LAMMPS by means of removing or adding a W or He atom in the simulation box. Then the simulation box was relaxed with an energy minimization method in LAMMPS to get stable energy states and structure. The strain field was applied to the box to investigate the effects on the formation energy of defects. Results are shown in Figs. 1 and 2.

It can be found from Fig. 1 that the self-interstitial formation energy decreases and formation energy of vacancy increases with strain from compress to expand. The most stable configuration for self-interstitials is the crowdion or dumbbell along $<111>$. Fig. 2 shows that the single He interstitial and substitution formation energy decreases with strain, which is similar to the self-interstitials. The stable position for single He interstitial is tetrahedral sites and a He atom is preferred to be trapped by a vacancy comparing with interstitial sites.

These results can be explained by the reason that the interaction between defects and local strain field changes the formation energy of defects. The formation of interstitials would lead to local lattice sites in compressive state, thus the average volume for each atom in local lattice decreases. The application of expanding strain increases the average atom volume, making it easier for the formation of interstitials, thus the formation energy decreases. While the formation of vacancies would increase the average atom volume, so the compressional strain decreases the vacancy formation energy.

Based on the above results, we can conclude that the strain field affects a lot on the formation of defects in tungsten. For tungsten used in divertor plates in fusion reactor, it is suggested to be pre-compressed to limit the production of interstitials, extending its lifetime under radiation environment.

References

[1] S. Plimpton, J. Comp. Phys, 117(1995)1.

[2] N. Juslin, B. D. Wirth, J. Nucl. Mater, 432(2013)61.

3 - 7 Effect of Strain Field on Defect Formation under Irradiation in bcc Metals

Gao Ning, Gao Xing, Wang Dong and Wang Zhiguang

When an energetic particle interacts with a lattice atom, different processes would be initiated sequentially in time (up to 10^{-12} ~10^{-11} s)[1]. Except the mobile process of defects in the last step, the others are largely athermal. Thus, the formation and stability of defects produced by irradiation in metals depends on various parameters. The effect of temperature has been studied for years, especially by computers simulations for displacement cascade. The higher temperature is, the less stable Frenkel pairs (interstitial - vacancy) are left[2]. In addition to temperature, the strain or stress field would also be contributed to the formation of defects, since the formation energy is affected by these fields. In this report, we firstly present the results of strain field effect on formation of different defects and critical displacement energy. The discussion is then given in the end.

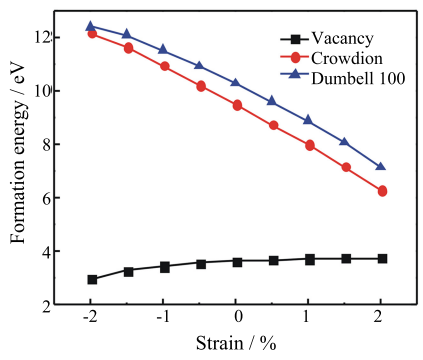

Fig. 1 (color online) The formation energy of single tungsten for crowdion, $<100>$ dumbbell and vacancy with different strain values.

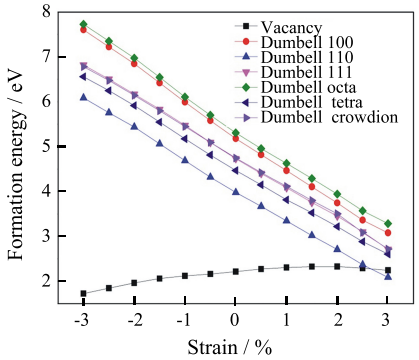

Fig. 2 (color online) Formation energies of different defects in bcc Fe with strain calculated with VASP.

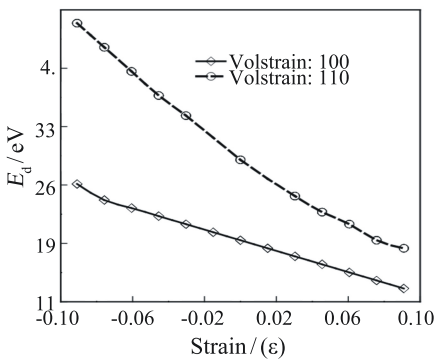

Fig. 3 The critical displacement energies along [100] and [110] directions with different strains.

