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Evaluation of the threshold displacement energy in tungsten by molecular dynamics calculations

Mosab Jaser Banisalman, Sehyeok Park, Takuji Oda*

Department of Nuclear Engineering, Seoul National University, 1 Gwanak-ro, Gwanak-gu, Seoul 151-742, South Korea

HIGHLIGHTS

- The threshold displacement energy of tungsten was determined by molecular dynamics calculations to be 85 eV, which reasonably agree with the ASTM recommendation, 90 eV.
- A possible error was estimated to be 4.5% by systematic investigations on the effects of calculation settings such as the system size and the number of sampled recoil directions.
- We explained the reasons why large discrepancies in the threshold displacement energy were observed in previous studies.

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ABSTRACT

The threshold displacement energy (TDE) is an important quantity used to determine the number of defects formed by irradiation of high-energy particles. For the TDE of tungsten, different values have been reported and then used in previous studies, which has caused inconsistencies in calculated damage amounts. In the present study, we evaluate the TDE using molecular dynamics calculations, where the TDE is defined as the average value of the minimum displacement energies for creating a stable defect over all recoil directions. To determine the TDE accurately, the effects of calculation settings, such as the simulation cell size, the number of sampled recoil directions, the increment step of the recoil energy in searching the threshold value, and the thermal vibration of atoms, were analyzed. A TDE of 85 eV was obtained for tungsten with an estimated error of 4.5%. This TDE value is close to the one recommended by the American Society for Testing and Materials (ASTM), 90 eV. Consequently, we conclude that 90 eV is a reasonable choice for the TDE of tungsten.

1. Introduction

Tungsten (W) is a promising candidate material for plasma-facing components in fusion reactors because of its high melting point, low sputtering yield, low tritium inventory, etc. Since the plasma-facing components are exposed to 14 MeV neutron irradiation, radiation damage processes and effects in the materials need to be sufficiently understood. In previous studies, several neutron irradiation experiments have been performed to clarify defect structures [1] and radiation effects on the mechanical properties [2,3] and on the tritium inventory [4,5].

The radiation damages are basically determined by two factors: (i) how many and what kind of defects are created in collision cascades and then (ii) how the defects evolve with time. For the determination of the number of created radiation defects, the threshold displacement energy (TDE) is one of the most important quantities. The TDE is defined as the minimum recoil energy required to form a stable Frenkel pair. The TDE is used in theoretical models such as the Kinchin–Pease model [6] and the NRT model [7] to estimate the number of defects created by collision cascades. Although there are some flaws in these theoretical models, such as an underestimation by the NRT model for a high-energy collision cascade in which the linearity between the damage energy and the defect number is broken [8], the models are still widely used to quantify radiation damage in the unit of displacement-per-atom (dpa) and to then compare the radiation effects of materials irradiated under different conditions.

As for the TDE of W, however, there is a discrepancy in previous studies: 45–61 eV [9] and 98 eV [8], determined by molecular

* Corresponding author.
E-mail address: oda@snu.ac.kr (T. Oda).

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dynamics (MD) calculations; 55.3 eV [10], obtained with a theoretical interpolation model [11] using a few available experimental values [12]; and 90 eV, recommended by the American Society for Testing and Materials (ASTM) [13]. The discrepancies in the TDE values cause inconsistencies in the evaluation of dpa and the number of created radiation defects. Indeed, different TDE values were sometimes employed for the damage evaluation in previous studies: for example, 55.3 eV in Ref. [14], 90 eV in Ref. [15] and some others, and values not specifically mentioned in many other studies.

In the present study, we aim to determine the TDE of W using the MD method as accurately as possible through careful analysis of the effects of MD calculation settings. We also aim to clarify the reason why the large discrepancies appeared among the previous studies. To achieve these aims, the first step of research is to define the TDE in the MD method. Indeed, the definition of the TDE is not very specific: it depends on the purpose and the method, as systematically discussed in a previous study for bcc-Fe [16]. In the present study, we define the TDE as the average value of the threshold displacement energies for all recoil directions, which has often been used as the definition of the TDE in previous MD studies. Hereafter, this average value is denoted $E_{d,avg}$, which is equivalent to $E^{av}{}_{d,ave}$ in Ref. [16].

The remaining part of this paper is organized as follows. In Section 2, methods employed in this study, including the calculation settings of MD recoil simulations and the procedure to search the threshold value, are described. In addition, calculation settings that affect $E_{d,avg}$ are explained. In Section 3, the MD simulation results used to evaluate the effects of four calculation settings, namely, (i) the simulation cell size, (ii) the number of sampled recoil directions, (iii) the increment step of the recoil energy in searching the threshold value, and (iv) the thermal vibration of atoms, are presented and analyzed. Moreover, the result of an additional analysis on the effect of direction deviation for the recoils of some typical directions, such as <100>, is provided. Subsequently, in Section 4, the most probable $E_{d,avg}$ value with an estimated error is presented. In addition, we discuss the reasons why there are apparent inconsistencies between the present study and previous studies in the obtained TDE values. Finally, the paper is closed with concluding remarks in Section 5.

