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# Displacement cascades and defects annealing in tungsten, Part I: Defect database from molecular dynamics simulations

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## HIGHLIGHTS

- Two energy regimes of defect production, each with a distinct characteristic slope.
- Profound SIA and vacancy clustering asymmetry at high temperatures.
- Formation of ⟨100⟩ SIA loops during displacement cascade.

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## ABSTRACT

Molecular dynamics simulations have been used to generate a comprehensive database of surviving defects due to displacement cascades in bulk tungsten. Twenty-one data points of primary knock-on atom (PKA) energies ranging from 100 eV (sub-threshold energy) to 100 keV ($\sim 780 \times E_d$, where $E_d$ = 128 eV is the average displacement threshold energy) have been completed at 300 K, 1025 K and 2050 K. Within this range of PKA energies, two regimes of power-law energy-dependence of the defect production are observed. A distinct power-law exponent characterizes the number of Frenkel pairs produced within each regime. The two regimes intersect at a transition energy which occurs at approximately $250 \times E_d$. The transition energy also marks the onset of the formation of large self-interstitial atom (SIA) clusters (size 14 or more). The observed defect clustering behavior is asymmetric, with SIA clustering increasing with temperature, while the vacancy clustering decreases. This asymmetry increases with temperature such that at 2050 K ($\sim 0.5T_m$) practically no large vacancy clusters are formed, meanwhile large SIA clusters appear in all simulations. The implication of such asymmetry on the long-term defect survival and damage accumulation is discussed. In addition, ⟨100⟩{110} SIA loops are observed to form directly in the highest energy cascades, while vacancy ⟨100⟩ loops are observed to form at the lowest temperature and highest PKA energies, although the appearance of both the vacancy and SIA loops with Burgers vector of ⟨100⟩ type is relatively rare.



## 1. Introduction

One of the challenging issues in fusion materials is determining the effects of neutron damage in tungsten plasma facing components under fusion relevant conditions. The challenge stems from the unavailability of a high flux 14-MeV fusion neutron source. Therefore, development of models to predict neutron damage through computer simulations is essential for designing and interpreting experiments performed in fission reactors and linear plasma devices. An example is the extensive effort to develop an open-source code, XOLOTL-PSI [1], to simulate plasma-surface interactions with tungsten. Being a multi-scale simulation tool, XOLOTL-PSI requires input from lower-level atomistic simulations. In this effort, a recently formulated W potential [2] is adopted to gather knowledge of atomistic processes for XOLOTL-PSI. This paper is concerned with the development of a database of primary defect states of radiation damage in tungsten. Along the way, several discoveries are made including a transition energy that separates different regimes of energy associated with different defect survival mechanisms, as well as asymmetric defect clustering behavior (i.e. strong differences in self-interstitial atom vs. vacancy clustering).

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Cascade damage databases at 300, 1025 and 2050 K are compiled. A systematic study of cascade energy ranging from 100 eV to 100 keV is performed at each temperature to better sample the full recoil energy spectrum of the primary-knock-on atom (PKA) due to fusion neutrons. As such, this paper presents the most comprehensive molecular dynamics (MD) database of cascade simulations in tungsten to date [3–6]. The range of PKA energies covers sub-threshold, low- and high-energy regimes. Data at 2050 K allows the investigation of the influence of temperature on defect production and morphology to be performed up to 0.5 of the melting temperature, $T_m$. With this comprehensive set of PKA energies and temperatures, we are able to reveal the profound effect of temperature on the asymmetry of defect clustering.

We have performed both displacement cascade and defect annealing simulations in tungsten. The results are presented in two parts. This paper reports on the primary damage production. Molecular dynamics simulations, with the LAMMPS code [7], have been used to perform the cascade simulations. A companion paper focuses on modeling the long-term evolutions of the resulting defect structures using an object kinetic Monte Carlo (OKMC) technique. That research involved both the development of modular and versatile OKMC software, kSOME and the simulations to determine the fate of the cascade damage, both of which are presented in a companion paper as Part II [8].

## 2. Methods

The W potential used in this study [2] is derived from the Ackland–Thetford potential [9]. A new modification hardens the potential at short distances for radiation damage simulations and improves the potential at distances of relevance to self-interstitial configurations. Prior to cascade simulations, all systems are thermalized for 30 ps at zero pressure with a Nosé–Hoover thermostat to obtain a proper distribution of atom positions and velocities. A cascade is initiated by giving a random PKA near the center of the simulation cell an initial velocity with a random direction. The PKA initial kinetic energy is denoted as $E_{MD}$. The cascade is simulated using a microcanonical ensemble for the first ~10 ps and subsequently thermostated in a constant volume so that the target temperature is achieved within the next 1 ps. A typical total simulation time is ~50 ps. The effect of the thermostat setting on defect counting and clustering is negligible. An adaptive time step is used, allowing a maximum displacement of 0.005 Å per step. Sufficiently large simulation cells are used to ensure no displaced atoms cross the periodic boundaries. Displaced atoms are defined as those beyond $0.3a_0$ of any lattice site, where $a_0$ is the lattice constant at the corresponding temperature. The calculated lattice constants at 300, 1025 and 2050 K are 3.17, 3.18 and 3.22 Å, respectively. Note that these temperatures represent homologous temperatures of 0.07, 0.25 and 0.5 for the potential, respectively.

