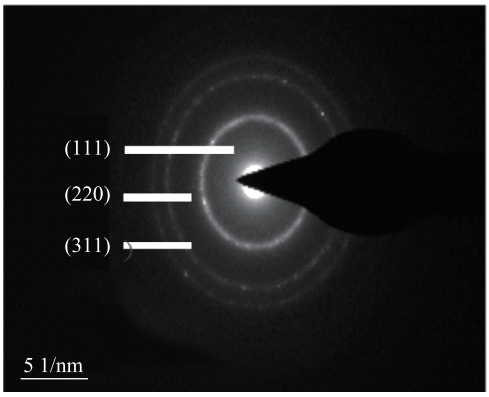

Fig. 1 Diffraction pattern from the unirradiated fiber.

Phases in the SiC fibers were determined by X-ray powder diffraction (XRD),as shown in Fig. 2. All XRD patterns were acquired using copper K-α radiation. Cu K-α radiation via a rotating anode was used; Cu K-α_2 and a continuously increasing background were removed from the XRD patterns using JADE software. The typical diffraction peaks at $2\theta = 35.8°$, 60.4°, and 72.1°, attributed to the (111), (220), and (311) lattices of 3C-SiC according to the JCPDS card (29-1129), respectively.

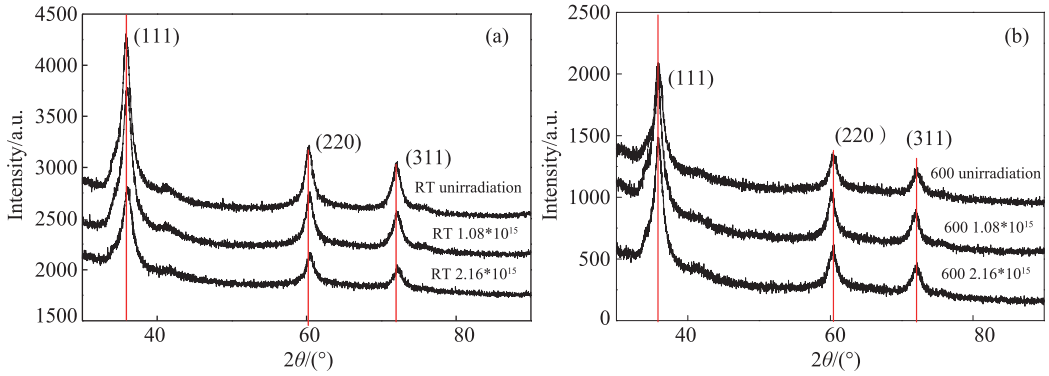

Fig. 2 (color online) XRD spectra of irradiated and non-irradiated SiC fibers. (a)at RT(b)at 600 ℃.

The XRD spectra of non-irradiated fibers at 600 ℃ show a significant evolution in comparison to non-irradiated one at room temperature. These differences concern the local structure modification. As the dose increases the peak intensity decreases, and the peak position moves to the right at the room temperature. The XRD spectra of irradiated fibers at 600 ℃ is different with the room temperature. In general XRD spectra suggest that SiC fiber has great irradiation resistance at the fluence of 2.16×10^{15} ions/cm^2.

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4 - 9 First-principles Investigation of Vacancy and Self-interstitial Atom Segregations at Grain Boundaries in Tungsten

He Wenhao, Gao Xing and Wang Zhiguang

Materials served in nuclear energy systems usually expose to high irradiation doses of particles. Projectile particles lead to creations of a large numbers of vacancies (Vs) and self-interstitial atoms (SIAs) in materials. The SIAs may gather to form dislocation loops and stacking-fault tetrahedrons, and the Vs usually gather to form voids. These defects contribute to material swelling, hardening, amorphization and embrittlement, and may accelerate material failure under irradiation[1]. As recombination center of Vs and SIAs, grain boundaries (GBs) are able

to enhance the radiation resistance of materials[2]. However, experimental investigation show that point defects sink strengths might depend on GB structures. The vacancy sink efficiency of the twin boundary $\sum 3(110)[111]$ is significantly lower than that of other GBs[3−5]. Moreover, the nano-crystalline copper contained a high fraction of twin boundary $\sum 3(110)[111]$ was not enhanced the radiation resistance[6]. Usually, GBs that have atomic configurations such that both the ability to trap intrinsic point defects and Frenkel pair annihilation rates are high will be good sinks for Vs and SIAs. Here, we mainly study the atomic configurations around GBs effects on the ability to trap Vs and SIAs.

