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### **International Atomic and Molecular Code Centre Network on A Database of Atomic Configurations Formed in Collision Cascades**

#### **Summary Report of the 5th Biennial Technical Meeting**

IAEA Headquarters, Vienna, Austria

16–17 November 2017

Prepared by

A.E. Sand, S.L. Dudarev and C. Hill

August 2018

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### **Abstract**

The International Code Centre 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 Unit in order to discuss computational and scientific issues associated with code developments. The 5th technical meeting was held 16–17 November 2017 and eleven experts in the field of molecular dynamics simulations of radiation damage were invited to discuss plans for a database of atomic configurations generated by MD simulations of collision cascades. This database is to be hosted by the Atomic and Molecular Data Unit and will provide 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. It is hoped that the database will be used in a crowdsourcing exercise in identifying defect structures such as dislocation loops formed in collision cascades. Longer term plans for a computing project to further simulate the evolution of materials on longer timescales were discussed.

August 2018



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## 1. Introduction

Computational modeling of the response of materials to bombardment by energetic particles is a crucial part of research directed towards the construction of a viable nuclear fusion reactor. Only a limited amount of data is accessible to experiment or is found in the literature, and computations are essential to generate adequate data in the search for materials with the right properties. The basic approach of classical Molecular Dynamics (MD) modelling in solids is well-understood and much used, but 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, initially forming a crystal lattice, with particles with keV or MeV energies.

The international Code Centres Network (CCN) is coordinated by the IAEA A+M Data Unit in order to gather, compare, validate, and provide access to computational codes relevant for modelers in fusion and plasma sciences. Starting with a consultants' meeting on "Establishment of Atomic and Molecular Computer Code Network" in 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.

The Unit organized the 5<sup>th</sup> Technical Meeting on the international Code Centres Network (CCN5) held at IAEA headquarters from 16 – 17 November 2017 where 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.

The need for a database of atomic configurations generated in collision cascades has long been recognized, and such databases, not open to the global research community, were created at LLNL and ORNL in the 1990s, driven by the needs of computational projects exploring the evolution of materials under neutron and ion irradiation. The content of these databases has never been made public, however they were used in order to generate peer-reviewed journal publications where the dynamics of evolution of defect configurations produced in cascades was explored.

The primary reason for the desirability of creating an open database at the IAEA stems from the long and established track record of IAEA as a recognized international centre that assembles and maintains data on the cross sections of neutron interaction with nuclei, atomic data and particle-material interactions. Atomic configurations generated by molecular dynamics simulations of high-energy cascade events are known to represent a reasonably well defined "stationary" state of a material, where the rates of evolution slow down significantly in comparison with the timescale of development of a cascade itself (~10ps). The subsequent evolution of cascade configurations, driven by the motion and reactions between the defects formed in a cascade, involves timescales ranging from 10ns to 10000s, or even longer. Simulation algorithms required for modelling evolution on such extended timescales, often involve a combination of molecular dynamics with other methods, for example a search for transition pathways, or simplification of representation of defects as classes of objects, suitable for application of Object kinetic Monte Carlo simulations. Simulating the evolution of defects interacting through long-range elastic forces still remains a major challenge.

The creation of a cascade configuration database will enable the more rapid development of such algorithms by providing standardized and verified initial conditions for running the simulations. It is also expected that this will provide a strong boost to research in modelling microstructural evolution of irradiated materials, which is one of the major weakness in the global multiscale simulation approach to fusion and fission materials.

An open database provides the added benefit of gathering together simulation results generated by different research groups, using different interatomic potentials and different simulation methods. The reliability of predictions from molecular dynamics simulations is subject to the quality of the interatomic potential, hence comparison between the predictions of different potentials is a key step in assessing the uncertainties in the data. Ideally, different potentials, if accurate, should produce the same results for the same simulation conditions. In addition to different potentials, results are also sensitive to the various methods that are currently in use to extend classical MD in order to simulate the highly non-equilibrium cascade events. Since the damage produced in individual cascades varies immensely, the data can only be evaluated through general features of the statistics from numerous simulations. One of the challenges currently facing attempts to compare results in the literature is the different ways in which the data is analyzed and presented, often making direct comparison from published work impossible. An open database will allow systematic analysis of data from different sources, and thereby facilitate direct comparison.

