4 - 3 A molecular Dynamics Study on Helium-vacancy Complexes in Tungsten under Strain Fields

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Tungsten (W) is a promising candidate as the plasma-facing materials in fusion reactors, which suffers from helium (He) and stresses from the reactor, *etc.* The coupling effects of He and stress in W is an important issue for its application. In this paper, He bubble growth was investigated by molecular dynamics (MD) simulations in body-centered cubic (BCC) W under different strain fields.

The simulation model containing 16 000 W atoms was built as the matrix to include He atoms. The values of the hydrostatic strains were from −2% to 2%. The initial model contained one vacancy and was relaxed at 300 K. Then He atoms were introduced one by one in the model and relaxed at 300 K and 0K. With increasing He atoms in He_nV, the pressure increases in the cluster and the surrounding tungsten would be distorted and then self-interstitial atoms (SIAs) were emitted at a certain He_nV. The binding energies of He and $He_{n-1}V$ and the first SIA emission under different strains were studied in our work.

The binding energy of He to $He_{n-1}V$ cluster with increasing n is defined as follows:

$$E_b^{\mathrm{He}}(n) = E_{\mathrm{He}}^f + E_{\mathrm{He}_{n-1}V}^f - E_{\mathrm{He}_nV}^f.$$

The binding energies were calculated and given in Fig. 1. The energies under 0 strain were similar with DFT simulation, which were 4.57, 3.11, 3.28, 2.61, 1.44 and 2.08 eV when n was 1 to 6, respectively. This indicates that our simulation results were correct. Under different strains, the binding energies of He and V were the highest and the binding energies of He and $He_{n-1}V$ showed a decreasing trend with increasing n before the first SIA emission. The large increases of binding energies with increasing n corresponded to the first SIA emission. When n was less than 9, the binding energies decreased with increasing strain.

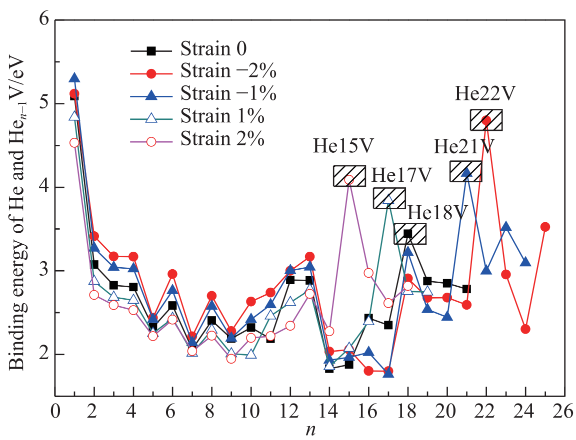

Fig. 1 (color online) The binding energies of He and $He_{n-1}V$ under different strains. The inserted boxes corresponds to the first SIA emission.

Under different strains, the first SIAs are <111> crowdions which were the most stable interstitial configurations in tungsten. The first SIA emission in He15V under the 2% strain was shown in Fig. 2. We can see from the figure that a $[1\ 1\ \bar{1}]$ crowdion was punched around the He bubbles. The first SIAs under strains of −2%, −1%, 0, 1% and 2% were emitted at $He_{22}V$, $He_{21}V$, $He_{18}V$, $He_{17}V$ and $He_{15}V$. With increasing strains, the number of He in He bubbles needed to punched the first SIA decrease. The W lattice atoms suffered from both the applied strains and strains induced He bubbles. The work needed to emit the first SIA was constant in W. With increasing applied strains, the work from He bubbles needed for the first SIA will decrease and then the number of He atoms will also decrease.

In summary, the applied strains will affect the binding energies and the first SIA emission. The elastic interaction between the external applied strain and the strain induced by He bubble were the main reasons.

