Dislocation- Defect Interactions in Iron

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Objectives

• To address the mechanical properties of iron in irradiated environments
• To develop a capability that predicts the aging and failure of the material under irradiation

Goals

• Distinguish the critical parameters in which failure occurs
• Study the dislocation – defects interaction mechanisms
• Study the mechanical behavior of bcc iron inhibited with prismatic loops and voids

Key Materials

• Dislocation: an irregularity within a crystal structure that strongly influence the properties of materials
• Vacancies: point defects in crystalline materials and are missing atoms
• Point Defects: vacancies and interstitials created by radiation undergo reactions and aggregation
• Like defects cluster and anti-defects annihilate

Method

• A dislocation is formed by removing a half plane of atoms and equilibrating the system. The resulting dislocation lies on a [110] type plane and moves along a <111> direction.
• A prismatic loop or a void is generated by removing atoms from the structure. The prismatic loop is of [100] type.
• A shear stress is applied and a dislocation moves and interacts with defects. The resulting mechanisms and the stress-strain curves are extracted and studied.
• Tools used are LAMMPS (MD Simulations) and AtomEye (visualization).

Results

I. Dislocation - prismatic loop interaction

• Temperature: 350K Diameter of loop: 4 nm
• After each pass the prismatic loop shrinks in size and the dislocation leaves a new defect behind.

II. Dislocation – void interaction

• Temperature: 350K Diameter of loop: 4 nm
• As the dislocation moves closer to the void, the void’s free surface attracts the dislocation. The radius of the void is 3 nm.

• The void begins to shear after the dislocation passes through.

• As the size of the void increases, the motion of the dislocation becomes more difficult, leading to the hardening of the material.

• The graph of the slope of the stress-strain curve versus the radius size shows a linear relationship.

Conclusions

• When a dislocation interacts with a prismatic loop, the loop shrinks in size with each pass and defects are left. The defects can cluster to form voids or prismatic loops.
• As the radius of the void increases, it becomes harder for the dislocation to move and the material hardens at a quicker rate. The relationship between radius size and hardening is linear.

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