15:50	Virtual Coffee Break
15:50 – 16:20	**Fei GAO**, *Department of Nuclear Engineering and Radiological Science, University of Michigan, United States of America* Radiation Resistance in Multicomponent Equiatomic Alloys
16:20 – 16:50	**Wahyu SETYAWAN**, *Pacific Northwest National Laboratory, United States of America* Cascade simulations in W-Ni-Fe heavy alloys and DFT study of He interaction with transmutation solutes in nano ferritic alloys

Tuesday, 19 October 2021

14:00 – 14:30	**Huiqiu DENG**, *Hunan University, China* Interatomic potentials and displacement cascade simulations for W and W-based alloys
14:30 – 15:00	**Christophe DOMAIN**, *EDF R&D Lab Les Renardières, France* Statistical analysis of displacement cascades in Fe, W and Ni ; solute segregation at grain boundaries in Fe
15:00 – 15:20	Virtual Coffee Break
15:20 – 15:50	**Christian HILL**, *IAEA, Austria* The IAEA CascadesDB and DefectDB databases
15:50 – 16:20	**Utkarsh BHARDWAJ**, *Computational Analysis Division, Bhabha Atomic Research Centre, India* Integration of CSaransh with CascadesDB
16:20 – 16:50	**Manoj Kumar WARRIER**, *Computational Analysis Division, Bhabha Atomic Research Centre, India* Defect Cluster Classification, Morphology and Stability Studies from Molecular Dynamics Simulations of Collision Cascades

Wednesday, 20 October 2021

14:00 – 14:30	**María J. CATURLA**, *Department of Applied Physics, University of Alicante, Spain* Collision cascades in the presence of dislocations
14:30 – 15:00	**Alexandra GORYAEVA**, *(CEA Saclay), France* Machine learning for atomistic materials science
15:00 – 15:30	**Jiting TIAN**, *Institute of Nuclear Physics and Chemistry (CAEP), China* Computational studies of high-dose radiation damage in hcp Zirconium
15:30 – 15:50	Virtual Coffee Break
15:50 – 16:20	**Daniel MASON**, *Culham Centre for Fusion Energy, United Kingdom* Simulated irradiation in the high-dose limit
16:20 – 17:00	Discussion (all participants)

Appendix 3: Presentation Abstracts

Integration of CSaransh with CascadesDB

Utkarsh Bhardwaj[1], Christian Hill[2] and Manoj Warrier[1]
1. Bhabha Atomic Research Centre, India; 2. International Atomic Energy Agency

Cascades Saransh (CSaransh) is an open source project for collision cascades analyses and visualization. We recently integrated CSaransh with IAEA's open database of collision cascades, CascadesDB. CSaransh has two modules. The first module, AnuVikar, takes the xyz files and meta information as input, and outputs a cleaned json file having defect coordinates and other properties such as defect morphologies and sizes, cascade volume and sub-cascade measure etc. for each cascade. It has a number of new algorithms that involve SaVi [1], a Graph based defect morphology identification algorithm, Unsupervised Machine Learning method to visualize and search for similar defect morphologies [2] etc. CSaransh features a single page modern web application to visualize defects and their morphologies, find patterns and correlations, and plot statistical trends. The output of AnuVikar can be loaded to CSaransh web application.

We processed over 2000 cascades from CascadesDB with AnuVikar. It processed this data with size over 140GB in under an hour and produced a 40 MB output file. The dataset that we have currently consists of all the cascades that are initially perfect and have no-surface defects. As with any large dataset, there were also cases where the data had inconsistencies and errors. The errors and warnings are written by AnuVikar in a log file after it processes the data. The errors range from general file corruption to errors in schema, to domain specific errors and inconsistencies between xyz files and meta information. These errors can either result in inability to process cascade or make it stand out as an outlier in the database. AnuVikar can estimate various parameters such as box-dimension, origin, lattice-constant if it finds the given parameters inconsistent with the Xyz file.

