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Migration and nucleation of helium atoms at (110) twist grain boundaries in tungsten

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HIGHLIGHTS

- The preference sites for the He interstitial on three typical twist grain boundaries (TGBs) plane are obtained.
- The dislocation network in the LAGB is a good sink for defects, which can attract and bind defects in the grain boundary.
- The magnitude and dimensionality of He migration in TGBs are reduced and influenced by grain boundary structure.
- Compared with the bulk, TGBs have higher cluster densities, smaller cluster sizes and more SIAs at high temperature.

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ABSTRACT

The migration and nucleation of He atoms at three typical (110) twist grain boundaries (TGBs): the low-angle grain boundary (LAGB), the ordinary high-angle grain boundary (HAGB) and the Σ3 TGB in W are investigated using molecular dynamics simulations. The presence of TGBs can absorb He atoms from bulk and impede the growth of He bubbles. Moreover, different grain boundary (GB) structures behave differently when interacting with He atoms. The LAGB can control the He distribution on the GB plane through its screw dislocation network, suggesting a promising approach for design of radiation tolerant materials. The ordinary HAGB presents a strong trap effect due to its disordered GB structure, which may induce a large He retention at the GB and embrittlement. The Σ3 TGB can provide a diffusion path for He atoms, although the diffusion rate is not as fast as it in bulk.

1. Introduction

One of the most important challenges for the successful commercialization of fusion power is the development of plasma facing materials (PFMs) that can tolerate the extreme conditions of elevated temperatures and high flux of plasma present in fusion reactors. Tungsten (W) is regarded as a promising candidate for PFMs because of its high melting temperature, high thermal conductivity and low sputtering erosion [1–3]. However, there are still many challenges in its future application. One of the major challenges is its exposure to large fluences of helium (He) plasma generated by (n, α) reactions, which can precipitate into clusters and bubbles [4–9], promote swelling, hardening and embrittlement [10,11], and eventually degrade mechanical properties and lifetime of structural materials [12,13].

Grain boundaries (GBs), severing as effect sinks for radiation-induced defects, can significantly improve the radiation resistance of materials and heal the crystal [14–17]. To date, extensive researches have covered the interaction between GBs and He atoms [18–22]. Bai et al. [16] investigate the defect-GB interaction mechanism in Cu and find that the Σ11 tilt GB can absorb interstitials and reemit them to annihilate bulk vacancies, leaving a healed crystal. The self-healing mechanism is also verified through first-principle calculations by Liu et al. [17]. Furthermore, Valles et al. [21] study the influence of a high GB density on the amount, size and distribution of defects produced by pulsed He irradiation in W and reveal that the He retention at GBs increases with the GB density. Among different GBs, twist grain boundaries (TGBs) draw more and more attention for their unique GB structures [23,24]. In our previous work [25], the energy and structure of (110) twist

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grain boundaries in W have been systematically investigated. According to the analysis of dislocation, (110) TGBs can be divided into three types: low-angle grain boundaries (LAGBs), intermediate-angle grain boundaries (IAGBs) and high-angle grain boundaries (HAGBs). When the twist angle $\theta \leq 16.10°$, a regular dislocation network consisting of $\frac{1}{2}[111]$, $\frac{1}{2}[\bar{1}\ 11]$ and $[001]$ screw dislocations exists in LAGBs. And the size and shape of meshes in the network vary with increased twist angles. The regions separated by dislocations are body-centered cubic arrangement regions (referred as normal regions in this work). In IAGBs, with $17.23° \leq \theta \leq 22.22°$, both atomistic structures and dislocations are disordered and dislocations do not form a regular network. The TGBs with $\theta \geq 23.5°$ are HAGBs, where no dislocation is observed. The HAGBs can be divided into three sub-types further: special boundaries with low Σ, boundaries in their vicinity with similar structures as the corresponding special boundary in local regions as well as ordinary HAGBs consisting of periodic patterns.

Previously, molecular statics, molecular dynamics and experiments have been combined to study the He bubble nucleation at LAGBs in Au and Cu [26,27]. The results indicate that He bubbles preferentially nucleate at screw dislocation nodal points and a He bubble superlattice is formed, which implies a potential approach for the design of radiation tolerant materials. Kumar et al. [28] simulate the shear deformation of {110} LAGB in α-Fe with and without He bubbles and reveal that the presence of He has a predominantly impact on the mechanical response of this particular dislocation structure, inducing hardening and possibly embrittlement. Despite the valuable resources provided by these early studies, we still lack a comprehensive understanding of the behavior of He atoms in different TGBs.

