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4 - 13 First-principles Investigation of Helium Adsorptions at Grain Boundaries in Tungsten

He Wenhao, Gao Xing and Wang Zhiguang

The tungsten was deemed to be the most promising candidates as plasma facing material (PFM) due to its high melting temperature, good thermal properties, low sputtering yield[1]. The PFMs will be exposed to a high flux of helium atoms escaping from the plasma. Helium easily are trapped by vacancies, dislocations, grain boundaries (GBs) to form helium bubbles, which can significantly degrade the mechanical properties of materials. One well-known example is the high-temperature helium embrittlement (HE), which is the drastic embrittlement of metal at temperatures above 0.5 T_{m} (T_{m}: melting temperature) due to helium bubbles formation at GBs, even at extremely low overall helium concentration. To enhance the HE resistance of metal, it is necessary to study adsorptions of helium atoms at GBs firstly.

In this study, first-principles calculations of total energy were carried out with the Vienna Ab initio Simulation Package (VASP) based on the density function theory (DFT). The projected augmented wave (PAW) pseudopotentials were used within the generalized gradient approximation (GGA) with Perdew and Wang functional for the exchange and correlation energies in the calculations. A cutoff energy of 400 eV was used for the plane-wave expansion. The internal structure relaxations were considered to finish when residual forces on each atom is less than 0.01 eV/Å. By least-square-fitting total energies to the 4$^{\mathrm{th}}$ Murnaghan's equation of state, the calculated equilibrium lattice parameter of the body centered cubic tungsten was 3.19 Å. A 4×4×4 supercell (128 atoms) with calculated lattice parameter was employed to calculate the helium adsorption energies in tetrahedron (TET) and octahedron (OCT) interstitial sites in the bulk. To investigate the adsorption behavior of helium at GBs, eight low sigma number symmetric tilt GBs with [001], [110], and [111] as tilt axes were constructed with the CSL model. The interstitial sites at grain boundaries are identified with five types of deltahedra, that is, TET, OCT, pentagonal bipyramid (PBP), cap trigonal prism (CTP), and bitetrahedron (BTE)[2].

The helium adsorption energy $E_{He}^{\mathrm{ad},i}$ in the i^{th} type interstitial site at GBs (bulk) can be calculated by

$$E_{\mathrm{He}}^{\mathrm{ad},i} = E_{\mathrm{GB(bulk)}}^{\mathrm{He},i} - E_{\mathrm{He}}^{\mathrm{iso}}, \tag{1}$$

where $E_{\mathrm{GB(bulk)}}^{\mathrm{He},i}$ is the total energy of the supercell with a helium atom in the i^{th} type of interstitial site at a GB (bulk), $E_{\mathrm{GB(bulk)}}^{\mathrm{Perf}}$ is the total energy of the supercell containing clean GB (bulk), and $E_{\mathrm{He}}^{\mathrm{iso}}$ is the energy of a helium atom in vacuum. In this study, a 10 Å *10 Å *10 Å supercell containing one helium atom was used to calculate $E_{\mathrm{He}}^{\mathrm{iso}}$.

At the top of Fig. 1 (a), the helium adsorption energies versus types of interstitial site are plotted. Clearly,

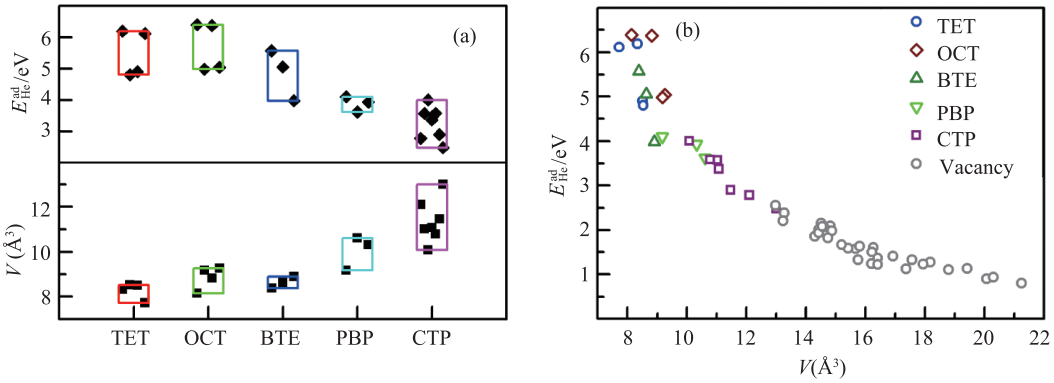

Fig. 1 (color online) (a) Helium adsorption energies $E_{\mathrm{He}}^{\mathrm{ad}}$ as well as the volume V of each polyhedral interstitial site. (b) The relationship between $E_{\mathrm{He}}^{\mathrm{ad}}$ and V.

