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

Summary Report of the 6th Biennial Technical Meeting of the Code Centres Network

IAEA Headquarters, Vienna, Austria
16 – 18 October 2019

Prepared by

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January 2020

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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 6th Technical Meeting described in this report, 11 experts in the field of Molecular Dynamics (MD) simulations of radiation damage reviewed CascadesDB, a database of atomic configurations generated by MD simulations of collision cascades. This database is developed and hosted by the AMD Unit and provides a central repository for the results of MD simulations of the evolution of a material's structure following an impact by a high energy particle. Further plans to extend and enhance CascadesDB, and to establish a new database resource, DefectDB, containing density functional theory calculations of defect structures were also discussed.

January 2020

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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 5th Technical Meeting on the International Code Centres Network (CCN5) at IAEA Headquarters from 16 – 17 November 2017. This meeting is described in detail in the International Nuclear Data Committee (INDC) report INDC(NDS)-0753 available at https://www-nds.iaea.org/publications/indc/indc-nds-0753/ and online at https://amdis.iaea.org/meetings/ccn-5/. Experts in Molecular Dynamics simulations discussed the construction of 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. This database resource has been realised as CascadesDB.

This report documents the 6th CCN meeting, which was held at IAEA Headquarters from 16 – 18 October 2019 to review CascadesDB project and to propose enhancements and extensions to the service. The following sections contain the meeting proceedings (Section 2), details of discussions (Section 3), and a summary and list of recommendations made by the participants (Section 4). Appendix 1 provides a template for the metadata model for DefectDB, a proposed database of DFT calculations of defect structures in nuclear materials which is described in Section 3.4. Appendices 2, 3 and 4 list the participants, the meeting agenda, and abstracts of the participants' presentations.

2. Proceedings

The 6th Code Centres Network Meeting was opened by 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 3).

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 development and deployment of the CascadesDB database initiated by the previous CCN meeting (https://

amdis.iaea.org/meetings/ccn-5/). CascadesDB, at the time of writing, contains 132 GB of data in 1532 simulations across 176 archives and is available at on the IAEA's website at https://cascadesdb.iaea.org.

S. L. Dudarev (UKAEA, UK) provided a summary of recent developments in atomistic density functional theory, molecular dynamics and elasticity-based simulations, which form a foundation for the Virtual Tokamak model. The new capabilities offered by the availability of the IAEA CascadesDB database were detailed.

A. E. Sand (University of Helsinki, Finland) presented an analysis of the main sources of uncertainty in the predictions of molecular dynamics simulations of collisional cascades, particularly in relation to the variation predicted for different metallic materials. She discussed the available experimental data and its use in validating such theoretical simulations, and outlined future directions for improving the accuracy of these simulations.

R. Voskoboynikov (Kurchatov Institute, Russia) provided a summary of research at the Kurchatov Institute into ordered materials in nuclear engineering and other radiation technologies. The effect of composition on interstitial stoichiometry and predictions of the radiation resistance of α_2-Ti_3Al, γ'-Ni_3Al and γ- TiAl were reported.

A. Nomoto (Materials Science Research Laboratory, Central Research Institute of Electric Power Industry, Japan) described experimental studies of radiation damage in reactor pressure vessel steels.

W. Setyawan (Pacific Northwest National Laboratory, USA) described a molecular dynamics study of various fcc W-Ni-Fe composite alloys, proposed materials with improved fracture toughness and ductile-to-brittle transition temperature properties for use in future experimental fusion devices.

M. Serrano (Centro de Investigaciones Energeticas, Medioambientales y Tecnologicas (CIEMAT), Spain) summarized the work of the Division of Materials for Energy, highlighting the activities of the Horizon-2020 M4F (Multiscale Modelling for Fusion and Fission Materials) project in relation to the scope of the meeting. She also outlined the Horizon-2020 project proposal, ENTENTE (European Database for Multiscale Modelling of Radiation Damage) and plans for collaboration with the community of the CCN.

M. Warrier (Bhabha Atomic Research Centre, India) provided a summary of his research group's activities in multi-scale modelling of material damage in nuclear materials due to surrogate ion irradiation (as a proxy for neutron irradiation). These simulations involve a combination of binary-collision approximation Monte Carlo (BCA-MC) and molecular dynamics techniques, and have recently been extended by the inclusion of electronic stopping and utilising methods from machine learning (ML) to classify defect structures.

M. C. Marinica (DEN – Service de Recherches de Métallurgie Physique, CEA, France) continued the theme of machine learning with a description of his group's recently-developed package MiLaDy (Machine Learning Dynamics) to explore the energetic landscape of defects in materials. He further detailed work on semi-supervised ML to identify and classify defect structures.

M. Caturla (University of Alicante, Spain) reviewed the different types of materials and conditions that are useful in a collisional cascades database, highlighting the need for cascade simulations for pre-damaged materials. She then discussed how to improve the access of different researchers working on multi-scale models with these data, with a focus on analysis tools, recommendations and data processing.