Tungsten (W) and its alloys have important application prospects in future advanced nuclear energy systems. In this study, the abilities to trap Vs and SIAs of eight symmetric tilt GBs in tungsten are investigated through first-principles calculations. The eight symmetric tilt GBs in tungsten are constructed by the coincidence site lattice (CSL) model[7]. Our results provide a sound theoretical guide to design favorite GBs to enhance segregations of intrinsic point defects.

Segregation energy $E^{\mathrm{S}}_{\mathrm{V(SIA)}}$ of V (SIA) is able to indicate the GB capability to trap intrinsic point defects. The Vs and SIAs prefer to segregate to the sites with the lowest formation energy. Accordingly, the segregation energy $E^{\mathrm{S}}_{\mathrm{V(SIA)}}$ of V (SIA) at a GB can be defined as,

$$E^{\mathrm{S}}_{\mathrm{V(SIA)}} = E^{\mathrm{f}}_{\mathrm{GB,V(SIA)}} - E^{\mathrm{f}}_{\mathrm{bulk,V(SIA)}}, \tag{1}$$

where $E^{\mathrm{f}}_{\mathrm{(GB,V(SIA))}}$ and $E^{\mathrm{f}}_{\mathrm{bulk,V(SIA)}}$ are the lowest formation energy of V(SIA) at the GB and in bulk, respectively. The larger segregation energy is, the less easily the point defect segregates to the GB. Figure 1(a) the relationship between the $E^{\mathrm{S}}_{\mathrm{V}}$ and GB energy γ. It can be seen that $E^{\mathrm{S}}_{\mathrm{V}}$ decreases as the γ increases. Figure 1(b) the relationship between the $E^{\mathrm{S}}_{\mathrm{SIA}}$ and the excess volume (V_{GB}/S). The excess volume (V_{GB}/S) of GB can be defined as[8]

$$V_{\mathrm{GB}}/S = \left(V - \frac{V_0}{n_0} \times n\right) / (2 \times S), \tag{2}$$

where V_0 and n_0 are the volume and the number of atoms in perfect bulk, respectively. V, n and S are the volume, the number of atoms and the cross sectional area in supercell contained the GB, respectively. It is obvious that $E^{\mathrm{S}}_{\mathrm{SIA}}$ monotonically decreases as the V_{GB}/S increases. Among all the GBs studied here, the twin GB $\sum 3(110)[111]$ has the weakest capability to trap Vs and SIAs due to its lowest GB energy and smallest excess volume.

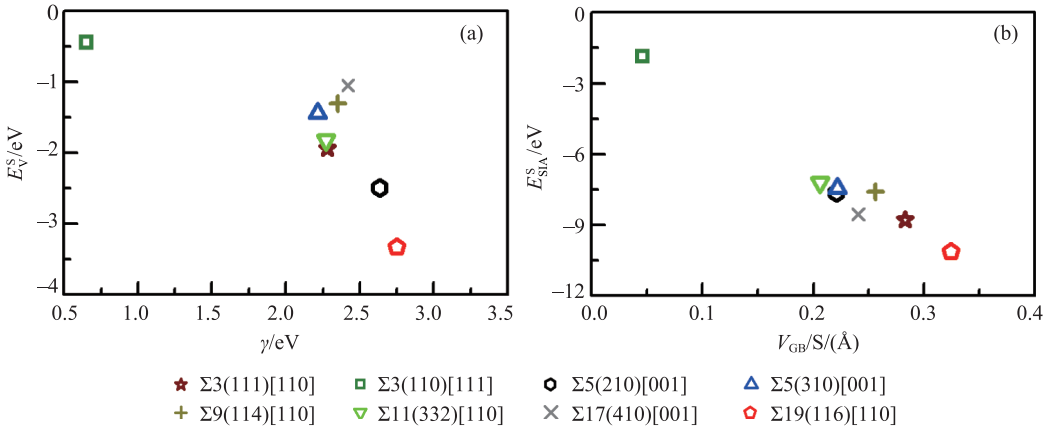

Fig. 1 (color online) (a) Dependence of the segregation energy $E^{\mathrm{S}}_{\mathrm{V}}$ of V on GB energy γ and (b) dependence of the segregation energy $E^{\mathrm{S}}_{\mathrm{SIA}}$ of SIA on excess volume V_{GB}/S of GB.

Experimental investigations have shown that vacancy sink efficiency varied for the different GBs[3,4], and the twin GB $\sum 3(110)[111]$ had the lower vacancy sink efficiency[3−5]. Our calculations also show that the ability to trap Vs and SIAs varies for different GBs. It is easily to understand that the strong ability to trap both Vs and SIAs of GB can provide a high possibility of recombination between them at/near the GB. Compared to other GBs, the ability of the twin GB $\sum 3(110)[111]$ to trap both Vs and SIAs is the weakest due to the lower GB energy and the smaller excess volume. This may be one key factor to induce that the twin GB $\sum 3(110)[111]$ has the lowest vacancy sink efficiency.

