Nuclear Instruments and Methods in Physics Research B 384 (2016) 68–75

Contents lists available at ScienceDirect

Nuclear Instruments and Methods in Physics Research B

journal homepage: www.elsevier.com/locate/nimb

Effect of strain field on displacement cascade in tungsten studied by molecular dynamics simulation

D. Wang [a,b], N. Gao [a,*], Z.G. Wang [a,*], X. Gao [a], W.H. He [a,b], M.H. Cui [a], L.L. Pang [a], Y.B. Zhu [a]

[a] Institute of Modern Physics, Chinese Academy of Sciences, Lanzhou 730000, China
[b] University of Chinese Academy of Sciences, Beijing 100049, China

ARTICLE INFO

Article history:
Received 16 June 2016
Received in revised form 11 August 2016
Accepted 11 August 2016

Keywords:
Strain field
Tungsten
Molecular dynamics
Displacement cascade

ABSTRACT

Using atomistic methods, the coupling effect of strain field and displacement cascade in body-centered cubic (BCC) tungsten is directly simulated by molecular dynamics (MD) simulations at different temperatures. The values of the hydrostatic and uniaxial (parallel or perpendicular to primary knock-on atom (PKA) direction) strains are from −2% to 2% and the temperature is from 100 to 1000 K. Because of the annealing effect, the influence of strain on radiation damage at low temperature has been proved to be more significant than that at high temperature. When the cascade proceeds under the hydrostatic strain, the Frenkel Pair (FP) production, the fraction of defect in cluster and the average size of the defect cluster, all increase at tensile state and decrease at compressive state. When the cascade is under uniaxial strain, the effect of strain parallel to PKA direction is less than the effect of hydrostatic strain, while the effect of strain perpendicular to PKA direction can be negligible. Under the uniaxial strain along ⟨1 1 1⟩ direction, the SIA and SIA cluster is observed to orientate along the strain direction at tensile state and the uniaxial compressive strain with direction perpendicular to ⟨1 1 1⟩ has led to the similar preferred nucleation. All these results indicate that under irradiation, the tensile state should be avoided for materials used in nuclear power plants.

1. Introduction

Due to the high melting temperature, high thermal conductivity, relatively low neutron activation and low sputtering yield, tungsten and tungsten-based alloys have been selected as one of candidate materials for the divertor and plasma facing components (PFC) in future fusion reactors [1]. Under the extreme environment in fusion reactors, tungsten will not only be exposed to high energy particles such as hydrogen, helium and neutron, leading to the heavy radiation damages, but also suffer from the high heat flux, the related thermal stress and other external mechanical loads. The stresses can influence the formation, migration and the other properties of radiation-induced defects. The threshold displacement energy (E_d) of tungsten is also found to be affected by local stresses [2]. Hence, the coupling effect of radiation and stress may influence the kinetic process of defects created by the radiation damage, e.g. the defect production rate, clustering behavior and the change of microstructure configuration. Therefore, the understanding of displacement cascade under the effect of stress/strain field is of great importance and need to be studied comprehensively.

Previous studies of displacement cascade in tungsten mainly focused on the following factors: the primary knock-on atom (PKA) energy [3–6], the PKA directions [7] and the irradiation temperature [4,5,8,9]. The reported results provide good understanding of the surviving defect number after cascade, defect properties and cluster behavior with regard to PKA energy, direction and annealing temperature. However, the influence of stress/strain fields is less studied as stated by Beeler et al. [10]. Until now only several papers are published about this topic for metals, including the face-centered cubic (FCC) copper [11,12], hexagonal close-packed (HCP) zirconium [13] and body-centered cubic (BCC) iron [10,14,15]. In FCC copper, as investigated by Miyashiro et al. [11,12], defect production rate in cascade increased under both uniaxial tensile and compressive strain. The largest increase was observed under isometric strain. The radiation damage of HCP zirconium under <a> or <c> strain studied by Di et al. [13] revealed that the external strain mainly affected the size of defect clusters rather than the total number of defects. For BCC iron, three studies were performed to understand such effects. Kirsanov et al. [14] found that non-uniform loads can decrease the number of