C. Domain (EDF R&D Lab Les Renardières, France) presented work carried out by EDF in assembling a large database of density functional theory calculations of defect and solute clusters in important nuclear materials (with applications both for fission and for fusion). The huge number of such calculations that are needed to characterize all the possible interactions in materials such as reactor pressure vessel steels was emphasized.

M. Warrier (Bhabha Atomic Research Centre, India), presenting on behalf of U. Bhardwaj, described CSaransh, an open source application that builds upon CascadesDB and provides a suite of browser-based data exploration and interactive visualization tools (see also Section 3.3).

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

- Prospects for improvement and expansion of CascadesDB;
- Provision and exploitation of experimental and theoretical data sets of relevance to radiation damage;
- Practical aspects: data availability, upload, validation, provenance and licensing; Formulation of future plans and roadmap.

A summary of these discussions is given in the following section.

The abstracts of the participants' presentations are given in Appendix 4 and are available on the AMD Unit's website at https://amdis.iaea.org/meetings/ccn-6/.

3. Discussions

3.1 Current status of CascadesDB

The CascadesDB database initiated by the 5th Code Centres Network meeting is a fully-functioning service, hosted by the IAEA at https://cascadesdb.iaea.org/. At the time of writing it hosts about 132 GB of data in 1532 simulations across 176 archives and includes collisional cascades simulations in W, Fe, Cu, Au, Ag, Ni, Pd and Pt utilising 14 different interatomic potentials. Data has been provided by five research institutes, and the need for more contributions was communicated.

A browser-based search interface can be used to query the database by author name, publication DOI, material chemical formula, initial temperature, PKA energy and archive name. An XML Schema describing the metadata has been developed; the metadata itself is stored in a relational database and can be output in XML, HTML or plain text formats.

Further information and resources are available on the CascadesDB website at the page https://cascadesdb.iaea.org/cdbmeta/doc.

3.2 Extensions to CascadesDB

Extensions to the existing CascadesDB were discussed in particular to address questions of radiation damage in complex microstructure and at high dose. In relation to this, it can be noted that the original specification for the database included the possibility of contributing results of cascade simulations in non-perfect crystal, which in the domain of collision cascades on the molecular dynamics time scale addresses both of these questions. However, current data entries only consist of simulations performed for initially perfect crystals. A number of the meeting participants hence agreed to contribute existing data for cascade damage in simulation cells including one-dimensional defects (point defects and small clusters), dislocation lines, grain boundaries and surfaces. Adding the main classes of "dislocation line" and "grain boundary" as optional attributes in the metadata (analogously to "surface" currently included in the metadata specification), in the event that non-perfect initial crystal is first indicated, was considered potentially useful.

Another possible extension in terms of a database of potentials was discussed, including properties of those potentials, such as predicted defect formation and migration energies, etc. While such a database would indeed be valuable, it was tacitly agreed that this would constitute a technically separate project, and should thus take lower priority compared to pushing for the growth and visibility of the CascadesDB. As an aside, a similar project already exists (https://catalog.data.gov/dataset/nist-interatomic-potentials-repository), and one might consider instead the possibility of linking to this database where appropriate, and/or encouraging CascadeDB contributors to supply the potential, if possible, in this existing database.

In order to increase visibility of the CascadesDB, as well as to lower the threshold to adoption for potential users, it was suggested to extend the functionality of CascadesDB to include visualization. This could be done semi-automatically, for example with a script that can take as input the file type as required by the database specification, and run an analysis (for example using CSaransh or Ovito) of the atomic configurations; these can then be stored in the database alongside the atomic coordinate file, and used to directly visualize the defect content of the particular entry. Visualization could be implemented either as a static picture, or through a dynamic visualizer embedded in the website.

The CascadesDB database has the potential to become a valuable resource to the nuclear materials community, but requires more, and more varied data. The participants in this meeting have a variety of research interests spanning many different relevant materials and structures and have offered to provide data sets described in Table 1.

Table 1. *Collisional cascades data offered by meeting participants*

Participant (initials)	Material
A. S.	Au, Cu, surfaces, defective structures
M. C.	Fe, Cu, cascades on dislocations
S. D.	Highly-irradiated steels
R. V.	Metal-metal alloys, Zr, Cu
M. W.	W, Fe
C. D.	W, Fe, (Ni, fcc alloys, …)
M. C. M.	Highly-irradiated Fe
B. L.	W, W-Re
A. N.	Fe

The difficulty of providing data where it has been archived was noted. In some cases, only compressed binary files are available, from which the required plain-text .xyz files would have to be reconstructed. In the most extreme cases, only the positions of atoms in the immediate vicinity of identified defect structures were retained: in this case, the data sets are unlikely to be suitable for inclusion in CascadesDB.