In this presentation we will introduce CSaransh with a live demo of the web-application from https://cascadesdb.org/csaransh. With integration of CSaransh one can easily browse through the CascadesDB data, and look for different patterns, statistics, and correlations. CSaransh with CascadesDB, provides an easy way to draw data-driven conclusions on collision cascades. We will then discuss the issues we found in the CascadesDB dataset after its validation with CSaransh. The integration of CSaransh with CascadesDB will help in mitigating errors in the database automatically, which becomes more crucial as the data grows.

Collision cascades in the presence of dislocations

María José Caturla
Department of Applied Physics, University of Alicante, Spain

Since the first calculations of collisions cascades, there has been a large amount of data compiled for the formation of defects in metals and semiconductors due to energetic primary knock-on atoms with energies from a few eV to several hundreds of keV. Most of the calculations existing in the literature are performed in pristine samples. Only a few examples exist where collision cascades are performed next to grain boundaries and even less next to dislocations.

In this presentation, we review a few of the latest calculations of irradiation of Cu and Fe in the presence of edge dislocations. We observe that, in the case of f.c.c. metals such as Cu, the presence of the dislocation enhances the formation of stacking fault tetrahedra defects and strong interactions between self-interstitial clusters and the dislocations are also observed including change of orientation of motion of these clusters. In Fe the most striking effect is the induced motion of edge dislocations by the shock wave produced by the collision cascade as well as the enhanced formation of vacancy clusters.

Interatomic potentials and displacement cascade simulations for W and W-based alloys

Huiqiu Deng[1], Yangchun Chen[1], Lixia Liu[1], Rongyang Qiu[1], Jingzhong Fang[1], Bowen Huang[1], Wangyu Hu[1], Ning Gao[2], Fei Gao[3]

[1] Hunan University, Changsha 410082, China

[2] Shandong University, Qingdao 266237 , China

[3] University of Michigan, Ann Arbor, MI 48109, United States

Tungsten (W) and W-based alloys are considered as the most promising plasma-facing materials for future fusion reactors due to their excellent performance. In this presentation, we will talk about some recent work in our group as following. First of all, a series of interatomic potentials for W, W-based alloys (such as W-Mo/Re/Ta/V) and W-V/Mo/Ta-He systems were developed for the displacement cascade simulations; then we performed systematic investigations on the displacement cascades in bulk W and W-base alloys with molecular dynamics simulations. Based on our potentials and molecular dynamics simulations, the displacement cascade database for W has been constructed, including seven typical PKA directions with 11 PKA energies ranging from 1 keV to 300 keV, totally 1700+ cascade events. The nucleation of C15 clusters has been observed in W bulk, and a new formation mechanism of <111> interstitial loops via the collapse of C15 clusters will be discussed. We also found that temperature gradient field will result in the directional diffusion of <111> dumbbell and 1/2<111> interstitial loop in W from the cold to the hot region, while stress gradient field will let the <111> dumbbell and 1/2<111> interstitial loop move toward the region where the stress is concentrated. The effects of transmutation elements, such as Re and Ta, on the generation and evolution of defects were analyzed. It was found that both the presence of Re and Ta atoms do not significantly affect the number of surviving defects, while the Re atom segregation has pinning effect on the mobility of defect clusters, and the presence of Ta inhibits the transition from <100> dislocation loops to 1/2<111> ones at high temperature. These results can provide important acknowledge for predicting the microstructural evolutions of W-based materials under radiation.