An important consideration for the purpose of validation and uncertainty assessment of the cascade configuration data is the format of the metadata describing the database entries. It is necessary that the metadata contain all information which may be relevant to fully describe the simulation method. It should be general enough to cover different practices in use among modellers, yet specific enough to be searchable; concise, yet detailed enough for the method to be reproducible. These are questions that the current meeting aimed to address.

This report contains an introduction in Section 1, proceedings of the meeting in Section 2, and discussions and recommendations in Section 3. The list of participants is provided in Appendix 1 and the meeting agenda in Appendix 2. The abstracts of presentations are provided in Appendix 3.

## **2. Proceedings**

The CCN meeting was opened by the new head of the Atomic and Molecular Data Unit, C. Hill, welcoming all participants. After introductions and some administrative formalities, the general meeting objectives were detailed by S. L. Dudarev (CCFE, UKAEA) and A. E. Sand (U. Helsinki). The agenda was adopted (Appendix 2). The abstract of each presentation is attached in the Appendix 3 and presentations are available at Unit's home page <https://www-amdis.iaea.org/CCN/Meetings5/>.

Andrea Sand of Helsinki University introduced her research on modelling energetic cascades in tungsten, noting the sensitivity to interatomic potentials and the agreement found with experimental results for the frequency distribution defect cluster size.

Wangyu Hu of Hunan University presented an account of the analytic embedded atom method as applied to computer simulations of radiation damage, with a particular focus on helium trapping in various metals.

Roman Voskoboynikov of NRC Kurchatov Institute discussed Molecular Dynamics studies of primary damage in materials subject to fast particle irradiation, noting in particular that an evaluation of the minimum size of the sampling set used to statistically analyse such simulations is essential to their proper validation.

María Caturla of Alicante University detailed a set of Molecular Dynamics simulations of the influence of the initial defect distribution on the collisional cascade microstructure evolution. The need for data relating to cascade damage in alloys was discussed.

Naoki Soneda of CRIEPI introduced the work of his group on the characterization and statistical distribution of defect clusters in a database of simulations for primary knock-on atom (PKA) energies up to 50 keV in bcc-Fe.

Fei Gao of Michigan University presented results from his group's studies of vacancies and interstitial loops generated by high-energy cascades in Fe. The violation of Burger's conservation law in the predicted interaction of a smaller  $\frac{1}{2}\langle 111 \rangle$  loop with a larger  $\frac{1}{2}\langle 111 \rangle$  loop containing a  $\langle 100 \rangle$  segment was described.

Kai Nordlund of Helsinki University gave a detailed account of Molecular Dynamics simulations of collisional cascades since 1993, including a description of the phenomenological technique of accounting for the energy loss to electronic excitations in the crystal atoms by the inclusion of a "frictional force" in their velocities. He estimated the size of a single cascade series simulation storing all the frames to be 14 GB and stressed the importance of using a non-binary format for storing data.

Wahyu Setyawan described MD simulations of cascade morphologies in bcc metals, noting that the atom mass has no effect on the displacement threshold energy,  $E_d$ , in these models.

Christophe Domain of EDF R&D described the effect of differing interatomic potentials on cascade simulations in metals and stressed the importance of including a specification of the interatomic potential in the metadata associated with each simulation in the planned database.

Manoj Kumar Warriar of the Bhabha Atomic Research Centre presented results of the post-processing of MD simulations to identify defects and other phenomena in data produced with LAMMPS.

On Day 2 of the meeting, Sergei Dudarev from the Culham Centre for Fusion Energy discussed real space models of crystal microstructure and stressed the need for a cascade database for validation and comparison of MD simulations.