It was further agreed that CascadesDB would benefit from frequent and widespread advertising, for example in conjunction with presentations at conferences and/or international meetings. Relevant upcoming events were identified as:

- The 19th International Conference on Fusion Reactor Materials (ICFRM-19), to be held in November in La Jolla, CA, USA. Kalle Heinola will represent the IAEA at this meeting and present the CascadesDB project.
- The 15th Conference of Computer Simulation of Irradiation Effects in Solids (COSIRES-2020) meeting in Porquerolles in June 2020.
- The 24th International Conference on Plasma-Surface Interactions in Controlled Fusion Devices (PSI-24) in Jeju, South Korea in May 2020.
- The Nuclear Materials conference, NuMat, to be held in Ghent in October 2020.
- The 10th Multiscale Materials Modelling conference (MMM), to be held in October 2020 Baltimore, USA.

Note: The COVID-19 pandemic outbreak that started in January 2020 has led to many of these events being postponed to 2021.

The joint publication, that was agreed upon during the first cascades database meeting held two years ago, will now be pushed through to submission, providing a permanent link to the CascadesDB in the literature. Such a permanent link should hence be set up and confirmed before final publication of the paper.

3.3 Analysis, validation and visualization software tools for CascadesDB

This section describes the CSaransh software tool developed by the group of M. Warrier and offered for deployment on the CascadesDB database.

The initial version of CSaransh lays the foundation for exploring radiation damage database for patterns, correlations and comparisons. Unlike existing tools which focus on analyzing one cascade at a time, CSaransh has been built with the primary focus on working with a complete database, extracting patterns from it using machine learning (ML) techniques and enabling qualitative assessment of the results and statistical patterns to guide further development of methods. Some of the new parameters that it introduces using ML are pattern matching of clusters present in the database, their classification, number of sub-cascades and volumes of cascades, etc.

Another important enhancement required for CascadesDB is the automatic validation of data submitted to the database. This is to ensure adherence to the specifications and recommendations set by the data model and so to improve the reliability and quality of the database for users. The CSaransh software tool is a significant step towards this goal.

Extending understanding of existing parameters

CSaransh aspires to be not limited to certain set of algorithms but to be a platform on which different algorithms can be statistically and qualitatively assessed from the cascades database. An example of this is the presence of different features such as triad-angles, pair-wise distances and adjacency for cluster shape pattern matching and classification. Future plans include the extension of the functionality to include point-cloud based features and neural network based features, amongst others. This is also true for basic parameters such as number of defects and number of sub-cascades which are ambiguous and not standard. It is anticipated that the comparison of techniques on an open web platform might prove to be very helpful; the use of the JSON format which is interoperable between languages makes it easy to add parameters with algorithms implemented in any language of choice or by using existing tools.

Adding new parameters

The data exploration features currently available concerning defect morphology and geometry will soon be augmented with others such as cascade and sub-cascade shape, pattern matching and classification. These new additions would be accompanied by new suitable interactive visualizations. The output results are directly useful to multi-scale modelling by providing, for example, the distance distribution of defects with cluster class distribution for each sub-cascade. Some of the feature additions proposed are:

- Determining whether a particular high-energy cascade is composed of sub-cascades that are similar to cascades formed by lower energy PKAs? If so, can low-energy cascades that look similar be found in the database?
- Adding physical properties of cluster shapes for each class of clusters such as thermal stability, diffusion, dislocation.

Scaling up and development

Another aspect of the development would be to make CSaransh more scalable, efficient, accessible and easy to use. Adding a JSON database system without changing the existing code can enable it to scale to huge databases. Work continues on these areas, and contributions for improving documentation and help features for the CSaransh interface are welcomed. Csaransh in its present form provides an online, interactive Python notebook to select data points, process, summarize and sample within the CascadesDB database without any installation. This allows users to look at the statistics and patterns in the database using traditional or machine learning techniques, and can be achieved using online Python notebook server environments such as, for example, Binder (https://jupyter.org/binder) or Google's Colab environment (https://colab.research.google.com/). With these accessible modern technologies in-place, it is hoped that community engagement, allowing researchers to easily experiment with the database, can be facilitated.

3.4 DefectDB: a database of DFT calculations of defect structures

A new data resource, tentatively named DefectDB, was proposed to catalogue DFT calculations of radiation-induced defect structures in materials of interest to nuclear fusion and fission applications. A browser-based search interface and relational database backend for the resource will be developed and deployed at the IAEA, with the assistance of M. C. Marinica and colleagues. Three main types of calculation will be initially considered:

(a) Structural relaxation (geometry);

(b) Pathway minimization;

(c) Molecular dynamics.

The defects considered are to be divided into the following two broad categories.

- Point defects:
    - Self-interstitials
    - Vacancies
    - Solute-interstitials
    - Solute-substitutionals
- Extended defects:

- Surfaces
- Edge dislocations
- Screw dislocations
- Loops and mixed dislocations
- Grain boundaries
- Stacking faults
- Twin defects

Full attribution and source information for the data is required, along with details concerning the method of calculation and pseudopotential employed. A template for the plain-text version of the metadata that can be used by data providers wishing to upload their calculation output files to the database is provided as Appendix 1.

4. Summary and Recommendations

1. A permanent location for the CascadesDB database on the IAEA's domain should be obtained and established as the official website for the project. *Note*: this has now been set up and the database is accessible from https://cascadesdb.iaea.org/.

