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Effect of collision cascades on dislocations in tungsten: A molecular dynamics study

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ABSTRACT

Tungsten (W) is the prime candidate material for the divertor and other plasma-facing components in DEMO. The point defects (i.e. vacancies and self-interstitials) produced in collision cascades caused by incident neutrons aggregate into dislocation loops (and voids), which strongly affect the mechanical properties. The point defects also interact with existing microstructural features, and understanding these processes is crucial for modelling the long term microstructural evolution of the material under fusion conditions. In this work, we performed molecular dynamics simulations of cascades interacting with initially straight edge dislocation dipoles. It was found that the residual vacancy number usually exceeds the residual interstitial number for cascades interacting with vacancy type dipoles, but for interstitial type dipoles these are close. We observed that a cascade near a dislocation promotes climb, i.e. it facilitates the movement of point defects along the climb direction. We also observed that the dislocations move easily along the glide direction, and that kinks are formed near the centre of the cascade, which then facilitate the movement of the dipoles. Some dipoles are sheared off by the cascade, and this is dependent on PKA energy, position, direction, and the width of dipole.

1. Introduction

Tungsten (W) and W-alloys are the primary candidate materials for plasma facing components in the extreme operating conditions of fusion reactors. Besides high temperature and corrosion, they are also exposed to intense irradiation from neutrons, photons, electrons, various atoms and ions. The exposure will continuously displace atoms from their perfect lattice sites generating a supersaturation of point defects, and thereby create vacancy clusters, dislocations loops, voids and even microscopic bubbles, which influence the mechanical properties and degrade the performance and lifetime of fusion components.

Dislocation movement, including glide and climb, is one of the key processes in the evolution of radiation damage, e.g. dislocation loop punching has been regarded as one of the crucial mechanisms for the nucleation and growth of gas bubbles in metals [1,2]. The subsequent evolution will change the surface morphology of materials. Jia et al. [3,4] have experimentally demonstrated that the blister formation model based on plastic deformation can explain the orientation dependence of blisters. However, dislocation loop evolution is frequently complicated. The interaction between loops, glide usually being easier than climb, and self-climb being faster than vacancy-mediated climb all strongly affect the evolution of loops [5,6]. The continuing irradiation also affects the evolution of the existing loops. Therefore, it is necessary to understand these processes from atomic point of view, and to know how collision cascades affect dislocation motion, which is also crucial for modelling the long term microstructural evolution of the material under fusion conditions.

As the key theoretical tool for understanding how microstructural effects in materials occur at the atomic level, molecular dynamics (MD) simulations have been used to investigate collective phenomena, such as transport phenomena [7–11], plastic deformation [12], and radiation damage [13,14]. In this work we focus on MD simulations of cascades interacting with initially straight edge dislocation dipoles. It was found that cascades can facilitate the movement of the dipoles toward the centre of cascades, promote the movement of point defects along the climb direction, and shear off the dipoles in some cases. The rest of the paper is organized as follows. In Section 2, we will describe MD details, including potentials and box creation. In Section 3, we will

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present the simulation results and discuss the effect of collision cascades on dislocations in tungsten.

2. Simulation method

Potential selection is one of the key ingredients in MD simulation. Currently, there have been many published interatomic potentials [15–22] used to describe the W-W interaction. Based on the benchmark by Bonny et al. [23], EAM4 produced by Marinica et al. [21] (abbreviated as Marinica4) was used in this work, since the Marinica4 potential clearly reproduces dislocation behaviour. As was performed earlier [7,13,24–26], the potential was first connected with a ZBL universal potential [27] to ensure short-range reliability.

All MD simulations were performed using MDPSCU, which was originally written by Hou et al. [28]. In this MD package, any process can be accelerated by multiple graphic processing units (GPUs) in parallel. The MD simulator was extended through the addition of some functional modules, such as box creation [7]. In an MD simulation, system information (i.e. atomic positions and velocities), generated by integrating the classical equations of motion, can be used to analyze equilibrium and transport properties. We used the velocity-Verlet algorithm [29] to integrate the equations of motion. Common neighbor analysis and the Wigner-Seitz method were used to identify the point defects, and the open visualization tool (OVITO) [30] was used to visualize the atomic structure and point defect configuration. Simulation boxes were prepared as illustrated in Fig. 1. A dipole, containing two dislocations of opposite sign on different slip planes, was constructed in the middle of x–y plane. Through inserting (extracting) one plane of W atoms (in the blue region), interstitial (vacancy) type dipoles were created. The x, y, and z axes of the simulation box are $\langle 1\,1\,1\rangle$, $\langle 1\,1\,0\rangle$, and $\langle 1\,1\,2\rangle$, respectively. The x-axis corresponds to the dislocation glide direction, and the y-axis is the climb direction. Periodic boundary conditions (PBCs) were used in all 3 dimensions to deal with finite-size effects. The width of the dipole along the y direction was $4\times[1\,1\,0]$, $6\times[1\,1\,0]$, or $10\times[1\,1\,0]$. As shown in Table 1, the atomic number (N_{atom}) in one simulation box was about 240,000 or 1,080,000 W atoms, depending on the kinetic energies of the primary knock-on atoms (PKAs).