2. Method

2.1. MD calculation settings

MD simulations were performed by using the LAMMPS code [17]. The interatomic interactions between W atoms were described with an embedded-atom method (EAM) [18] potential that was originally parameterized by Derlet et al. [19] and then modified by Björkas et al. [20] for recoil simulations.

A bcc-W crystal was modeled with supercells of various sizes under periodic boundary conditions. In bcc metals, since the <111> collision sequence often occurs, the damage region and reentered atoms along the <111> collision sequence could overlap if a cubic supercell is used. To avoid the overlap, we utilized orthorhombic $(2n_{size}) \times (2n_{size}) \times (3n_{size})$ supercells with an integer n_{size}, such as a $6 \times 6 \times 9$ supercell with $n_{size} = 3$, where the total number of atoms in the supercell (N_{atom}) is equal to $24n_{size}^3$.

Before starting a recoil event, the systems were equilibrated at 0 Pa and 30 K under an NPT ensemble of the Nose-Hoover thermostat [21,22], where 0 Pa is practically equivalent with the atmospheric pressure. For example, the volume difference between 0 Pa and 10^5 Pa is just around 0.00005% in bcc-Fe according to the bulk modulus of bcc-Fe (210 GPa). Additionally, 30 K is within a typical temperature range of recoil simulations for the TDE evaluation.

Recoil MD simulations were performed under the NVE ensemble. Each recoil event was initiated by giving a recoil energy, as an additional kinetic energy, to an atom, which is regarded as the primary knock-on atom (PKA). The total energy of the system is conserved after the introduction of the recoil energy. In the present study, we always selected the same atom as the PKA. Electronic stopping was not considered because the utilized recoil energies were not high.

An adaptive timestep implemented in the LAMMPS code was used. Specifically, in every 5 steps, the timestep was first estimated so that the maximum displacement (x_{max}) of atoms per step became less than 0.01 Å. Then, if the estimated timestep was larger than t_{max}, which was 2 fs in the present study, the timestep was reset to t_{max}. We confirmed that this adaptive scheme with $x_{max} = 0.01$ Å and $t_{max} = 2$ fs is accurate enough for the purpose of the present study by comparing the results for some different x_{max} and t_{max} values.

Each recoil MD simulation was performed up to around 5 ps after the onset of the recoil event. For the last structure of each recoil simulation, whether a defect was formed in the system or not was judged by the Wigner-Seitz defect analysis [23] using the LAMMPS Voro++ package [24]. Specifically, we first defined Wigner-Seitz cells with respect to the initial atomic configuration, which is a perfect bcc-W lattice at 30 K. Then, in recoil simulations for which there was a Wigner-Seitz cell that did not contain an atom, the cell was regarded as a vacancy, and we judged that a defect was formed. It should be noted that if the size of the supercell is small, the system starts to significantly move/drift when a recoil event is initiated because the introduction of a recoil energy induces a momentum in the system under the NVE ensemble. The movement/drift of the system sometimes causes a misjudgment in the Wigner-Seitz defect analysis. Therefore, to avoid this, the center of mass of the system was fixed during recoil simulations. We confirmed in some test cases that the Wigner-Seitz defect analysis with a fixed center of mass appropriately detects a defect in comparison with visualization analysis of the MD results.

To determine the minimum displacement energy for each recoil direction, we conducted the following two steps:

- ✓ (Step-1) The recoil energy was first set to 25 eV, and it was then increased by ΔE_{step} eV until a defect was first detected;
- ✓ (Step-2) After the first detection of a defect, the recoil energy was decreased by 1 eV to determine the minimum energy for defect formation.

The minimum energy for a specific recoil direction is denoted as $E_{d,i}$ hereafter, where the index i indicates the recoil direction. We also use a similar notation to represent the $E_{d,i}$ value for a specific recoil direction: for example, $E_{d,<100>}$ represents the $E_{d,i}$ of the <100> recoil direction.

2.2. Calculation settings that affect $E_{d,avg}$

The $E_{d,avg}$ value determined by MD calculation depends on (1) the system size, (2) the number of sampled recoil directions, (3) the ΔE_{step} value used in searching the threshold, (4) the thermal vibration effect, (5) the potential model, and (6) the temperature. In the present study, the effects of (1)–(4) were investigated.

The effect of (5) the potential model was not examined because we consider the potential model used in the present study to be one of the best W potential models available for recoil simulations. As will be presented in Section 3, this potential model gives $E_{d,<100>}$ and $E_{d,<111>}$ values comparable with experiment: 43 eV and 41 eV in the MD simulation with the present potential model and 42 ± 1 eV