2. Efforts should be made to further populate the database with suitable collisional cascades simulations, starting with the data sets offered by the meeting participants (Table 1).

3. The CascadesDB service should be augmented with further analysis and visualization tools. The research group of M. Warrier have already made progress with compatible software tool, CSaransh, which is compatible with the data standards of CascadesDB; a consultancy visit to the IAEA is planned for May 2020 for deployment of this tool as a service on the CascadesDB server. *Note*: this visit has been postponed until later in 2020 because of the global COVID-19 pandemic.

4. The CascadesDB project will continue to be promoted at relevant international conferences and meetings, and an article detailing its development and current status written and submitted to a suitable journal.

5. A new database, DefectDB, should be established as a repository for DFT calculations of defect structures in materials of relevance to nuclear engineering, and deployed by the IAEA with a similar, searchable online interface. The group of M. C. Marinica have already initiated a project to define a suitable data model for this database; a consultancy visit to the IAEA in January 2020 is planned to develop this model for deployment. *Note*: a prototype website is available at https://db-amdis.org/defectdb.

6. A further meeting, the 7th Code Centres Network Meeting, should be held in October or November 2021 to review progress on the project, with a particular focus on uncertainty

quantification and propagation and the role of the CascadesDB and DefectDB data services in the ENTENTE project, if this is successfully funded.

Appendix 1: Template for DefectDB metadata

The first version of a template for providing metadata to DefectDB is given below. Metadata is provided either on a single line, or in the case of multi-line entries on one or more lines within text blocks delimited by three or more hyphens.

```
# Lines starting with a '#' symbol are treated as comments and not read in.

Attribution
===========

name: XXX                       [Single author name; optional]
institution: XXX                [one-line string; optional]]
email: XXX                      [valid email address]
url: XXX                        [valid URL; optional]

attribution-comments:           [Multi-line string; optional]
-----------------------
XXX
...
-----------------------

acknowledgements:               [Multi-line string; optional]
-----------------------
XXX
...
-----------------------


Source
======

source-doi: XXX                 [valid DOI or doi.org URL; optional]
source-url: XXX                 [valid URL; optional]


Content
=======

system-composition: XXX         [A_p B_q C_r ...; see note {3}]
matrix: XXX                     [chemical formula of dominant species in
                                 the material]
structure: XXX                  [fcc|bcc|hcp|dia|amorphous|liquid|other]
structure-comment: XXX          [specification of "other"; optional if
                                 "structure" is provided]
content-comment:                [Multi-line string; optional]
-----------------------
XXX
...
-----------------------

point-defect: <defect-type> <number> <matrix-atom> <defect-atom> [see note {4}]
point-defect: <defect-type> <number> <matrix-atom> <defect-atom> [see note {4}]
...

extended-defect: <defect-type>  [see note {5}]
extended-defect: <defect-type>  [see note {5}]
...


Calculation
===========

calculation-type: XXX           [structural relaxation|pathway minimization|
                                 molecular dynamics|other; see note {6}]
code-name: XXX                  [name of code, e.g. VASP]
code-version: XXX               [full version number of code]
exchange-correlation: XXX       [GGA|LDA|meta-GGA|hybrid-GGA|VOSKOWN|GGA+U]
exchange_correlation_comment:   [multi-line string; optional if
                                 "exchange-correlation" is provided]
-----------------------
```

```
XXX
...
-----------------------


kpoints: XXX                    [N N N S S S; mesh size along each direction
                                 and fractional shift; see note {7}]
kpoints-density: XXX            [D S; mesh density and fractional shift; see
                                 note {7}]
Ecut: XXX                       [Kinetic energy cut-off in eV; float]
smearing-type: XXX              [Fermi|Gaussian|Methfessel-Paxton|
                                 Partial occupancy|Tetrahedron]
smearing-energy: XXX            [Smearing energy in eV; float]

pseudopotential-name: XXX       [name of pseudopotential]
pseudopotential-class: XXX      [norm-conserving|ultrasoft|paw|all-electrons]
pseudopotential-url: XXX        [valid URL; one-line string; optional]
pseudopotential-semicore: XXX   [True|False]

convergence-criterion: XXX      [Tolerance criterion for electronic
                                 convergence; float]
magnetism-included: XXX         [True|False]
calculation-comment:            [multi-line string; optional]
-----------------------
XXX
...
-----------------------


Additional Fields
=================

archive-path: XXX               [Path to data files; see note {8}]
bulk-path: XXX                  [Path to bulk (reference) data files; optional;
                                 see note {9}]


Footnotes
---------
{1} All fields are mandatory unless indicated as optional

{2} Blank lines, and lines starting with the character '#' are ignored;
    Multi-line fields are entered between lines consisting entirely of three
    or more hyphens: '---'

{3} system-composition: one-line string of the form A_p B_q C_r ...: space-
delimited sequence of unique atom symbols (A, B, C) and number of atoms
(p, q, r) for each atom type


{4} point defects are specified on one or more lines with each line:
       <defect-type>: XXX      [self-interstitial|vacancy|solute-interstitial|
                                solute-substitutional]
       <number>: XXX           [number of this type of defect; integer > 0]
       <matrix-atom>: XXX      [A|B|C|...: identity of missing atom
                                (for vacancy defects) or substituted atom
                                (for solute substitution)]
       <defect-atom>: XXX      [identity of interstitial atom or identity of
                                substituent atom]

{5} extended defects are specified on one or more lines with each line:
       <defect-type>: XXX      [surface|edge-dislocation|screw-dislocation|
                                loops-mixed-dislocations|grain-boundary|
                                stacking-fault|twin]

{6} if other is specified for calculatiom-type, then the calculation-comment
    field must be completed

{7} specify exactly one of kpoints and kpoints-density

{8} paths are specified from and including the uploading user's data directory:
    e.g. marinica/Fe_SIE/Fe_bulk. Use Unix-style separators ('/') and do not
    use paths which include spaces. Do not include a leading slash. The path
    specified is to a directory containing the data files which will be
```

```
    turned into a bzip2-compressed tar archive; i.e. the downloaded data will
    be available from <URL>/marinica/Fe_SIE/Fe_bulk.tar.bz2

{9} If the calculation involves defects, optionally specify the path to an
    calculation of the bulk structure here. The path must exist already: ie
    the bulk calculation data must already be in the database
```