* Corresponding authors.
E-mail addresses: ning.gao@impcas.ac.cn (N. Gao), zhgwang@impcas.ac.cn (Z.G. Wang).

http://dx.doi.org/10.1016/j.nimb.2016.08.006
0168-583X/

stable defects, change the threshold displacement energy and also the cascade region structure. Gao et al. [15] investigated the displacement cascade of α-iron under uniaxial tensile strain along ⟨1 1 1⟩ direction, revealing that the number of defects decreased in the tensile state (strain <1%) and the fraction of interstitials aligned parallel to the strain axis increased with increasing strain. Recently, Beeler et al. [10] have studied the effects of hydrostatic strain, uniaxial strain, monoclinic shear and tetragonal shear strains on the radiation damage production, finding that the volume-conserving shear strains yielded no significant changes in the stable number of defects produced, while the volume changed strains did the opposite. However, for BCC tungsten, few studies were performed about the stress and strain effects on the radiation damage. Our previous work [2] provided evidences that hydrostatic strains significantly affect the formation energies of defects and E_d in tungsten. Changing the strain from compression to tension decreases the self-interstitial atoms (SIAs) formation energies but increases the vacancy formation energy. Similar to the SIA formation energy, E_d is also found to decrease with the strain from compression to tension for hydrostatic case. Since the formation energies of defects and E_d are both affected by strains applied on the system and also these two properties play important roles in understanding the displacement cascade, therefore, it is necessary to study the strain effect on displacement cascade in tungsten for completeness of our understanding of coupling effect of strain and radiation for future development of radiation resistant materials used in fusion reactors.

It should be noted that the previous studies [10–15] only focused on the effect of strain on number of defects created by the displacement cascade in copper, zirconium and iron. The detail of coupling effect has not been explored, especially the effect from the combination of the directions of applied strain and PKA. In this work, displacement cascade under different applied strains, the hydrostatic strain and uniaxial strain either parallel or perpendicular to PKA directions, will be simulated by molecular dynamics (MD) simulation to investigate the impact of strain and effect of above combination on defect production, cluster fraction and size in BCC tungsten. The details of simulations are firstly described in Section 2. Then the information of the Frenkel Pair (FP) production, cluster fraction and size and rotation of ⟨1 1 1⟩-crowdions during the collision cascade under strains in tungsten are presented in Section 3. The results are discussed in Section 4. Finally, the conclusions are given in Section 5.

2. Method

The molecular dynamics simulations are performed using LAMMPS [16] software package. The interatomic interaction between W atoms in this work is described by a modified version of Ackland-Thetford potential [17] developed by Juslin and Wirth [18]. It has been shown in previous studies [2,18] that Juslin-potential provides good fittings of defect properties to DFT results [19,20] and threshold displacement energy. Periodic boundary conditions are applied along three directions in all simulations. The PKA energy is set to 5 keV for all simulations. In BCC crystal system, since the ⟨1 0 0⟩, ⟨1 1 0⟩ and ⟨1 1 1⟩ directions are highly symmetrical, the ⟨1 3 5⟩ direction is usually selected as the direction representing the average behavior of displacement cascade [21]. In the present work, the PKA directions are chosen along ⟨1 0 0⟩, ⟨1 1 0⟩, ⟨1 1 1⟩ and ⟨1 3 5⟩ to get representative data for BCC tungsten, which can also be compared with previous studies [10,15]. The hydrostatic and uniaxial strains applied in the simulations are from −2% to 2%. It should be noted that negative values correspond to compressive strain and positive values correspond to tensile strain. For hydrostatic style, the same strains are applied in X, Y and Z axes of simulation cell, and the hydrostatic strain is then defined as $\varepsilon_{hyd} = 1/3Tr(\varepsilon)$, where ε is the externally applied strain tensor. For uniaxial style, the strains are applied either parallel ($\varepsilon_{\parallel} = \varepsilon_{xx}$, in X axis) or perpendicular ($\varepsilon_{\perp} = \varepsilon_{yy}$, in Y axis) to PKA directions, where ε_{xx} and ε_{yy} is the strain tensor along X and Y axis. It should be noted in this work, the uniaxial and hydrostatic strain instead of stress are mainly considered as the primary factors. One example of box deformation with 2% strain is listed in Table 1. After the cell has reached the preset strain, its size would be kept for the following simulations. In order to investigate the coupling effect of temperature and applied strain, the simulations are also performed at four different temperatures, 100 K, 300 K, 500 K, 1000 K, with same strain range.