Jean-Christophe Sublet of the Nuclear Data Services Unit at the IAEA gave a technical account of the IAEA neutron cross section database and an overview of IT at the IAEA Nuclear Data Section.

### **3. Discussions**

Discussion sessions in this meeting were primarily concerned with the practicalities of establishing a workable data model for representing Molecular Dynamics simulation data and the hardware, security and administrative implications of running a database from the IAEA.

#### **Scientific Challenges and Accumulation of Data**

Andrea Sand and María Caturla led the discussion on the technical and scientific challenges involved in establishing a database of collisional cascade molecular dynamics simulation data. A few general principles were agreed:

1. Generally, all data entered into the database should be associated with a peer-reviewed publication describing in detail the methods used to generate the data.
2. There should be a scientific committee associated with the database and to set standards around the metadata necessary for its precise description. The committee should include, *inter alios*, S. L. Dudarev, A. E. Sand, and the AMD Unit Head.
3. Submissions to the database should be vetted by a human expert (presumably someone on the scientific committee), except perhaps in the case of submissions by well-established members of the database community. "Well-established" could, for example, be automatically assessed

by the submission system as a data provider whose data has already been cited an average of  $n$  times for some suitable choice of  $n$ .

4. The database should provide a mechanism for data users to leave comments on data sets.
5. A browser-based frontend to the database providing easy visualization of submitted data would be welcome.
6. It was agreed that the initial configuration of the material should be stored for any simulation that did not start from a perfect crystal lattice. This allows the data in the database to be analysed to assess the effect of pre-damage, grain boundaries, surfaces, etc. on the cascade, as well as catering for the needs of simulations of alloys.
7. The database should not seek to identify any defects that may have been identified in the microstructure so as not to prejudice subsequent analysis.

The data format for the file holding the atom positions was discussed.

1. This file should be in ASCII plain-text format
2. The file should consist of a variable number of space-delimited columns.
3. The meaning of each column should be described in the metadata associated with the file. This metadata description should be particularly careful to specify the units of any physical quantities.
4. The first four columns are mandatory and should hold the atom's element symbol and its  $x$ ,  $y$ , and  $z$  positions.
5. Possible entries in subsequent columns include an index (assuming the MD simulation keeps track of individual atoms and in case this index is not given by the atom's row position in the file); and the atom's velocity components,  $v_x$ ,  $v_y$  and  $v_z$ .

The necessary metadata for the faithful description of the parameters used in a MD simulation was the subject of some discussion. It was decided that a minimal set of metadata should be considered mandatory, with a much larger, but structured set considered optional; data providers are to be strongly encouraged to include as much of this optional metadata as possible. A list of metadata entries is given below.

1. Atomic number of PKA
2. Whether the PKA is a recoil or implanted ion
3. Material
4. Lattice Structure
5. Lattice parameters, box size and crystal orientation
6. Temperature
7. Methods (electronic effects, thermostats)
8. Interatomic potential: should there be a separate repository for tabulated potentials? In some simulations it may not be possible to provide a tabulated potential but a reference should be considered mandatory
9. MD code name and version
10. The input file to the MD simulation run
11. Citations and acknowledgements (bibliography)
12. How to cite the data (for data users)
13. URI(s) for the data file(s) themselves
14. A description of the meaning of the columns in the data files, to include a full specification of the units of any physical quantities
15. Information about the PKA direction should be available, either in comments or in the code input file

Although it may not be possible in the short term to assign DOI-like identifiers to data sets, the presence of this cascades database online makes it possible to assign to them a URI (Uniform Resource Identifier) which may well simply be the URL of the resource at the domain of the database.

Some time was spent discussing how many data (xyz) files may share a single metadata description, in view of the large number of xyz files that may be produced in a simulation which differ only in the recoil direction. Many felt that the information about the recoil direction, which can be obtained from the MD simulation input file should be omitted from the metadata description to allow large numbers of xyz data files to share a single metadata description.