Appendix 2: Meeting Participants

Matteo BARBARINO, IAEA Division of Physical and Chemical Sciences, Physics Section, Vienna International Centre, A-1400 VIENNA, AUSTRIA

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Appendix 3: Meeting Agenda

Wednesday, 16 October 2019

Session 1: Session I

Chair: Christian HILL

09:30 – 10:00	**Arjan KONING**, **Christian HILL**: Welcome, introduction of the participants, adoption of the agenda
10:00 – 10:30	**Christian HILL**, *IAEA, Austria* Background and current status of radiation damage data services of the Atomic and Molecular Data Unit
10:30 – 11:00	**Sergei DUDAREV**, *Culham Centre for Fusion Energy, United Kingdom* Radiation defect data for a Virtual Tokamak Model
11:00 – 11:30	Coffee Break
11:30 – 12:00	**Andrea SAND**, *Department of Physics, University of Helsinki, Finland* Variation and uncertainty in cascade damage predictions from simulations
12:00 – 12:30	**Roman VOSKOBOYNIKOV**, *Kurchatov Institute, Russia* Ordered materials in nuclear engineering and radiation technology
12:30 – 14:00	Lunch

Session 2: Session II

Chair: Andrea SAND

14:00 – 14:30	**NOMOTO Akiyoshi**, *Materials Science Research Laboratory, Central Research Institute of Electric Power Industry (CRIEPI), Japan* Atom probe tomography of reactor pressure vessel steels
14:30 – 15:00	**Wahyu SETYAWAN**, *Pacific Northwest National Laboratory, United States of America* Displacement Cascade Simulations in FCC Ni-Fe Solid Solutions
15:00 – 15:30	**Marta SERRANO**, *Centro de Investigaciones Energeticas, Medioambientales y Tecnologicas, Spain* CIEMAT contribution to the IAEA Code Centres Network (CCN)
15:30 – 16:00	Coffee Break
16:00 – 16:30	**Manoj Kumar WARRIER**, *Computational Analysis Division, Bhabha Atomic Research Centre, India* Multi-scale modeling of surrogate ion irradiation damage
16:30 – 17:00	**Mihai Cosmin MĂRINICĂ**, *Université Paris-Saclay, France* Up-to-date approaches for atomistic material science
19:00 – 21:30	Social Dinner

Thursday, 17 October 2019

Session 3: Session III

Chair: Sergei DUDAREV

09:00 – 09:30	**María J. CATURLA**, *Department of Applied Physics, University of Alicante, Spain* How can we make the best use of collision cascade data for multiscale models?
09:30 – 10:00	**Christophe DOMAIN**, *EDF R&D Lab Les Renardières, France* High throughput DFT calculations in metals: synergy of irradiation defects and solutes and combinatorial configurations
10:00 – 10:30	**Manoj Kumar WARRIER**, *Computational Analysis Division, Bhabha Atomic Research Centre, India* Analysis and Visualization of collision cascades data
10:30 – 11:00	Coffee Break
11:00 – 12:30	Discussion (all): Prospects for improvement and expansion of CascadesDB
12:30 – 14:00	Lunch

Session 4: Session IV

14:00 – 17:00	Discussion (all): Provision and exploitation of experimental and theoretical data sets of relevance to radiation damage

Friday, 18 October 2019

Session 5: Session V

Chair: Christian HILL

09:00 – 11:00	Discussion (all): Practical aspects: data availability, upload, validation, provenance and licensing; Formulation of future plans and roadmap
11:00 – 11:30	Coffee Break
11:30 – 12:30	Recommendations and drafting of meeting report
12:30 – 13:00	Final Comments and Review; Adjournment of Meeting