Radiation Resistance in Multicomponent Equiatomic Alloys

Fei Gao
Department of Nuclear Engineering and Radiological Sciences, University of Michigan,
Ann Arbor, MI 48109, USA

Multicomponent equiatomic alloys, including medium- and high-entropy alloys (MEAs and HEAs), have been demonstrated notably high irradiation resistance, which is commonly attributed to their extraordinary interstitial behaviors or chemical disorder. The recent progress in simulating radiation damage and microstructural evolution in multicomponent equiatomic alloys will be discussed and some interesting results will be highlighted. These simulations provide the detailed mechanisms on the generation and evolution of irradiation-induced defects in face-centered cubic MEAs and HEAs to understand the new mechanisms of their irradiation tolerance. As compared with Ni, the primary radiation damage produced by displacement cascades in a HEA-NiCoCrFe exhibits delayed defect accumulation and enhanced defect suppression, which is attributed to the stronger thermal spike, lower thermal conductivity, and smaller binding energy of interstitials. In addition, the interaction of the displacement cascades with a pre-existing stacking fault tetrahedron (SFT) in a MEA-NiCoCr and Ni is employed to understand their differences of void swelling. The probability for SFTs to directly transfer to voids under irradiation in the NiCoCr MEA is much smaller than that in Ni, which is due to their lower formation energy and higher binding energy relative to those of voids in the NiCoCr MEA. This probably provides a novel pathway for void swelling resistances in MEAs and HEAs, as observed in experiments. The correlation between the defect behaviors and irradiation resistance is found to play an important role in controlling material performance under irradiation, thus providing significant insights and strategic guidance for developing MEAs and HEAs for nuclear applications.

Keywords: High entropy alloys; Medium entropy alloys; Displacement cascade; Radiation resistance; Defect evolution

Machine Learning for Atomistic Materials Science

A.M. Goryaeva[1], T. D. Swinburne[2], C. Lapointe[1], J. Baima[1], J. Dérès[1], M.-C. Marinica[1]

[1]DEN - Service de Recherches de Métallurgie Physique, CEA, Université Paris-Saclay, F-91191 Gif-sur-Yvette, France
[2]CNRS, Centre Interdisciplinaire de Nanoscience de Marseille (CINaM), Université Aix-Marseille, France

Multi-scale approaches in materials science face a traditional dichotomy in the choice of the atomistic force fields: robust, accurate and numerically expensive *ab initio* methods against less transferable but fast empirical methods. The ML methods propose a third avenue that allows control of the balance between the accuracy and numerical efficiency. Moreover, the ML-based vision of fundamental concepts in materials science, such as structural defects, can augment and revise traditional interpretations.

We will present recent advances in atomistic material simulations by means of machine learning and data-driven approaches.

Machine learning (ML) methods cannot fully replace traditional approaches in physics and/or materials science. The phase space in physics / materials science has a well defined structure and is too vast and complex to be described only by the inherent statistical correlations within the data points. Statistical methods trained on the physical data can be of great help when the traditional approaches are limited and/or their direct application is hindered by factors such as high computational cost.

In metals, the interaction and transformation of crystal defect networks give rise to an extraordinarily diverse range of defect morphologies [1]. Using the recently developed package MiLaDy (Machine Learning Dynamics) [2]: (i) we redefine the concept of defects in materials science [3]; (ii) we provide reliable force fields for complex defects such as interstitial, dislocation loops, dislocations; (iii) we are able to explore the atomistic free energy landscape of point defects in metals with *ab initio* accuracy up to the melting temperature [4], and, finally, (iv) we are able to propose surrogate models that bypass the traditional approaches [5]. We exemplify and discuss, in the framework of experimental findings, the case of energetic landscape of defects in body-centered and face-centered cubic metals.

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[2] M.-C. Marinica, A. M. Goryaeva, T. D. Swinburne *et al*, MiLaDy - Machine Learning Dynamics, CEA Saclay, 2015-2021 ; A.M. Goryaeva, J.-B. Maillet, M.-C. Marinica. Comp. Mater. Sci. **166**, 200 (2019)
[3] A. M. Goryaeva *et al*. Nature Commun. **11**, 4691 (2020)
[4] C. Lapointe *et al*. (to be submitted); T.D. Swinburne, M.-C. Marinica, Phys. Rev. Lett. **120**, 135503 (2018)
[5] C. Lapointe, T. D. Swinburne *et al*. , Phys. Rev. Materials **4**, 063802 (2020); F. Bruneval *et al*. J. Chem. Theory Comput. **16**, 4399 (2020)