B. Braams raised the issue of the various use cases for a cascades database. In addition to the planned crowdsourced activity on the identification of interesting features in the xyz data, there is scope for the application of machine learning techniques to the evolution of material damage. This can be promoted by allowing the storage of “snapshots” of the simulation, for example a frame (xyz file) every 100 fs.

### **Active Points and Next Steps**

The discussion sessions led to broad agreement about the outline of the data model behind CascadesDB. It was proposed that a prototype database be developed and populated with example data from the research groups of the meetings participants. As outlined below, the development of the data model will be informed by the needs of these data, and when finalized should be codified in a publicly accessible document.

The meeting participants will work together over the first few months of 2018 to develop the data model and prototype database, which will be implemented on IAEA servers as soon as possible.

## **4. Summary and Recommendations**

The objective of the meeting was to initiate the implementation of an online database of atomic configurations generated by Molecular Dynamics simulations of collisional cascades. The assembled participants reached an agreement over the data standards and methodological approach for this database and development of a prototype database and online application will begin in 2018.

### **Recommendations**

- A Scientific Committee should be established to guide the implementation and development of CascadesDB.
- The CascadesDB data model should be informed by the needs and existing data of members of the Technical Meeting and should be published in a suitable journal after peer review.
- The online application serving as the database frontend should be publicly released after consultation with and advice from the MT-IT department of the IAEA.
- The database should be implemented in such a way that it meets the requirements of the FAIR (=Findable, Accessible, Interoperable, and Re-usable) principles (see, for example, <https://www.nature.com/articles/sdata201618>).

Overall, the coordinating effort of IAEA was very welcomed and the meeting was considered as very useful and productive by all the participants.



## APPENDIX 1: Participants

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## APPENDIX 2: Meeting Agenda

Thursday, 16 November 2017

Meeting Room C5

- 09:30 – 09:45**      **Christian Hill:** Opening Remarks  
**09:45 – 10:00**      **Sergei L. Dudarev and Andrea E. Sand:** General Meeting Objectives

### *Session I. Chair: C. Domain*

- 10:00 – 10:30**      **Andrea E. Sand,** University of Helsinki, Finland  
“Energetic cascades in tungsten: sensitivity to interatomic potentials and electronic effects”
- 10:30 – 11:00**      **Wangyu Hu,** Hunan University, Changsha, China  
“The analytic embedded atom method and its application to computer simulations for radiation damage”
- 11:00 – 11:15*      *Coffee break*
- 11:15 – 11:45**      **Roman Voskoboynikov,** NRC Kurchatov Institute, Moscow, Russia  
“An MD study of primary damage in structural materials exposed to fast particle irradiation in the nuclear stopping power regime”
- 11:45 – 12:15**      **María J. Caturla,** University of Alicante, Alicante, Spain  
“Damage distribution in f.c.c. and b.c.c. metals from molecular dynamics and its influence on microstructure evolution”
- 12:15 – 14:00*      *Lunch*

### *Session II. Chair: A. E. Sand*

- 14:00 – 14:30**      **Naoki Soneda,** Central Research Institute of Electric Power Industry, Japan  
“Displacement cascade database for PKA energies up to 50 keV in bcc-Fe”
- 14:30 – 15:00**      **Fei Gao,** University of Michigan, Ann Arbor, USA  
“Formation of Nano Size <100> Interstitial Loop within High Energy Cascades and Their Migration in Iron”
- 15:00 – 15:30**      **Kai Nordlund,** University of Helsinki, Finland  
“Molecular dynamics simulations of collision cascades: method development and results from 1993 on”
- 15:30 – 15:45**      *Coffee break*

### *Session III. Chair: M. J. Caturla*

- 15:45 – 16:15**      **Wahyu Setyawan,** Pacific Northwest National Laboratory, USA  
“Cascade Morphologies in bcc Metals”
- 16:15 – 16:45**      **Christophe Domain,** EDF R&D, France



“Cascades by molecular dynamics in metals: interatomic potentials and BCA comparison, statistics”

