

## 5 - 33 A Kinetic Monte Carlo Simulation of the Effect of Temperature on the Irradiated Microstructure of a Reactor Pressure Vessel\*

Li Jianyang, Zhang Chonghong and Yang Yitao

It is well known that the dose rate, primary knock-on atom (PKA) spectrum, nuclear reaction products, and irradiation temperatures may influence the microstructure of irradiated materials. The invariance theory of shifting the irradiation temperature to compensate for the effect of dose rate on irradiation damage was first proposed by Mansur in the 1990s<sup>[1]</sup>. While this model mainly studied the point defect absorption and irradiation swelling, computational simulations of complete fine microstructures have been less reported. This work carried out Object kinetic Monte Carlo (OKMC) simulations to study the influence of dose rate and temperature on the irradiation microstructure of a dilute FeMnNi alloy, which is a model alloy of reactor pressure vessel (RPV) steel, operating service temperature of about 573 K. Our model reasonably considered the production of <100>-type self-interstitial atom (SIA) loops<sup>[2]</sup>, which is often neglected in previous computational simulations of Fe-based alloy. Figure 1 presented the density of SIA loops, vacancy clusters, and the ratio of <100>-type SIA loops changed with temperature and the dose rate. It is found that a certain irradiation temperature shift at a higher dose rate ( $1 \times 10^{-4}$  dpa/s) could bring overall similar irradiation microstructure as a lower dose rate ( $1 \times 10^{-7}$  dpa/s) in a large dose range. This suggests that temperature shifts could have some compensation for the dose rate effect in temperature regions dominated by kinetic processes. However, high-energy ion irradiation is also accompanied by higher electron energy loss and lattice temperature rise due to electron-phonon coupling, so the compensation of the dose-rate effect between neutron and ion irradiation is not straightforward and needs further investigation<sup>[3]</sup>. For more results and discussion, please refer to our recent work<sup>[2]</sup>.

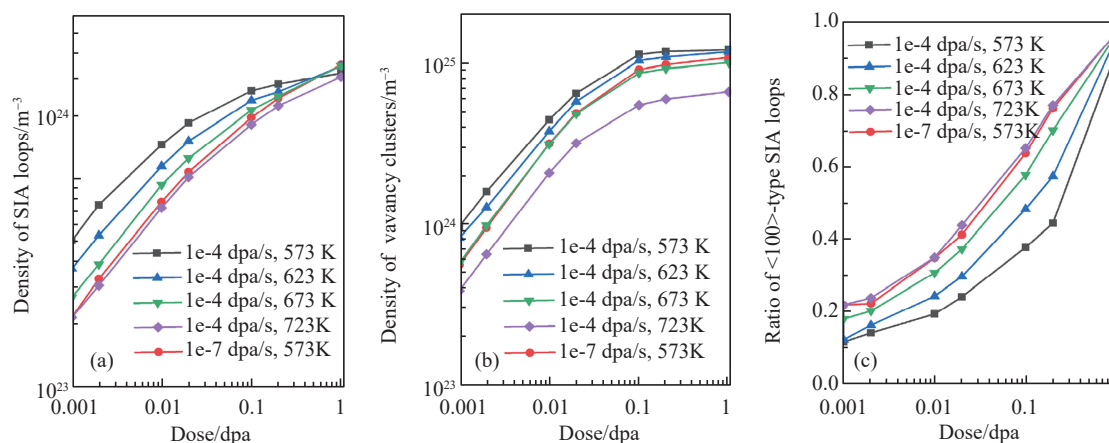


Fig. 1 The number density of (a) SIA loops and (b) vacancy clusters, (c) the ratio of <100>-type SIA loops for different irradiation conditions.

### References

- [1] L. K. Mansur, J. Nucl. Mater., 206(1993)306.
- [2] J. Y Li, C. H. Zhang, Nuclear Engineering and Technology, 55(3)(2023)958.
- [3] Okan K. Orhan, Mohamed Hendy, Mauricio Ponga, Acta Materialia, 244(2023)118511.

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