The formation energy result calculated by MD simulation for single tungsten is shown in Fig. 1. It can be found that the interstitial formation energy decreases with strain value for crowdion and dumbbell, while increases for

vacancy case. The DFT results calculated with VASP for bcc iron are shown in Fig. 2. The results for bcc Fe are similar to W. One possible reason for these results is elastic interaction between defects and strain filed, leading to the change of elastic formation energy of these defects.

Since the strain field affects the formation of defects, the critical displacement energy should also be affected. One case is shown in Fig. 3. The critical displacement energies decrease with strain for [100] and [110] directions, which can be explained by strain effect on formation energy as shown in Figs. 1 and 2.

Based on above results, one conclusion can be given that when the materials work under compressive condition in reactor, the lifetime would be extended. Thus, the materials with pre-compression stress may be one of good candidates for radiation-resistance application.

References

[1] H. Ullmaier, W. Schilling, Physics of Modern Materials, 1, IAEA, Vienna, (1980).

[2] D. J. Bacon, J. Nucl. Mater, 276(1999)1.

3 - 8 Thermal Desorption and Surface Modification Induced by Helium Implantation in Tungsten

Cui Minghuan, Wang Zhiguang, Yao Cunfeng, Pang Lilong, Shen Tielong, Sun Jianrong, Zhu Yabin, Sheng Yanbin, Zhu Huiping, Wang Ji and Zhang Hongpeng

Plasma-facing materials (PFMs) for a fusion reactor suffer hydrogen/helium plasma bombardment, neutron irradiation and high temperature, *etc.* Tungsten is a promising candidate PFM due to its low sputtering yield for the light elements, high thermal conductivity, high mechanical strength, and high melting point. Helium could be introduced by helium bombardment and neutron irradiation and trapped in tungsten at different sinks. It is possible that the trapped helium atoms re-emit to the core plasma due to thermal desorption which affects the safety. In this work, the thermal desorption behavior of helium implanted into tungsten at different temperatures was investigated.

The tungsten specimens with high purity of 99.99% were implanted with 100 keV helium ions at room temperature (RT), 400, 600 and 800 °C. Helium implantation experiments were performed at 320 kV multi-discipline research platform for Highly Charged Ions equipped with an ECR (Electron Cyclotron Resonance) ion source in the Institute of Modern Physics, Chinese Academy of Sciences (IMP, CAS), Lanzhou. The beam was swept at two directions of X and Y in order to get a uniform beam. The mean flux was about 4.7×10^{13} ions/(cm^{2}s). The fluence was 1.0×10^{18} ions/cm^2. After implantation, He desorption behavior was investigated by Thermal Helium Desorption Spectroscopy (THDS) and Scanning Electron Microscope (SEM) was used after THDS test to identify the surface modification. In the thermal desorption process, the temperature increased first with a ramp rate of 2 K/s to 175 °C, then with a ramp rate of 3 K/s to 900°C, kept 100 s at the temperatures of 175 and 900 °C and at last cooled down to RT.

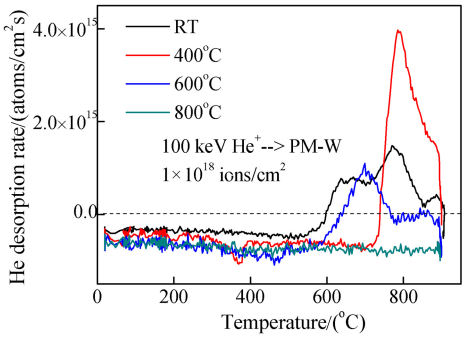

Fig. 1 (color online) THDS of specimen implanted with 100 keV He$^+$ to 1×10^{18} ions/cm^2.

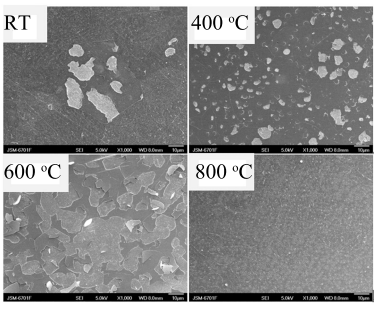

Fig. 2 Surface modification of specimens implanted with 100 keV He$^+$ to 1×10^{18} ions/cm^2 after THDS test, implantation temperatures are indicated in each figure.

Thermal helium desorption spectra are shown in Fig. 1. It should be illustrated that the He desorption rates below zero are considered as background, *i.e.* zero, and only those data above zero will be discussed. When the implantation temperature was RT, helium desorption started at about 598 °C and four peaks appeared below 900