**16:45 – 17:15**

**Manoj Kumar Warriar**, Bhabha Atomic Research Centre, India

“Post-processing MD simulations to identify defects, their trajectories and clustering in LAMMPS”

19:00

*Dinner*

**Friday, 17 November 2017**

Meeting Room C5

*Session IV: Objectives and Methodology*

**09:30 – 10:00**

**Sergei L. Dudarev**, UKAEA, UK

“Real-space models for microstructure and the need for a cascade database”

**10:00 – 10:30**

**Jean-Christophe Sublet**, Nuclear Data Services Unit, IAEA

“The structure of the IAEA neutron cross section database”

**10:30 – 11:00**

**Andrea E. Sand** (lead)

*Discussion*: Scientific challenges and accumulation of data

**11:00 – 11:15**

*Coffee break*

**11:15 – 12:15**

**Andrea E. Sand** (lead)

*Discussion* (continued): Scientific challenges and accumulation of data

**12:15 – 14:00**

*Lunch*

*Session V: Implementation*

**14:00 – 14:15**

**Christian Hill**, Atomic and Molecular Data Unit, IAEA

“Accumulation of data at the IAEA and means of access of the database”

**14:15 – 15:30**

**Andrea E. Sand and Sergei L. Dudarev** (leads)

*Discussion*: Active points and next steps

**15:30**

Concluding remarks

**15:30 – 17:00**

AOB; closure of the meeting

## **APPENDIX 3: Abstracts**

### **Energetic cascades in tungsten: sensitivity to interatomic potentials and electronic effects**

Andrea E. Sand, Division of Material Physics, Department of Physics, University of Helsinki

The walls of fusion reactors will be subjected to energetic neutron irradiation, leading to microstructural modification of the material and possible long term degradation of the reactor components. Collisions between neutrons and the atoms in the material give rise to recoils of varying energy, leading to collision cascades that form nano-scale defects. Very energetic recoils will be much more prevalent in future fusion reactors than in current fission reactors. It is therefore important to understand the effects of these energetic events.

This presentation highlights some of the challenges related to simulating energetic collision cascades, with focus on tungsten. The outcomes of molecular dynamics (MD) simulations of energetic collision cascades vary much more strongly than for similar lower energy events. For this reason, a full description of the defect production relevant for fusion devices may require up to hundreds of individual cascade simulations for each recoil energy, with each simulation of an energetic event taking over 1000 CPU hours on modern supercomputers. Molecular dynamics simulations are always subject to the limitations of the interatomic potential that is used. In energetic cascade simulations in tungsten, results show an unexpectedly strong sensitivity to the potential, with large differences even between recent, extensively fitted potentials of high quality. Another uncertainty in cascade simulations stems from the effects of electrons, which are not directly treated in MD simulations, but can be included through various simplified models. Different methodologies in treating electrons also lead to different results. Assessing the sensitivity of results to different methods, and validation of results through comparison to experiments, is therefore crucial, but this, again, requires massive amounts of data for each given potential and simulations method, since comparisons can only be made statistically.

## **An MD study of primary damage in structural materials exposed to fast particle irradiation in the nuclear stopping power regime**

Roman Voskoboynikov, NRC Kurchatov Institute

Collision cascades are the main source of radiation defects in materials subjected to fast particle irradiation in the nuclear stopping power regime. They are formed by the recoil of primary knock-on atoms with the energy of more than  $\sim 1$  keV. The cascade process is characterized by the temporal and spatial scale of the order of  $ps$  and  $nm$ , respectively, which is prohibitive for direct experimental investigation but can be studied by molecular dynamics (MD) simulations.

In this report, we overviewed a few adjustments to conventional MD simulation techniques that make them more suitable for studying collision cascades. In order to optimise numerical integration of the equations of motion, the interatomic potentials are tabulated and interpolated by cubic splines over  $r^2$  (not  $r$ ) where  $r$  is the interatomic distance. At the initial stage of a collision cascade, significant acceleration of MD simulations is achieved by splitting the ensemble atoms in the MD box into two subsets of “hot” and “cold” atoms that are treated separately.