As the combination of strain and PKA directions may affect the simulation results, four simulation cells are constructed by setting the X axes to be consistent with PKA directions. For the first case, the [1 0 0], [0 1 0], [0 0 1] are selected for X, Y and Z axes. The PKA is then along X [1 0 0] direction. For the other three cases, the different orthogonal systems are built for simulation cells for computational purpose as listed in Table 2. The cell size is chosen to keep the displacement cascade occurring in the center of the box instead of crossing the boundary. In the present work, the cells containing W atoms about 250,000, 245,000, 243,600 and 245,700, respectively, are built for above four cases (Table 2). As stated in above paragraph, the strain are mainly applied along X and Y directions for uniaxial strain state cases. Thus, the above combination effect can be then studied.

The total energy minimization of system is firstly performed to get a relaxed cell under the preset constant strain. The MD simulations are then followed at the given temperatures (100–1000 K) for 30 ps using NVT ensemble with a timestep of 1 fs. For different strain state, PKA direction and temperature, 20 simulations are performed for statistical analysis by changing the random seed in MD simulations. Following the method suggested by Setyawan et al. [22], the displacement cascade is simulated in an NVE ensemble for all atoms except the border atoms. The border atoms are those within Region-I as shown in Fig. 1, which is about 2 atomic layers from the box edges. To extract heat from system, the border atoms are applied with NVT ensemble at given temperature. An automatically adaptive time step method is used during the simulation by restricting the maximum atom displacement to 0.005 Å per step. For each case, the total simulation time of displacement cascade is ~20 ps. Thus, long-time thermal diffusion is not taken into account in this work. As stated above, the PKA position is carefully selected so that the displacement cascade is kept in Region-II (Fig. 1), ensuring the boundary will not affect the cascade results.

The Wigner-Seitz (WS) cell method is employed to analyze the state of the defects. An empty cell without W atom is identified as a vacancy, while two W atoms in a WS cell is identified as an interstitial and more than two W atoms in a WS cell is then regarded as an interstitial cluster. The defect cluster state are then obtained. In previous studies, the most commonly used cutoff radii in cluster analysis are the 2nd or the 4th nearest neighbor (NN2 or NN4) distance for vacancy, and the 3rd nearest neighbor (NN3) distance for interstitial defects [8, 23,24]. In this work, the mass center of a defect is used to identify the position of the defect. Considering

Table 1
Details of cell deformation for a representative 2% applied strain. ε_{hyd} is hydrostatic strain. $\varepsilon_{\parallel}$ is uniaxial strain parallel to PKA direction. $\varepsilon_{\perp}$ is uniaxial strain perpendicular to PKA direction. ε_{xx}, ε_{yy} and ε_{zz} are strain applied along X, Y and Z axis.

2% strain	ε_{xx} %	ε_{yy} %	ε_{zz} %	Volume change %
ε_{hyd}	2	2	2	6.12
$\varepsilon_{\parallel}$	2	0	0	2
$\varepsilon_{\perp}$	0	2	0	2