Simulated irradiation in the high dose limit

Daniel Mason, Fredric Granberg, Max Boleininger, Abdallah Reza, Felix Hofmann, Thomas Schwarz-Selinger and Sergei Dudarev

Modelling highly damaged materials – exposed to over 0.1 displacements per atom (dpa) – where saturation of damage is often observed, is difficult because a microstructure containing high density of defects evolves non-linearly as a function of dose. In this study we show how to determine both hydrogen retention and thermal diffusivity changes in tungsten exposed to high irradiation dose, using no adjustable parameters.

First, we generated converged high dose (>1 dpa) microstructures, using a combination of the creation-relaxation algorithm (CRA) and massively overlapping collision cascade molecular dynamics (MD) simulations. We make robust estimates of vacancy and void regions using a modified Wigner-Seitz decomposition. The resulting estimates of the void surface area is used to predict the deuterium retention capacity of tungsten as a function of radiation exposure. The predictions were compared to deuterium retention measured by nuclear reaction analysis.

The theory gives an excellent match to the experimental data, with both model and experiment showing that 1.5-2.0 at.% deuterium is retained in tungsten in the limit of high dose. We then make robust estimates of the total defect content by statistically comparing the atomic potential energy distribution to the expected thermal distribution. With the defect count identified, and a simple model relating electronic scattering rate to excess energy with a single parameter- the resistivity per Frenkel pair- we compute conductivity changes as a function of dose. These were compared to thermal diffusivity measurements made at low temperature using transient grating spectroscopy, and found to give an excellent match over the range of doses studied.

We conclude that combining CRA and MD generates high quality microstructures, and that from these we can make forward predictions for low-temperature engineering properties as a function of elastic boundary conditions and dose, without needing user reparameterization.

Electronic energy losses in collision cascade simulations

Andrea E. Sand
Aalto University, Finland

Electrons couple to atoms through two distinct processes, i.e. electronic stopping in the high energy limit and electron-phonon coupling in the low energy limit. In collision cascades, atoms transition smoothly from one regime to the other, and a clear physically motivated threshold between these two regimes cannot be determined. This gives rise to significant challenges for incorporating electronic effects in large scale atomistic simulations. In this talk, I present the latest developments towards this goal.

By extensive quantum mechanical calculations, we can determine the electronic energy losses in specific local environments, in particular, as a function of the local electronic density seen by the projectile or atom. Using a model that approximates the energy losses as a function of the electronic density modelled in the atomic system, we are able to simulate energetic collision cascades in multi-million atom systems with both electronic stopping and electron-phonon coupling, without imposing cut-off parameters. We find that two energy loss regimes during cascade evolution emerge from this model, with a transition in the rate of energy losses occurring between the early ballistic phase and later relaxation phase of the cascade. The two stages of energy losses clearly capture the two different coupling regimes, with energy losses corresponding to electronic stopping in the early phase of a cascade and electron-phonon coupling in the later phase.

Cascades in fcc Ni-Fe Solid Solution and He Interaction with Solutes and Impurities in Nano-structured Ferritic Alloys