Four different but complementary techniques are employed for identification and visualization of radiation defects created in collision cascades.

We also provided the outcomes of recent MD simulations of radiation effects in solids exposed to irradiation. Collision cascades in the bulk, near the surface and in the vicinity of edge and screw dislocations in elemental metals and intermetallic compounds were investigated. Overlapping of collision cascades under high dose irradiation conditions was considered as well. In order to validate MD simulations and get the statistically reliable number of residual defects, the optimal size of the sampling set was evaluated following a simple procedure.

It has been established that interatomic compounds demonstrate high resistance against the formation of primary damage. Understanding and controlling energy dissipation in intermetallic compounds under irradiation may pave the way for new design principles of radiation-tolerant structural materials for nuclear engineering applications.

Strong interaction of collision cascades with free surfaces, dislocation cores and residual radiation defects is observed under all simulation condition.

## **Damage distribution in f.c.c. and b.c.c. metals from molecular dynamics and its influence on microstructure evolution**

María J. Caturla, Departamento de Física Aplicada, Facultad de Ciencias, Universidad de Alicante

The damage distribution obtained from molecular dynamics simulations of collision cascades is the initial starting point to study microstructure evolution of materials under irradiation. These simulations are able to describe the production of defects and their evolution due to energetic recoils to time scales of a few picoseconds, where the population of defects produced reach a constant value. These defects, however, evolve over much longer time scales that are not computationally accessible with molecular dynamics. Therefore other methods are used to extend the time and length scales using the initial configurations of defects obtained from molecular dynamics. In this talk we describe how a database of collision cascades can help modeling microstructure evolution under irradiation, focusing on one particular tool: object kinetic Monte Carlo. We describe how, using this technique, we have been able to show that this initial defect distribution plays a key role in microstructure evolution. We show that the main differences observed experimentally between irradiated copper and iron can be traced back to the damage distribution in the collision cascade, and how this distribution could also explain differences in swelling measured in f.c.c. and b.c.c. materials. In this talk we also describe how the access to the full coordinates of atoms from molecular dynamics simulations of collision cascades can be used to simulate the image that one would obtained in transmission electron microscopy, making a direct connection between experiments and simulations.

## Cascade Morphologies in bcc Metals

W. Setyawan<sup>1</sup>, A. P. Selby<sup>2</sup>, R. E. Stoller<sup>3</sup>, B. D. Wirth<sup>2</sup>, and R. J. Kurtz<sup>1</sup>

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Energetic atom collisions in solids induce shockwaves with complex morphologies. In this presentation, we discuss the existence of a morphological transition in such cascades. The order parameter of the morphology is defined as the exponent,  $b$ , in the defect production curve as a function of cascade energy ( $N_F \sim E_{MD}^b$ ). The response of different bcc metals can be compared in a consistent energy domain when the energy is normalized by the transition energy,  $\mu$ , between the low- and the high-energy regime. We explore cascade morphological development for primary knock-on atom (PKA) energies up to 70, 200, 100, and 150 keV for Cr, Fe, Mo, and W, respectively. Using these data, an empirical formula for  $\mu$  as a function of displacement threshold energy,  $E_d$ , is presented for these bcc metals.

To explore the robustness of the empirical formula, five test systems are simulated. Four of the test systems are constructed by employing the Cr or W interatomic potential and by varying the mass of all atoms (lattice mass) or only the mass of the PKA. The fifth test is performed using a different W potential. The value of  $E_d$  for all nine systems is calculated by using systematic grids of PKA direction and is averaged based on the solid angle and the multiplicity of each direction. For a given interatomic potential, varying the lattice mass has a negligible effect on  $E_d$ . However, varying the PKA mass significantly affects  $E_d$ . The causes for these variations and their implication on  $\mu$  will be discussed. Empirical formulas for  $\mu$  with and without the test systems are presented. In addition, the effect of electronic loss will be discussed based on the available data.