Appendix 4: Presentation Abstracts

Analysis and Visualization of Collision Cascades Data

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As ever increasing computational power drives longer simulations generating more and more data, extracting knowledge from the data is becoming more relevant. Modern data exploratory techniques like supervised and unsupervised machine learning and reactive visualizations can provide effective ways to identify patterns and get new insights [1]. In the field of radiation damage, use of machine learning is restricted to using supervised learning for development of inter-atomic potential surfaces [2,3]. The potential of ML for exploratory data analysis using is now being explored [4,5,6]. **CascadesDB** lays the foundation for future efforts in this direction with a standard database of MD simulation data of collision cascades. **CSaransh** is an open source application that builds upon this and provides a whole suite of data exploration tools and modern interactive visualizations accessible directly from web.

CSaransh analyzes cascades database to explore patterns, correlations and comparisons of many new parameters such as sub-cascades, defect cluster shapes, cascade volume and surface area in addition to the essential properties like defects count, in-cascade clustering etc. It uses algorithms from the field of unsupervised machine learning, dimensionality reduction, computational geometry and other statistical techniques to find the new parameters while efficient methods have been developed for essential properties. The reactive GUI with modern web frameworks provides interactive visualizations and plots to explore the results qualitatively and quantitatively compare the different cascades or statistics calculated for a group of cascades across energies or elements.

The suite uses different tools for various tasks. C++14 is used to efficiently post- process big simulation outputs and has to be run only once for a given set of data. Python is used for the machine learning algorithms. HTML with React-js is used to develop the single page web application. JSON is used as the common data format between post-processors and GUI. The post-processing and web application both are modular such that new data-exploration parameters, plots and visualizations can be added seamlessly. *The initial results show effectiveness of new methods of data exploration to cascades and might open new avenues for better insights and possible refinement of higher scale models of radiation damage.*

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How can we make the best use of collision cascade data for multiscale models?

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The development of a database of collision cascades such as the IAEA CascadesDB [1] opens a great opportunity for researchers to have access to a large variety of conditions and materials that otherwise would be quite difficult to perform by each individual research group. But in order to have a good use of this data, a discussion is necessary on how to make this data more accessible to researchers working on multiscale models.

In this talk we will, first, give a brief review of the different types of conditions that one could find in this database, based on the simulations of collisions cascades performed by ourselves as well as existing in the literature: materials, boundary conditions or the presence of initial defects (dislocations, grain boundaries, defect clusters). Then we will focus on a discussion on how to improve the access of different researchers working on multiscale models to this data: analysis tools, recommendations, data processing, etc.

1. https://cascadesdb.org/

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High throughput DFT calculations in metals: synergy of irradiation defects and solutes and combinatorial configurations

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[3] EM2VM, Joint laboratory Study and Modeling of the Microstructure for Ageing of Materials

In a classical nuclear power plant, the components near the reactor, such as the cladding (made out of Zr alloys) or the internal structures (austenitic steels) and to a lesser extent the pressure vessel (bainitic / ferritic steels), are subjected to neutron bombardment. In a fusion reactor, high energy particles (H isotopes and He) as well as 14 MeV neutrons bombard the walls (ferritic martensitic steels) and the divertor (tungsten alloys).

In order to predict and understand the ageing of structural materials, a multiscale modelling approach is developed to simulate the microstructure evolution under irradiation. It is based on the key physical phenomena the material experiences. In this approach, there are two main inputs with a strong impact on the microstructure obtained: (i) the source term constituted by the formation of point defects and displacement cascades and (ii) the properties of the defect clusters and solute-defect clusters formed. The key properties of defects and defect clusters are their stability and mobility, e.g. binding energies and migration energies (the material evolution is described in terms of elementary physical mechanisms), which are the inputs of kinetic Monte Carlo models for the modelling of the microstructure evolution.

Industrial alloys are multi-component alloys and the number of possible interactions between solute and defect clusters increases rapidly with the number of solute present. A typical example is the reactor pressure vessel steels, where the main elements observed in the clusters formed under irradiation contain Cu, Ni, Mn, Si as well as P. In order to characterize all the possible interactions between these solutes and the point defects, to build cohesive models, a large number of DFT calculations are necessary, that represent thousands to tens of thousands calculations and billions of CPU hours.

Radiation defect data for a Virtual Tokamak Reactor Model

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Operation of a fusion or an advanced fission power plant is invariably associated with the accumulation of defects, produced by neutron and particle irradiation, in the bulk of reactor components. The accumulation of defects gives rise to strongly fluctuating spatially varying strain and stress fields, which on the macroscopic scale lead to irreversible deformations of components. Recent developments in the simulation methodology show how to relate the microscopic fields of defects to macroscopic strain and stress, and how to include these effects in the Finite Element Method simulation framework. This is expected to enable making the next step in the simulation methodology and develop an approach where a tokamak reactor design is evaluated, as an integrated evolving system, over its entire lifetime [1].