Wahyu Setyawan
Pacific Northwest National Laboratory, Richland, WA, USA 99352

Molecular dynamics is employed to simulate atomic collision cascades in a Ni-30at.%Fe fcc solid solution. Electronic stopping is modeled as a frictional force for atoms with kinetic energy > 10 eV. Cascades are performed at 700 °C, with a primary knock-on atom energy (E_{PKA}) up to 70 keV. Comparison of cascades initiated with Ni versus Fe PKAs shows that the defect production is similar. Both types of PKA also produce a similar fraction of Ni defects, which is approximately the same as the fraction in the alloy. The defect production curve as a function of E_{PKA} exhibits two regimes of power law, where the high-energy regime occurs for E_{PKA} > 10 keV. In the high-energy regime, > 80% of interstitial defects are clustered and the average size (number of interstitials) of the largest clusters is > 10. For small clusters (size < 10), the dominant Burgers vector is <100>, while for larger clusters (>10), it is <110>. Cascades in pure Ni are simulated with E_{PKA} = 20 and 50 keV for comparison. The results show that defect production and clustering in the alloy is smaller than in Ni. In the second part of this presentation, density functional theory is employed to study the interaction between He and transmutation products, alloy solutes, and impurities in 14-YWT nano-structured ferritic alloy. Strong attraction is found between a substitutional He with Y (binding energy = 1.24 eV), Mg (0.52), Ti (0.34), Si (0.34), Al (0.32), Ni (0.26), Ta (0.23), Mn (0.16), Mo (0.10). For an interstitial He, it is strongly attracted to Y (0.46), Mg (0.32), Ti (0.16). These interactions could potentially promote He bubble nucleation and increase the population of small He bubbles that are invisible under an electron microscope; yet contribute to void swelling. Interstitial He is also attracted to impurity O (0.33), C (0.15), and N (0.12). Under fusion neutrons, approximately 3-5 times more H is produced than He. Thus, the interaction with H is also studied. Hydrogen is found to be strongly attracted to substitutional He (0.56), suggesting that hydrogen may exacerbate the He bubble formation in these alloys.

Computational studies of high-dose radiation damage in hcp Zirconium

Jiting TIAN
Institute of Nuclear Physics and Chemistry (INPC), China Academy of Engineering Physics (CAEP), Mianyang, China

Heavy damage in materials induced by high-dose irradiation is important both for fundamental materials science and nuclear industrial applications. Benefited from recent developments of computational power, resources, and methods, it's possible now to simulate high-dose irradiation damage in metal crystals on the atomic scale. In this talk, I'll introduce our recent computational studies on high-dose radiation damage in hcp Zirconium (Zr), a widely-used material for fuel tubes in nuclear reactors. First, I'll show that a simple simulation of repeated collision cascades in the same box (i.e. cascade overlap) is able to give some novel insights on the formation of basal vacancy loops (<c>-type loops), which is a typical and important defect in heavily-irradiated Zr. Then I'd like to introduce another efficient method to simulate high-dose radiation, i.e., Frenkel pair accumulation (FPA) method, which is able to reach a dose level as high as several dpa. Using this method, I explore the extreme radiation damage in Zr, observing an asymptotic approach to a steady damage level, which features a high point defect content (~3%), nanoscale dislocation lines and loops, and significant anisotropic deformation strains. Finally I'd like to compare the defect accumulation in metals and non-metals from a potential energy landscape perspective.

Defect Cluster Classification, Morphology and Stability Studies from Molecular Dynamics Simulations of Collision Cascades

M. Warrier, U. Bhradwaj, A. Sand

A brief introduction to the earlier classification of defect clusters using artificial Intelligence techniques is presented [1]. A new method of classifying defects using a graph data structure has been developed [2]. The advantages of the new method, viz. (i) obtaining the internal morphology of the defect cluster (ii) orientation of its homologous components, etc., wil be discussed. We apply the new method to analyze collision cascades in W at 100 - 200 keV primary knock-on atoms (PKA) using three different ineraction potentials [3. Results of the distribution of different defect clusters for the three potentials show that there exist a basic set of six defect morphologies in W. The fraction of the different morphologies vary based on the potential used.

Preliminary results of the stability of the <100> defect clusters of varying sizes using the three interatomic potentials are then presented.

References

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Nuclear Data Section
International Atomic Energy Agency
Vienna International Centre, P.O. Box
100 A-1400 Vienna, Austria

E-mail: nds.contact-point@iaea.org
Fax: (43-1) 26007
Telephone: (43-1) 2600 21725
Web: http://nds.iaea.org