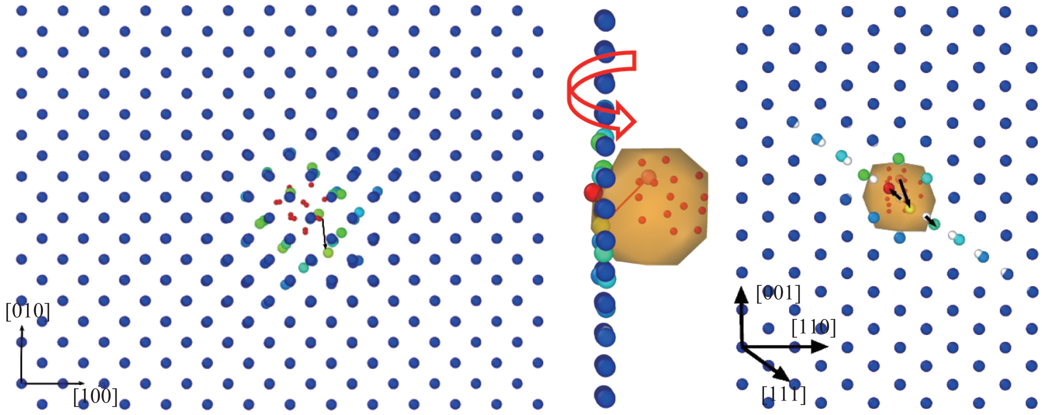

Fig. 2 (color online) The first SIA emission in He15V under the 2% strain. The white circles are initial W atoms in HeV. The red circles are He atoms. Other circles are the final W atoms in $He_{15}V$.

4 - 4 Enhanced Transmittance in Crystal $LiTaO_3$ by Heavy Ions Implantation

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In our experiments, we used congruent samples of 1 mm thickness, single crystal $LiTaO_3$. The samples were implanted at room temperature (RT) by 3.25 MeV Fe, 6 MeV Xe, 1 MeV Bi ions respectively, with projected ion ranges of 1.36, 1.23, 0.12 μm calculated by SRIM2008. Note that inert ion Xe is chosen for eliminating the potential effects of new phases resulting from chemical process during implantation, compared to metal ion Fe and Bi. The ion fluences were varied between 1×10^{12} and 2×10^{15} cm^{-2}. The optical transmission spectra of the implanted samples were measured by PerkinElmer Lambda 900 UV/VIS/NIR Spectrometer with a scanning step length of 1 nm. During measurement, the incidence non-polarized light was perpendicular to the surfaces of the samples. The surface morphology of samples was characterized by OM and AFM. Rutherford backscattering-channeling (RBS-c) and XRD were used to examine ion-induced structural changes in samples.

Figure. 1 shows the transmission spectra of $LiTaO_3$ implanted with Fe, Xe, Bi ions respectively at different fluences. It is very surprise that there is no extra optical absorption in all implanted samples comparing with un-implanted sample. However, the transmittance increases over a broad spectral range of 340 ∼ 2 500 nm when the fluences are over certain values. This is quite different from the previous reports that ion implantations cause the intense optical absorption, particularly in VIS region[1−3]. Note that some of transmittance curves at low fluences are not presented in this Figure, as they almost overlap with virgin. With increasing fluences, all transmittances increase but no-uniformly. In the case of Fe-ion implantation at a low fluence of 2×10^{14} cm^{-2}, however, the transmittance near ultraviolet region slightly decreases, even lower than the virgin. Finally, it increases and exceeds the virgin at high fluence, meanwhile, the transmittance curve shows oscillation that should result from optical interference. There is little difference between Fe and Xe, Bi ion implantations. Xe or Bi implantation seems to could create more effective transmittance increasing in UV region than infrared region. The transmittance increases maximum up to about 82.2% near 565 and 750 nm corresponding to Xe and Bi implantation respectively.

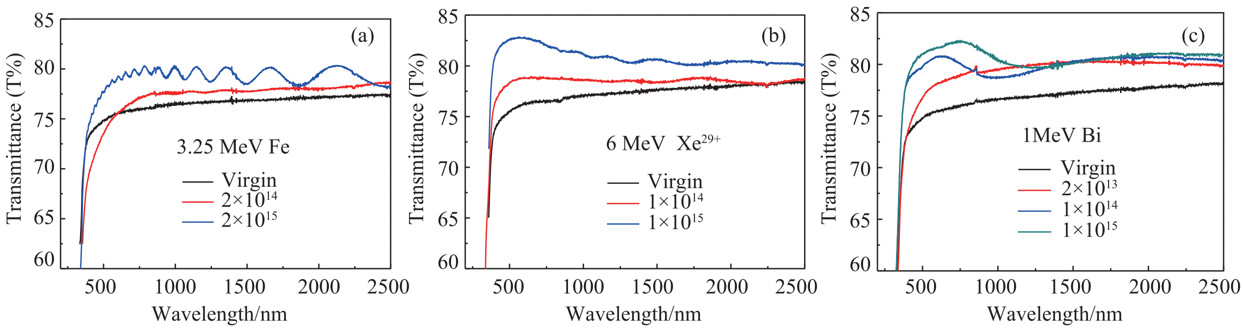

Fig. 1 (color online) The transmission spectra of $LiTaO_3$ implanted with Fe, Xe, Bi ions respectively at different fluences.