In this work, we focus on the He migration and nucleation behaviors at early stages in different TGBs. In the following, we will first describe the simulation method in section 2. The migration and nucleation behaviors of He atoms in different TGBs are presented in section 3, followed by the conclusions given in section 4.

2. Method

In this work, the potential for W-He system proposed by Juslin and Wirth [29] is used. They develop a new pair potential for W-He interaction and modify the Acaland-Thetford W-W potential [30] at short range. For He-He interaction, the Beck potential [31] with the short range fit by Morishita et al. [32] is adopted. Before MD simulations, we calculate the parameters for the W-He interaction using the present potential and compare them with those from experiment, DFT calculations and other potentials (Table 1). The comparison indicates that the present potential provide a good description for the W-He interaction. Besides, the present potential proposed by Juslin and Wirth has been widely used in the researches of the W-He interaction, such as He cluster growth [33], He diffusion on grain boundaries [34] as well as He behaviors near surface [35–37], which further prove its reliability.

To investigate the effect of GB structures on He migration and nucleation, three typical TGBs are studied: the LAGB with $\theta = 3°$, the ordinary HAGB with $\theta = 34.38°$ and the Σ3 TGB with $\theta = 70.53°$. The details of methodology used in construction of the simulation models of TGBs have been described elsewhere [25,48]. The upper and lower sections of a single crystal rotate about the $[1\bar{1}0]$ direction by $\frac{\theta}{2}$ clockwise and counterclockwise respectively. After rotation, the equilibrium GB structures are obtained via the combination of conjugate gradient energy minimization and quasi-dynamic quenching. Periodic boundary conditions are applied along the x and y directions, while a fixed boundary condition is applied along the z direction. The migration and nucleation of He atoms are investigated respectively through two independent simulations. In the first simulation, the mean square displacement (MSD) is used to analysis the migration of a He interstitial, which is randomly inserted in the TGB plane. MSD calculations are performed from 300 to 1200 K with migration time of 1 ns? For each TGB, five calculations are performed to reduce the statistics effect and their results are averaged. In the LAGB, the MSDs are calculated in the dislocation network and normal regions respectively for the apparent difference between them. In the second simulation, the nucleation process of He atoms in TGBs under different He

Table 1
Parameters of the W-He system determined from the present potential, in comparison with those form experiment, density-functional theory (DFT) calculations, the modified embedded atom method (MEAM) potential and the bond-order potential (BOP). a: the lattice constant (Å); E_c: cohesive energy (eV/atom); E_f: formation energy (eV); v: vacancy: SIA: self-interstitial atom; tet: tetrahedral interstitial; oct: octahedral interstitial; $db\langle ijk\rangle$: $\langle ijk\rangle$ dumbbell interstitial configuration.

	Present	DFT	Experimental	BOP	MEAM[j]
a	3.165	3.18[c]	3.165[d]	3.165[h,i]	3.164
E_c	−8.90	−7.406[i]	−8.90[e]	−8.906[h],−8.89[i]	−8.66
$E_{f,v}$	3.63	3.46[a],3.56[b]	3.7 ± 0.2[f]	3.52[h],1.68[i]	3.95
$E_{f,tet}^{SIA}$	10.31	11.64[a],11.05[b]		10.75[h]	
$E_{f,oct}^{SIA}$	10.41	11.99[a],11.68[b]		12.05[h]	
$E_{f,db\langle 100\rangle}^{SIA}$	10.29	11.74[a],11.49[b]		12.01[h]	
$E_{f,db\langle 110\rangle}^{SIA}$	10.18	10.10[a],9.84[b]		9.53[h]	8.98
$E_{f,db\langle 111\rangle}^{SIA}$	9.51	9.82[a],9.55[b]	9.06 ± 0.63[g]	9.33[h]	
$E_{f,subs}^{He}$	4.69	4.70[a]		4.70[h]	
$E_{f,tet}^{He}$	6.15	6.16[a]		6.21[h]	
$E_{f,oct}^{He}$	6.30	6.38[a]		6.39[h]	

[a] Ref. [38].
[b] Ref. [39].
[c] Ref. [40].
[d] Ref. [41].
[e] Ref. [42].
[f] Ref. [43].
[g] Ref. [44].
[h] Ref. [45].
[i] Ref. [46].
[j] Ref. [47].