This presentation provides a summary of recent developments in atomistic density functional theory and molecular dynamics, as well as elasticity-based simulations, which form a foundation for the Virtual Tokamak model, and relate it to the new capabilities offered by the availability of IAEA database of collision cascades.

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Up-to-date approaches for atomistic material science

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Machine learning (ML), a subfield of artificial intelligence, is currently used for various applications in materials sciences such as guiding chemical synthesis and discovery of new compounds, development of interatomic force fields and structural analysis of materials. This presentation proposes a review of ML techniques for an accurate description of the energy landscape and morphology of defects embedded into crystalline structure.

From atomic scale, multi-scale studies of properties 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 [1]. The ML methods propose an intermediate approach that allows the control of the balance between the accuracy and numerical efficiency. Here, using the recently developed package MiLaDy (Machine Learning Dynamics) [2,3], we exemplify the case of energetic landscape of defects in metals. The present approach merges ab initio - free energy - machine learning regression (Kernel, Gaussian Processes, Polynomial) and, therefore, can provide quantities that underpin many multi-scale models, such as atomistic formation free energies or diffusion transition rates [4,5].

Moreover, the state-of-the-art ML methods combined with atomic descriptors are applied for automatic detection and structural analysis of defects in solids. Traditionally, structural analysis of defects is performed using well-established techniques, such as Wigner-Seitz, Voronoi and bond-angle analysis, etc. Here, we have opted for using semi-supervised ML techniques based at novelty/outlier detection, such as Support Vector Machine and Minimum Covariance Determinant. We firstly learn the bulk environment using deformations or standard molecular dynamics of bulk, without defects, supercells. Then, we perform the detection of the defects using the outlier detection techniques. Furthermore, based on this structural analysis technique, we also propose a generic numerical tool to examine transferability of kernel ML potentials, prior to perform time-consuming molecular dynamics calculations.

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Variation and uncertainty in cascade damage predictions from simulations

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The first step in modelling radiation damage in materials consists in predicting the primary damage, which forms on picosecond time scales as a direct result of an elastic collision with an impacting particle. The collision cascades caused by the incoming particle, which give rise to structural damage on the nanometer scale, are highly non- equilibrium events, directly involving up to thousands of atoms in a complex non- linear process. Methods based on molecular dynamics have been developed which successfully handle many of the aspects of the dynamics in cascades. However, the predictive capacity of atomistic cascade simulations is still restricted by the level of accuracy of the models used [1, 2].

Cascades are highly stochastic in nature, with strong variation between events, which poses a significant challenge for the development of simulation methodology. In addition, the accuracy of predictions is often hard to determine, since the picosecond time scale effects are difficult to capture experimentally. In this presentation, I will describe the inherent variation in cascades and cascade damage in different metals, and outline the main sources of uncertainty in predictions from molecular dynamics simulations. I will present some of the ways in which simulation results can be directly compared to experiment [3, 4, 5], and discuss the related available experimental data and data needs. Finally, I will consider future directions for developing the simulation methodology and improving the accuracy of predictions from simulations.

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CIEMAT contribution to the IAEA Code Centres Network (CCN)

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As the Division of Materials for Energy of CIEMAT participates for the first time in this meeting, the presentation will highlight our objectives, structure and research lines, emphasising the type of data we could potentially provide in terms of experimental measurements and observations on steels, as well as, modelling data on iron alloys. In addition, the activities of the H2020 M4F (Multiscale modeling for Fusion and fission materials) project coordinated by CIEMAT will be presented, as they are consistent with the goals of the meeting. Finally, the H2020/ENTENTE (European Database for Multiscale Modelling of Radiation Damage) project proposal, just submitted to Euratom and also coordinated by CIEMAT, will be described. If approved, this project will pursue the creation of a database dedicated to the embrittlement of reactor pressure vessel steels, ranging from mechanical to microstructural and modelling data. Collaboration of ENTENTE with the community involved in the meeting, particularly if a CRP is launched, in particular concerning the CascadeDB, is accordingly considered possible and of mutual benefit.

Displacement Cascade Simulations in FCC Ni-Fe Solid Solutions

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Tungsten alloys and composites are actively researched in the fusion materials community to improve the fracture toughness and the ductile-to-brittle transition temperature of tungsten for use as plasma-facing materials. Among these materials, ductile-phase-toughened composites are particularly promising. W-Ni-Fe composites, consisting of tungsten particles embedded in a ductile face-centered cubic (fcc) Ni-Fe random solid solution with a Ni:Fe weight ratio of 7 :3, have been shown to exhibit a significantly higher fracture toughness (30-60 MPa√m) compared to pure tungsten (8 MPa√m) at room temperature [1]. However, the irradiation effects against fusion neutrons remain largely unknown. In this study, molecular dynamics (MD) is employed to simulate the displacement cascades in an fcc Ni-Fe solid solution. The cascades simulations are performed with a random Fe or Ni primary-knock-on atom (PKA) as a function of PKA energy to build a database of primary defects for future kinetic Monte Carlo simulations of damage accumulation. Irradiation-induced phase separation will be studied. Furthermore, the defect distribution will be compared to the data of pure Ni to elucidate the effect of Fe solute atoms on the cascades.