All the boxes were first quenched to move all atoms in the simulation to the nearest favorable site, where the box temperature is close to 0 K. Then the boxes were relaxed and finally were equilibrated for more than 100 picoseconds (ps). In these processes, the MD time step was set to 1 fs (fs). Temperature was confined based on thermalisation [7] firstly, and then by using electron phonon coupling (EPC) [31,32]. Fig. 2(a) shows the atomic configuration (projection along the z-axis) of box after relaxation. According to many trials, we found the two dislocations in one dipole can easily glide in the opposite glide directions at the beginning of relaxation and then equilibrate at close to 45° (θ is the angle between the plane including the two dislocation edges and the slip plane) as shown in Fig. 2(a), which is consistent with the prediction of elasticity theory [33]. In the equilibrium state, the variations of θ and the positions of dipole (x_p) are both rather small as shown in Fig. 2(b). Therefore, the dipole is stationary on the MD time scale if there is no external stress.

After full equilibration (more than 100 ps), the collision cascade event was initiated by imparting kinetic energy to the selected PKA

Table 1
PKA energy (E_{PKA}) and corresponding atomic number (N_{atom}) in one perfect simulation box. The atomic number in one simulation box with dislocations is close to N_{atom}.

E_{PKA}	10 keV	20 keV	30 keV
N_{atom}	240,000	1,080,000	1,080,000

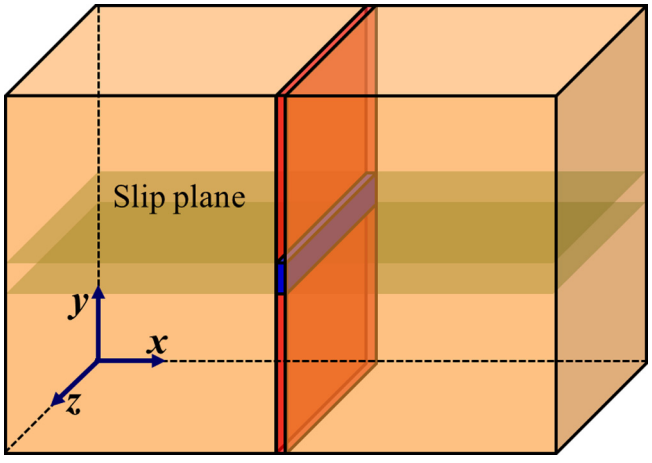

Fig. 1. Schematic representation of simulation box with dislocations. Vacancy or interstitial type dipole was constructed in the blue region. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

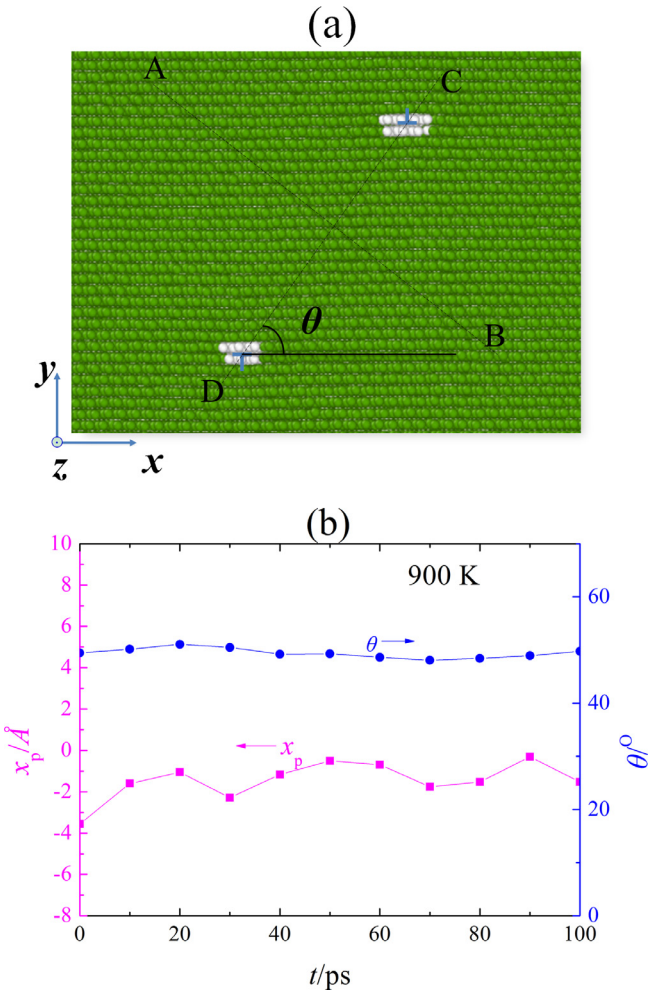

Fig. 2. (a) The atomic configuration near the dipole after relaxation. Green ball denotes body-centered cubic (bcc) atom, white non-bcc atom. PKAs were usually distributed in the AB and CD line. (b) The variations of θ and the positions of dipole (x_p) in the relaxation process. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)