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The interaction between the edge dislocation and the dislocation loop-bubble complex under shear stress in BCC

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Introduction

In the nuclear reactor, the structural materials need to provide sufficient mechanical support for the reactor device. In the state of stress for a long time, the shear force acting on the crystal for a long time will cause the crystal to deform. This affects the mechanical properties of the material.

- When shear stress makes the discrete crystal blocks slide against each other, the deformation mode changes from uniform deformation to plastic deformation.
- Dislocation slip is characterized by the displacement of a crystal in a specific crystallographic direction (called a slip direction) and a specific lattice plane (called a slip plane)
- Various types of defects will hinder the movement of dislocations to a certain extent when encountering slipping dislocations, thereby directly affecting the deformation mechanism of the material.
- Understanding the interaction between dislocations and various defects is very meaningful work for the practical application of materials.
- The simulation work in this paper is mainly divided into two parts: 1) Interaction between H bubbles and edge dislocations. 2)Interaction between the loop-bubble complex and the 1/2<111>{112} edge dislocation.

METHODS

- In this work, an embedded atom method (EAM) potential function developed by Ramasubramaniam et al[1] was applied to describe the Fe-H interaction. The portion of this potential function describing the Fe-Fe interaction is based on the potential published by Ackland et al [2].
- The upper region (orange part) represents the atomic layer on the upper surface of the substrate, and the atoms in this region will be applied with stress along the [111] direction (the x-direction) to move to the right by the set value. The middle region (white part) is the atoms inside the matrix, the atoms in this region can move freely. The atoms within the lower region (gray part) will always be fixed to their initial position and cannot be moved.
- We insert a 1/2<111>{112} edge dislocation in the middle region of the calculation box, Fig.2 shows the arrangement of atomic planes before the system is relaxed after inserting a half-atomic plane into the lattice. The 1/2<111>{112} edge dislocation can be obtained after the energy minimization of the system.
- we calculate the interaction of the dislocation loop-bubble complex with edge dislocation. As shown in Fig.3, three forms of loop-bubble complexes (labeled as C1, C2 and C3) were simulated.

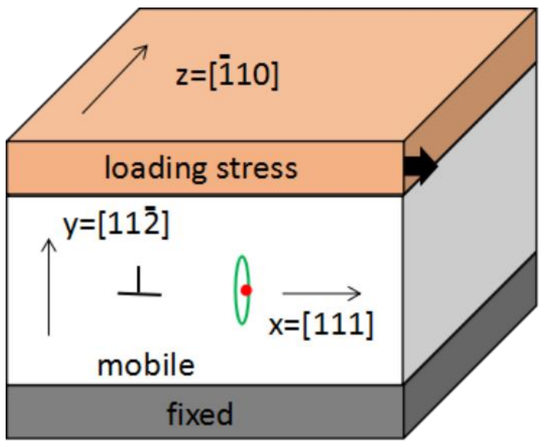


Fig.1 Computational box.

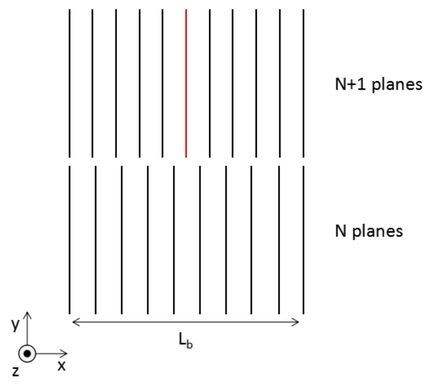


Fig.2 The arrangement of atomic planes after inserting a half-atomic plane(the red line) into the lattice..

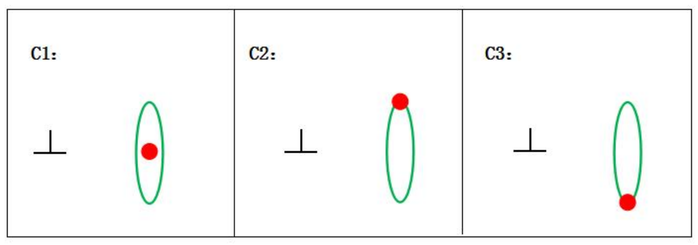


Fig.3 Three forms of loop-bubble complexes (labeled as C1, C2 and C3).

RESULTS

- ***Interaction between edge dislocations and H bubbles***

It can be seen from Fig.4 that with the increase of the size of the H-bubble, the CRSS value increases significantly. The pinning strength of 2nm bubbles to dislocations is directly more than twice that of 1nm bubbles, while the increase in pinning strength of 3nm bubbles is smaller. The effect of size effect on the CRSS value is very strong. However, with the increase of the H/V ratio in the H bubble, the CRSS value just has a slight upward trend.

