## THE INTERACTION BETWEEN THE EDGE DISLOCATION AND THE DISLOCATION LOOP-BUBBLE COMPLEX UNDER SHEAR STRESS IN BCC IRON

## <sup>1</sup>Y.X. Wei, M. Xu, P. F. Zheng, <sup>2</sup> L. P. Guo

<sup>1</sup>Southwestern Institute of Physics, Chengdu 610041, China;

<sup>2</sup>Key Laboratory of Artificial Micro- and Nano-Structures of Ministry of Education, Hubei Nuclear Solid Physics Key Laboratory, School of Physics and Technology, Wuhan University, Wuhan 430072, China;

## Email: minxu@swip.ac.cn

In the advanced fusion nuclear reactor, the structural materials need to provide sufficient mechanical support for the reactor device. In a state of stress for a long time, the shear force acting on the crystal for a long time causes it to deform, which affects the mechanical properties of the material. The movement of dislocations can be hindered by defects when they come into contact with each other, which directly affects the deformation mechanism of the material. In previous studies, the interaction between the dislocation, the loop and the bubble, as well as those between any two of them, have been investigated [1-5]. We have previously investigated the interaction between dislocation loops and H-bubbles in BCC iron, found that, dislocation loops and H-bubbles can form the morphology of a loop-bubble complex under certain conditions [6]. Then, as a new composite defect structure, the loop-bubble complex will have any effect on the slip of dislocation?

This paper mainly applies molecular dynamics methods to study the pinning behavior of loop-bubble complexes to edge dislocations. We calculate the interaction of the dislocation loop-bubble complex with edge dislocation. As shown in Fig.1, three forms of loop-bubble complexes (labeled as C1, C2 and C3) were simulated. By calculating the CRSS value [], we can quantitatively compare the pinning strength of dialoctions under different conditions.



Fig. 1, The initial relative position of the dislocation and loop-bubble complex in the simulation box, the red one represents the bubble and the green one represents the dislocation loop.

The results of the interaction between the above dislocations and C1, C2, and C3 show that the loop-bubble complex does obstacle the slip of dislocations, and the position of the bubble in the loop can greatly affect the block strength of the complex. The CRSS values indicate that the block strengths of the three loop-bubble complexes against edge dislocations are arranged as C2 (90Mpa) < C1 (120Mpa) < C3 (225Mpa). Take the interaction progress between dislocation and C2complex for example, as shown in Fig.2. When dislocations pass through the dislocation loop-H bubble complex, a part of the dislocation loop will be absorbed. The H bubble at the edge of the absorbed dislocation loop has the strongest hindering effect on the dislocation, followed by the dislocation loop. The internal H bubbles have a moderate hindering effect on dislocations, while the H bubbles at the edge of the unabsorbed part of the dislocation loop have the weakest hindering effect on dislocations. The hindering strength of loop-bubble complexes to edge dislocations is between that of dislocation loops and H-bubbles. We have conducted a detailed analysis of the mechanism behind the above results, and we believe that studies the interaction mechanism of multiple defects (the dislocation, loop, bubble)

will be helpful to further understand the microstructure evolution of structural materials after irradiation, as well as the comprehensive impact on the material mechanical properties.



Fig. 2 The process of the dislocation interacts with the loop-bubble complex C2. (a)-(d) show the changes in the shape and relative position of the dislocation and loop-bubble complexes at different stages. (e) shows a top view of the structure inside the dotted box in (c). The blue part of the dislocation line indicates the edge dislocation part, and the pink and white part indicates the screw dislocation part. The grey bubble represents the H bubble.

## REFERENCES

- K. Tapasa, D. J. Bacon, Y. N. Osetsky, Computer simulation of dislocation-solute interaction in dilute Fe-Cu alloys[J]. Modelling & Simulation in Materials Science & Engineering, 2006, 14(7):1153-1166.
- [2] D. Terentyev, D. J. Bacon, Y. N. Osetsky, Interaction of an edge dislocation with voids in α-iron modelled with different interatomic potentials[J]. journal of physics condensed matter, 2008, 20(44):445007.
- [3] Y. N. Osetsky, R.E Stoller, Y Matsukawa. Dislocation-stacking fault tetrahedron interaction: what can we learn from atomic-scale modelling[J]. Journal of Nuclear Materials, 2004, 329-333(part-PB):1228-1232.
- [4] M. Victoria, N. Baluc, C. Bailat, et al. Microstructure and associated tensile properties of irradiated fcc and bcc metals[J]. Journal of Nuclear Materials, 2000, 276(1-3):114-122.
- [5] S.M. Hafez Haghighat and R. Schaeublin, "Molecular dynamics modeling of cavity strengthening in irradiated iron", Proceedings of Third International Conference of Multiscale Materials Modeling, Freiburg, Germany, September 2006, p.729.
- [6] Y.X. Wei, N. Gao, et al. Interactions between hydrogen bubbles and prismatic interstitial dislocation loops in BCC iron, Computational Materials Science, 2020, 180, 109724