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Ordered materials in nuclear engineering and radiation technology

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Materials with ordered crystal structure are not just considered but have already been applied in a number of demanding nuclear power and radiation technology applications. For example, most existing research and test reactors are fueled with UAl_x or U_3Si_2 intermetallic fuel. Binary, ternary and quaternary intermetallic compounds of beryllium with Ti, V, Zr, Nb, Ta, Mo, W and/or Y are the main advanced breeder/multiplier candidates for use in blankets of future fusion reactors. γ'-Ni_3Al precipitates are a key strengthening component of the microstructure of Ni-based refractory alloys that affects their high temperature strength and creep resistance properties. Spinel ($MgAl_2O_4$) is a potential candidate for inert matrix fuels and a heterogeneous diluent of Pu and minor actinides (Am, Np and Cm) for subsequent transmutation/ incineration in fast-neutron reactors. Complex oxides with perovskite and pyrochlore crystal structure are reckoned as promising ceramic hosts for immobilization of high-level nuclear waste.

All structural and functional materials with ordered crystal structure usually last longer and outperform their elemental constituents as well as disordered solid solutions with the same chemical composition under simultaneous impact of high operating temperature, applied loading, thermal flux, corrosive/ oxidation environment and fast particle irradiation. Despite a rich diversity of chemical compositions, crystal lattices, defect subsystems, operating conditions, service properties, etc. ordered materials exposed to fast particle irradiation exhibit similar microstructural transformations. That provides an opportunity to gain a deeper insight into peculiarities of radiation effects in ordered solids by studying model materials with relatively simple microstructure and chemical composition. Afterwards, the obtained results can be extrapolated to the whole range of intermetallic alloys, spinels (AB_2O_4), perovskites (ABO_3), pyrochlores ($A_2B_2O_7$) and other complex oxides with fluorite-like crystal structures, *e.g.* δ-phases ($A_4B_3O_{12}$ and A_6BO_{12}).

A noticeable progress in the understanding of the governing mechanisms of radiation damage formation in ordered solids has been achieved by conducting molecular dynamics simulations of collision cascades in γ-TiAl, α_2-Ti_3Al and γ'-Ni_3Al intermetallic compounds and the corresponding disordered solid solutions with the same chemical composition. All three intermetallics demonstrate a higher resistance against radiation damage formation comparing to their disordered counterparts.

A strong disproportion in the partition of interstitials that exceeds the stoichiometric composition has been observed in collision cascades in the three intermetallic compounds. In the case of the disordered solid solutions, the discrepancy is even more radical.

In irradiated intermetallic compounds, heavier projectiles generate more disorder, whereas lighter projectiles with the same energy produce more primary radiation damage. A simple quantitative correlation between the number of antisites and the number of Frenkel pairs created in collision cascades in intermetallic compounds has been revealed.

A significant fraction of the original radiation resistance of α_2-Ti_3Al is retained even after complete disordering. In contrast to α_2-Ti_3Al, disordered γ'-Ni_3Al intermetallics loses completely its initial radiation tolerance. It is highly likely that the short-range and long-range order contributions to the overall radiation tolerance are different in the two intermetallic compounds. A robust proof of the proposed hypothesis has yet to be accomplished.

Multi-scale Model of Material Damage due to Surrogate Ion Irradiation (SII)

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Energetic ions of several MeV are used to bombard materials in order to study the effect of neutron irradiation on materials – hence this is also called surrogate ion- irradiation. This is because the primary damage mechanisms in both cases are same and SII causes the same amount of displacement per atom (DPA) in a couple of days as neutron irradiation does in years, albeit in a smaller volume. The primary damage mechanisms like (i) collision cascades, (ii) in-cascade clustering to form sessile and glissile clusters, and (iii) diffusive recombination of defects, are at least qualitatively similar in both cases. Therefore SII is a useful method to gain an understanding of the mechanisms and to validate the codes and models used to simulate primary irradiation damage. A multi-scale model to simulate material damage due to SII is presented, which involves the following:

- A combination of Binary Collision Approximation Monte Carlo (BCA- MC) and Molecular Dynamics (MD) is used to obtain the primary damage state for several MeV proton irradiation of FeCr /Nb.
- Electronic stopping has been added in LAMMPS as a frictional force with the co-efficient of friction being obtained using the Lindhard-Scharff model [1].
- Machine learning is employed on a MD database to classify the in- cascade clusters based on shape, size and dimensionality. This is the first step to identify sessile and glissile clusters. With this the primary damage state of a material subjected to SII is obtained. [2]
- MD is used to obtain the diffusion parameters of interstitials and vacancies [3,4,5] and these parameters are passed to higher scale Kinetic Monte Carlo (KMC) simulations. Initial KMC results are discussed.

The talk aims to focus on the parameters that need to be passed across scales/models .

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