## **Cascades by molecular dynamics in metals: interatomic potentials and BCA comparison, statistics**

C. Domain<sup>1,5</sup>, C.S. Becquart<sup>2,5</sup>, P. Olsson<sup>3</sup>, A. De Backer<sup>4</sup>

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<sup>3</sup> KTH, Stockholm, Sweden

<sup>4</sup> CCFE, Culham, UK

<sup>5</sup> 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, the source term constituted by the formation of point defects and displacement cascades has a strong impact on the microstructure obtained. Molecular dynamics associated to empirical potentials is the most appropriate method to estimate the source, with limitations on the PKA energy that can be accessible (even on HPC machines) and uncertainties associated to the cohesive model used (equilibrium part, hardening and the link with the equilibrium part of the potential).

Consequently we explore different strategies to improve the prediction of the primary damage. (i) BCA and MD techniques are combined in order to model the effect of high neutron (or heavy ion) energy. (ii) Sensitivity studies of the primary damage comparing different empirical potentials provide an evaluation on the uncertainty on the results and can help to understand the effect of the different part of the potential. (iii) As DFT method is state of the art atomic cohesive model for few hundreds to thousands of atoms; DFT calculations of threshold displacement energies are performed (thanks to HPC resources) as potential reference values to compare to experimental results. In this state of mind, a simple method has been developed, that we refer to as the quasi static drag method, to compare DFT and different empirical potentials. (iv) Large MD cascade databases are produced and analysed in order to obtain statistics in order to go beyond the total defect number and fully characterize the cluster size distribution for both vacancies and self interstitials. This is indeed one of the key input for mesoscale techniques such as object kinetic Monte Carlo or cluster dynamics simulations of the microstructure evolution.

## Post-processing MD simulations to identify defects, their trajectories and clustering in LAMMPS

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A Max-Space Clustering (MSC) method is used to identify a cut-off radius beyond which a self-interstitial atom (SIA) can be classified as an interstitial [1]. A union-find data structure has been used to cluster the atoms and a method to further analyze the clusters to avoid over-counting due to the presence of dumbbell and crowdion configurations is described [1]. It is seen that the cut-off radius to identify a SIA increases linearly with the temperature of the material and the intercept and slope of this dependence has been obtained for 5 bcc (Cr, Fe, Mo, Nb and W) and 6 fcc (Ag, Au, Cu, Ni, Pd and Pt) crystals [2]. In general, it is seen that the cut-off radii for the bcc crystals are higher than that of the fcc crystals [2]. Molecular Dynamics (MD) simulations of collision cascades in 200 random directions have been carried out in Cu & W for Primary Knock-on Atom (PKA) energies of 1-5 keV in steps of 1 keV using stiffened potentials that match the ZBL potential at small inter-atomic separations [3]. The average number of defects, their clustering and distribution, averaged over the 200 directions can be used as inputs to codes which can simulate radiation induced damage at larger length and time scales. It is seen that around 100 random directions are sufficient for the running average number of defects to saturate.

MD can also be used to study SIA diffusion to obtain the migration energies, pre-factor for diffusion and jump correlation lengths. These parameters can be used to simulate the diffusive recombination of defects (interstitials and vacancies) to either mitigate damage or to form interstitial/vacancy agglomerates thereby changing the microstructure of the material. Therefore, MD simulations are useful not only to simulate collision cascades, but also to obtain other parameters that are important for quantifying irradiation induced changes in material microstructures.

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## **Real-space models for microstructure and the need for a cascade database**

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The development of real-time models for microstructural evolution has been partially stimulated by the recent advances in molecular dynamics simulations.

MD simulations have been applied to modelling the formation and subsequent evolution of defects and clusters of defects, for example, nano-dislocation loops in iron and other metals. A hypothesis stating that clusters of point defects play a significant part in the microstructural evolution of irradiated materials was proposed in the 1990s within the framework of the “production bias” radiation damage model. However, it is only recently that direct observations confirmed the fact that mobile and immobile clusters of point defects form an integral part of the microstructure of an irradiated material.