the $E_{\rm He}^{\rm ad}$ depends largely on the shape of the interstitial site. The average value of the helium adsorption energy differs for different type of interstitial site, and the CTP sites hold the lowest average adsorption energy for helium in tungsten. Moreover, the $E_{\rm He}^{\rm ad}$ varies prominently even for the same type of interstitial site. To understand the large variation of the helium adsorption energies, volumes V of the interstitial sites at clean GBs without helium are measured and are plotted at the bottom of Fig. 1 (a). There is an obvious correlation between the helium adsorption energies and the volumes of the interstitial sites. That is, the larger the volume is, the lower the helium adsorption energy is. The $E_{He}^{\rm ad}$ versus V is plotted in Fig. 1 (b). To validate our final conclusion, the helium adsorption energies in vacancies around GBs are also plotted in Fig. 1 (b). It is obviously that the $E_{\rm He}^{\rm ad}$ exponentially decreases as the volumes of interstitial sites increase Helium is expected to occupy the interstitial sites with larger volume, since helium has a closed shell electronic structure and the bonding interaction is weak[3].

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4 - 14 First-principles Investigation of Helium Segregations at Grain Boundaries in Tungsten

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Tungsten is one of the promising candidates for plasma facing materials (PFMs), such as the first wall materials and divertor, of the magnetic confinement fusion reactor due to its high melting temperature, high thermal conductivity and low sputtering erosion. The PFMs will be exposed to a high flux of helium atoms escaping from the plasma[1]. The helium atoms in metals tend to assemble in vacancies, dislocations, and grain boundaries (GBs), and form helium bubbles, which can significantly degrade the mechanical properties of materials. One well-known example is the high-temperature helium embrittlement (HE). It has been experimentally demonstrated that the segregation of helium at GBs is sensitive to the morphology of GBs[2]. Therefore it is possible to enhance HE resistance of materials by increasing the fraction of certain kinds of GBs which are resistant to aggregation of helium atoms through GB engineering. To provide a rational guidance for the GB engineering, it is of fundamental importance to explore the relationship between the segregations of helium atoms at GBs and the characteristics of GBs.

First-principles calculations of total energy 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 structure relaxations stopped when the residual force on each atom was less than 0.01 eV/Å. By least-square-fitting total energies to the 4^{th} Murnaghan's equation of state, the calculated equilibrium lattice parameter of the body centered cubic tungsten was 3.19 Å. To investigate the segregation behavior of helium at GBs, eight low sigma number symmetric tilt GBs with [001], [110], and [111] as tilt axes were constructed with the CSL model. The interstitial sites at grain boundaries are identified with five types of deltahedra, that is, tetrahedron (TET), octahedron (OCT), pentagonal bipyramid (PBP), cap trigonal prism (CTP), and bitetrahedron (BTE)[3].

The helium segregation energy $E_{\rm He}^{{\rm seg},i}$ in the $i^{\rm th}$ type interstitial site at GBs can be calculated by

$$E_{\rm He}^{{\rm seg},i}=(E_{\rm GB}^{{\rm He},i}-E_{\rm GB}^{\rm Perf})-(E_{\rm bulk}^{\rm He}-E_{\rm bulk}^{\rm Perf}), \quad (1)$$

where $E_{\rm GB}^{{\rm He},i}$ is the total energy of the supercell with a helium atom in the $i^{\rm th}$ type of interstitial site at a GB, $E_{\rm GB}^{\rm Perf}$ is the total energy of the supercell containing clean GB, and $E_{\rm bulk}^{\rm He}$ is the total energy of the supercell with a helium atom in the TET interstitial site in bulk, $E_{\rm bulk}^{\rm Perf}$ is the total energy of the bulk without helium. For a GB, the helium prefers to segregate to the interstitial sites with the lowest segregation energy, which is defined as the helium segregation energy in the GB $E_{\rm He}^{\rm seg,GB}$. The $E_{\rm He}^{\rm seg,GB}$ in the eight GBs are listed in Table 1.

Table 1 The helium segregation energy $E_{\rm He}^{\rm seg,GB}$ in the eight GBs.

	$E_{\rm He}^{\rm seg,GB}$/eV	GBs	$E_{\rm He}^{\rm seg,GB}$/eV	GBs	$E_{\rm He}^{\rm seg,GB}$/eV
$\sum$3(110)[111]	−1.23	$\sum$5(310)[001]	−2.65	$\sum$3(111)[110]	−3.44
$\sum$5(210)[001]	−2.21	$\sum$11(332)[110]	−2.84	$\sum$19(116)[110]	−3.74
$\sum$9(114)[110]	−2.60	$\sum$17(410)[001]	−3.31		