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4 - 10 First-principles Investigation of Vacancy and Self-interstitial Atom Formation Energy at Grain Boundary in Tungsten

He Wenhao, Gao Xing and Wang Zhiguang

Materials served in nuclear energy systems usually expose to high irradiation doses of particles. Projectile particles lead to creations of a large numbers of vacancies (Vs) and self-interstitial atoms (SIAs) in materials. The SIAs may gather to form dislocation loops and stacking-fault tetrahedrons, and the Vs usually gather to form voids. These defects contribute to material swelling, hardening, amorphization and embrittlement, and may accelerate material failure under irradiation[1]. Extensive experimental results demonstrated that nano-crystalline materials generally showed good radiation resistance than common poly-crystalline materials because there existed a high fraction of grain boundaries (GBs) in nano-crystalline materials[2]. However, threshold stresses in Nabarro–Herring creep provided the earliest indication that point defects sink strengths might depend on GB structures[3]. Usually, GBs that have atomic configurations such that both the ability to trap intrinsic point defects and Frenkel pair annihilation rates are high will be good sinks for Vs and SIAs. Here, we mainly study the atomic configurations around GBs effects on the ability to trap Vs and SIAs. Tungsten is one of the promising candidates for plasma facing materials (PFMs), such as the first wall materials and divertor of magnetic confinement fusion reactor due to its high melting temperature, high thermal conductivity and low sputtering erosion. In this study, the abilities to trap Vs and SIAs of eight symmetric tilt GBs in tungsten are investigated through first-principles calculations. These GBs are constructed by the coincidence site lattice model[4].

First-principles total energy calculations were carried out with the Vienna Ab initio Simulation Package (VASP) based on the density functional theory (DFT). The projected augmented wave (PAW) pseudopotentials were employed in the calculations within the generalized gradient approximation (GGA) with Perdew and Wang functional for the exchange and correlation energies. A cutoff energy of 400 eV was used for the plane-wave expansion. The internal structural relaxations stopped when the residual force on each atom was less than 0.01 eV/Å. Both atomic positions and volumes of supercells were allowed to relax in all calculations.

The vacancy formation energy $E_{\mathrm{V}}^{\mathrm{f}}$ at each site around GBs (bulk) can be calculated by,

$$E_{\mathrm{V}}^{\mathrm{f}} = E_{(\mathrm{GB(bulk),V})} - E_{(\mathrm{GB(bulk)})} + e_{\mathrm{W}}, \tag{1}$$

where $E_{(\mathrm{GB(bulk),V})}$ is the total energy of the supercell containing a vacancy around the GB (bulk), $E_{(\mathrm{GB(bulk)})}$ is the total energy of the supercell containing the clean GB (bulk), and e_{W} is the energy of a tungsten atom in bulk environment.

The SIA formation energy $E_{\mathrm{SIA}}^{\mathrm{f}}$ in each interstitial site at GBs (bulk) can be calculated by,

$$E_{\mathrm{SIA}}^{\mathrm{f}} = E_{(\mathrm{GB(bulk),SIA})} - E_{\mathrm{GB(bulk)}} - e_{\mathrm{W}}, \tag{2}$$

where $E_{(\mathrm{GB(bulk),SIA})}$ is the total energy of the supercell containing a SIA in the interstitial site at a GB (bulk).

$E_{\mathrm{V}}^{\mathrm{f}}$ versus hard-sphere radius r_0 of the vacancy is shown in Fig. 1(a). In this study, the r_0 is defined as the largest hard-sphere radius which can be inserted into the vacancy. The hard-sphere radius of tungsten atom is defined as half the distance between the nearest neighbors in bcc tungsten, which is 1.38 Å in equilibrium bcc tungsten. As shown in Fig. 1(a), the $E_{\mathrm{V}}^{\mathrm{f}}$ rapidly increases as r_0 increases and reaches its largest value as the r_0 is 1.38 Å. Then the $E_{\mathrm{V}}^{\mathrm{f}}$ slowly decreases as the r_0 keeps increasing. This result is reasonably sound since the binding energy in bcc tungsten is the largest when the first nearest neighbor distance is 2.76 Å. Any shorter/longer distance between them will induce the decrease of the binding energy thus make the formation of a vacancy easier. The r_0 can refer to the atom density around GB. The smaller the r_0 is, the larger the atomic density is. According to the relation between $E_{\mathrm{V}}^{\mathrm{f}}$ and r_0, it is easily found that any denser/looser atomic configuration around GB than that in