Somewhat surprisingly, interpreting in situ real-time electron microscope observations remains genuinely problematic. The ten orders of magnitude mismatch between the nanosecond time scale accessible to an MD simulation and the 10–1000 s time scale of a typical experimental observation impedes meaningful quantitative analysis and interpretation of experimental findings. The need to develop a model, using which real-time observations could be simulated and interpreted, does not only stem from the fact that we now have available some high qualitative techniques for characterizing materials.

Recently, the question about how to model, in real time, the evolution of an ensemble of mobile interacting radiation defects has been brought into focus by the rapidly growing applications of ion-beam sources to simulating neutron irradiation damage effects in fission and fusion materials. The presentation illustrates applications of several models for evolving radiation-induced microstructure in real space and real time, and shows an essential part that a collision cascade database can play in the interpretation of experimental observations of radiation effects in a variety of materials, and also in the development of real space models for microstructural evolution in a variety of materials developed for nuclear fission and fusion applications.



## **The analytic embedded atom method and its application to computer simulations for radiation damage**

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The basic theoretical frame of our modified analytic embedded-atom method is introduced briefly. With these potentials, computer simulations for radiation damage is demonstrated for various systems, such as tungsten, helium doping iron, helium doping vanadium, NiMo binary alloy, and amorphous alloys. [1-8]

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## Formation of Nano Size $\langle 100 \rangle$ Interstitial Loop within High Energy Cascades and Their Migration in Iron

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Numerous computer simulations and experimental studies have been performed to understand the formation and evolution of SIA loops in irradiated iron. The formation mechanism of  $\frac{1}{2}\langle 111 \rangle$  loops, as revealed by a number of computer simulations, is well established within displacement cascades in Fe and these loops are known to be glissile parallel to their Burgers vector with an energy barrier of  $\sim 0.1$  eV. Therefore,  $\frac{1}{2}\langle 111 \rangle$  loops are highly mobile at all temperatures and can easily diffuse to and interact with microstructural features such as dislocations, grain boundaries, precipitates, voids, and free surfaces. However, the formation mechanism of  $\langle 100 \rangle$  interstitial loops becomes a long-standing puzzle because the formation energy of  $\langle 100 \rangle$  loops is higher than that of  $\langle 111 \rangle$  loops in Fe. Several mechanisms have been proposed to understand the formation of  $\langle 100 \rangle$  dislocation loops in irradiated iron, including  $\frac{1}{2}\langle 1-10 \rangle$  share of a faulted  $\frac{1}{2}\langle 110 \rangle$  loop, two gliding  $\langle 111 \rangle$  loops colliding to form one  $\langle 100 \rangle$  loop, transformation from  $\langle 111 \rangle$  loops at high temperature, and transformation from a C15 Laves phase interstitial cluster. Here, we report a direct observation of the formation of both interstitial and vacancy  $\langle 100 \rangle$  dislocation loops in high energy displacement cascades using large-scale molecular dynamics simulations (consisting of atoms up to 220 millions). This process occurs very quickly, just in a few picoseconds within the cascades. In addition, the process does not require any precursors other than point defects. However,  $\langle 100 \rangle$  loops are observed in the cascades with PKA energies higher than 200 keV, which suggests that their formation probability at lower energy cascades is very small. In addition, the self-adaptive accelerated molecular dynamics (SAAMD) have been applied to study the transition from a  $\frac{1}{2}\langle 111 \rangle$  loop to form a  $\langle 100 \rangle$  loop, as well as migration of the  $\langle 100 \rangle$  loop, which takes place at the times on the order of  $\sim 10^2$  s.

**Displacement cascade database for PKA energies up to 50 keV in bcc-Fe**

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**Molecular dynamics simulations of collision cascades: method development and results from 1993 on**

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**The structure of the IAEA neutron cross section database**

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