As usual, a self-interstitial-atom (SIA) or a vacancy is determined from the Wigner–Seitz cells occupancy. The list of PKA energies, simulation cell sizes and the number of simulation runs is presented in Table 1. When appropriate, the analysis presented in this paper is given as a function of PKA energy normalized by the average displacement threshold energy, $E_d$. The conversion to the reduced energies is included in Table 1 for convenience.

## 3. Results

### 3.1. Defect production

The number of surviving Frenkel pairs, $N_F$, is plotted in Fig. 1a as a function of reduced energy defined as $E^* \equiv E_{MD}/E_d$, where the calculated average displacement threshold energy is $E_d$ = 128 eV [2].

**Table 1**
List of PKA energies ($E_{MD}$), simulation cells (cubes with side length $L$ expressed in lattice constant $a_0$) and the number of simulations ($N_r$). The average displacement threshold energy is $E_d$ = 128 eV.

| $E_{MD}$ (keV) | $E_{MD}/E_d$ | $L$ $a_0$ | $N_r$ 300 K | $N_r$ 1025 K | $N_r$ 2050 K |
|---|---|---|---|---|---|
| 0.1 | 0.78 | 15 | 40 | 40 | 40 |
| 0.15 | 1.17 | 15 | 40 | 40 | 40 |
| 0.2 | 1.56 | 15 | 40 | 40 | 40 |
| 0.3 | 2.34 | 15 | 40 | 40 | 40 |
| 0.5 | 3.91 | 20 | 20 | 20 | 20 |
| 0.75 | 5.86 | 20 | 20 | 20 | 20 |
| 1 | 7.81 | 30 | 20 | 20 | 20 |
| 1.5 | 11.72 | 30 | 20 | 20 | 20 |
| 2 | 15.63 | 30 | 20 | 20 | 20 |
| 3 | 23.44 | 30 | 20 | 20 | 20 |
| 5 | 39.06 | 40 | 20 | 20 | 20 |
| 7.5 | 58.59 | 40 | 20 | 20 | 20 |
| 10 | 78.13 | 50 | 20 | 15 | 15 |
| 15 | 117.19 | 50 | 20 | 15 | 15 |
| 20 | 156.25 | 64 | 20 | 15 | 15 |
| 30 | 234.38 | 64 | 20 | 15 | 15 |
| 40 | 312.50 | 64 | 15 | 15 | 15 |
| 50 | 390.63 | 80 | 15 | 15 | 15 |
| 60 | 468.75 | 80 | 15 | 15 | 15 |
| 75 | 585.94 | 100 | 15 | 15 | 15 |
| 100 | 781.25 | 120 | 20 | 20 | 20 |
| | 300 K | 1025 K | 2050 K | | |
| $a_0$ (Å) | 3.167 | 3.184 | 3.216 | | |

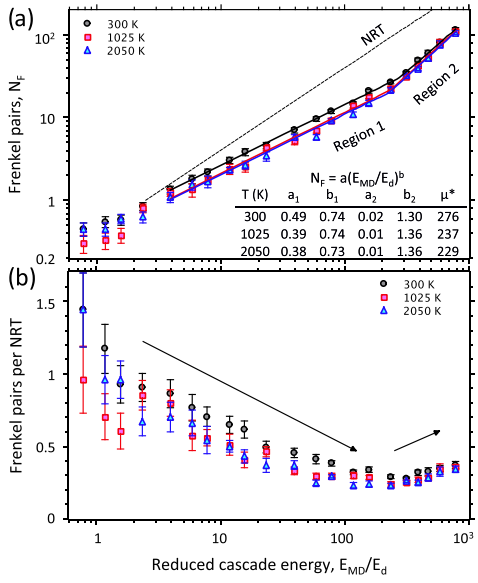


**Fig. 1.** (a) Plots of $N_F$ vs. $E_{MD}/E_d$ and power-law fits revealing two energy regimes with the transition occurring at a reduced energy $\mu^*$, (b) ratio of surviving MD Frenkel pairs to the number of displacements obtained from the NRT model.

The value of $E_d$ signifies the energy at which the probability to create a Frenkel pair is $P_F$ = 0.5. In each of the simulations with $E^* < 2$, $N_F$ is either zero or one, but never >1. Therefore, in this energy regime, $P_F = N_F$, i.e. $P_F$ can be directly read from the $N_F$ curve. Comparing the value of $N_F$ at $E^* = 1$ for different temperatures, we observe the following. At 300 K, the value of $N_F$ is ~0.5, indicating that $E_d$ remains unchanged for a relatively wide range of low temperatures from 10 K to 300 K in tungsten. It is known that a thermally activated Frenkel pair may recombine hence increasing the effective value of $E_d$. This phenomenon is likely responsible for the decrease of $N_F$ to 0.3 at 1025 K. On the other hand, temperature