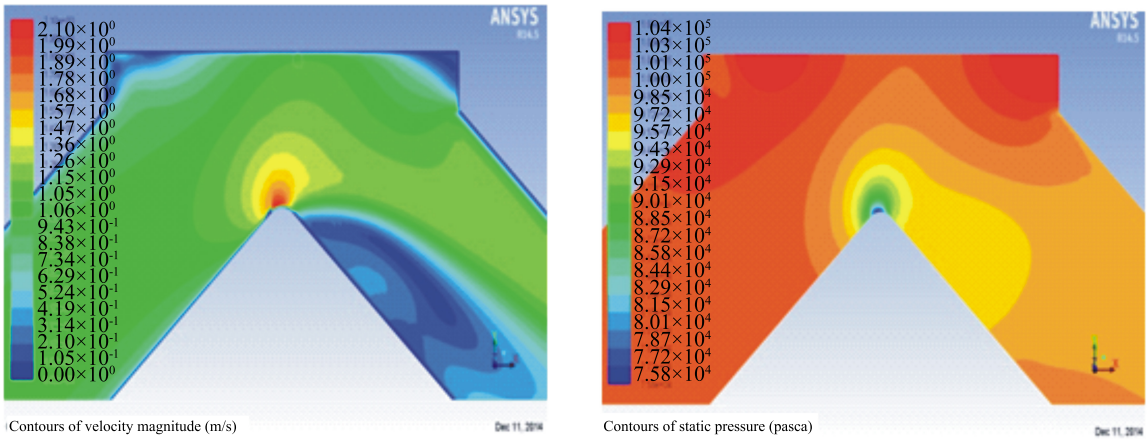

Fig. 2 (color online) Velocity (left) and pressure (right) distribution on the surface of sample calculated with RELAP5 code.

Now, the first corrosion test without irradiation was successfully conducted for 1 000 h without any failure. A study for synergetic effect of irradiation and LBE on the materials of interest for ADS will be carried out next.

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3 - 6 Molecular Dynamic Simulation of Point Defects under Strain Field in W

Wang Dong, Gao Ning, Gao Xing and Wang Zhiguang

Tungsten is one of the promising candidates for the divertor plate in International Thermonuclear Experimental Reactor (ITER) because of its high melting temperature, high thermal conductivity and low sputtering erosion. During the operation of ITER, it will be exposed to high energy particles: hydrogen, helium and neutron, producing high density of interstitials and vacancies which will change the structure and properties of materials. The formation of defects changes the local stress/strain field, and the external stress/strain field will also affect the properties of defects. In this work, we use the Large-scale Atomic/Molecular Massively Parallel Simulator LAMMPS[1] to study the formation of defects under strain field in tungsten.

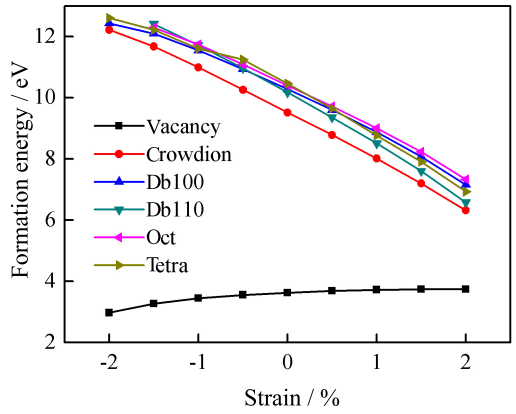

Fig. 1 (color online) Formation energy of vacancy and single self-interstitials with different strains in bcc W.

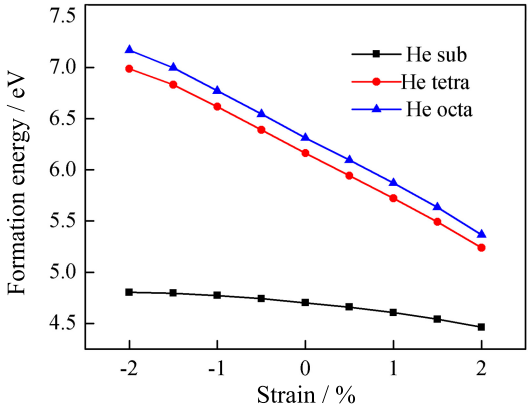

Fig. 2 (color online) Formation energy of different He interstitials with strain in bcc W.

A bcc lattice with 16 000 W atoms (20 × 20 × 20) was constructed as the simulation box. The potentials used for W-W and W-He both were developed by Juslin and Wirth[2]. The vacancy and interstitials were produced by

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

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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.

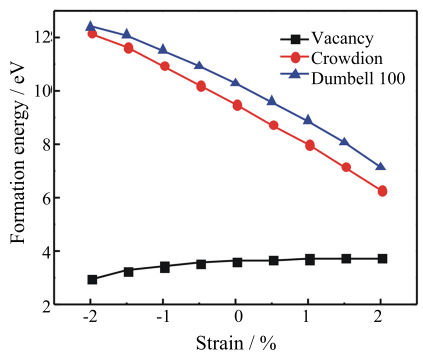

Fig. 1 (color online) The formation energy of single tungsten for crowdion, $<100>$ dumbbell and vacancy with different strain values.

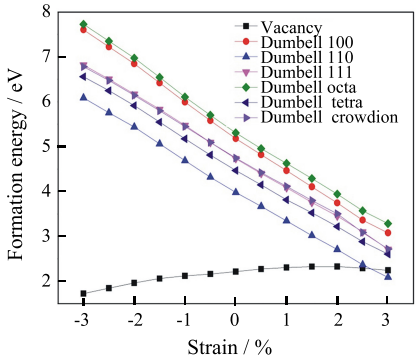

Fig. 2 (color online) Formation energies of different defects in bcc Fe with strain calculated with VASP.

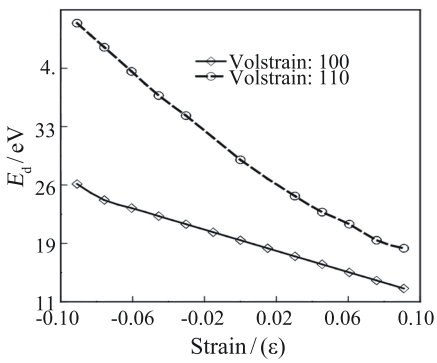

Fig. 3 The critical displacement energies along [100] and [110] directions with different strains.

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