Fig.4

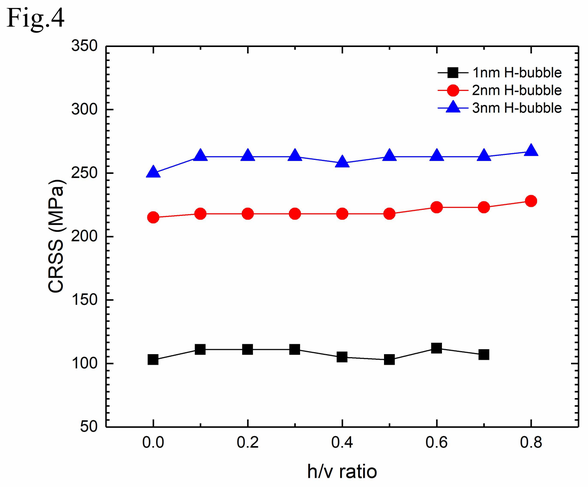
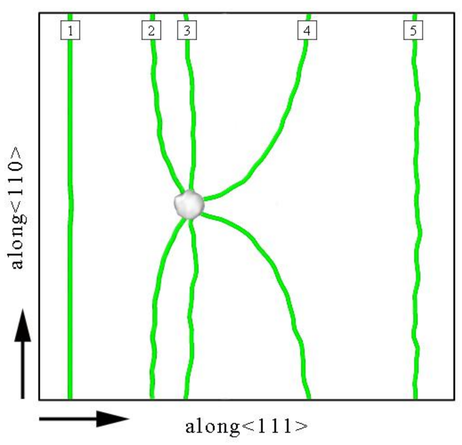


Fig.5



Where H/V equals 0, it represents the voids. The pinning strength of H bubbles to dislocations is almost equivalent to that of voids of the same size. Observing the simulation process, the hindering strength of the H bubble and the void to dislocation slip is consistent, and the interaction behavior of the two when the edge dislocation crosses the H bubble is also very similar to that when the edge dislocation crosses the void. There is no obvious bulge in the middle of the dislocation, indicating that the dislocation is break free from pinning by cutting through the H-bubble instead of climbing way. But in other simulations, dislocations can also climb through the H-bubble. Dislocations pass through H bubbles in the same way as through voids (both climb and cut through).

- ***Interaction between edge dislocations and dislocation loop-H-bubble complexes***

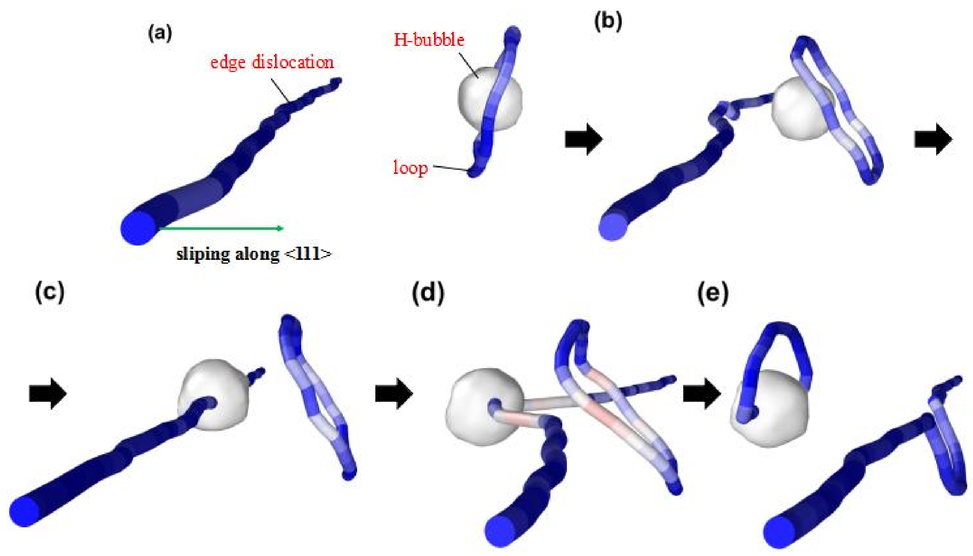


Fig.6 the state of dislocations and loop-bubble complexes after the entire system is relaxed in an unstressed state

After applying shear stress, the whole process of dislocations from the beginning of slippage to the complete unhindering of the loop-bubble complex can be described in three main stages. The results show that when a dislocation encounters a dislocation loop, it is very easy to absorb part or all of the dislocation loop to form a super-jog-like dislocation segment. However, when the edge dislocation slip plane is parallel to the dislocation loop Burg vector, it is difficult for the dislocation to contact 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.

Conclusion

- The pinning strength of H bubbles to edge dislocations is slightly stronger than that of cavities of the same size. The way the edge dislocations cross the H-bubble is in line with Orowan's theory.
- The results show that the dislocation loop-H-bubble complex does hinder the slip of edge dislocations, and its hindering strength varies greatly with the position of the H-bubble in the complex.
- 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 ring-bubble complexes to edge dislocations is between that of dislocation loops and H-bubbles.

Reference

[1] A. Ramasubramaniam, M. Itakura, E.A. Carter, Interatomic potentials for hydrogen in α–iron based on density functional theory, Phys. Rev. B. 79 (2009) 174101.

[2] G.J. Ackland, M.I. Mendelev, D.J. Srolovitz, S. Han, A.V. Barashev, Development of an interatomic potential for phosphorus impurities in α-iron, J. Phys.: Condens. Matter. 16 (2004) S2629–S2642.