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.

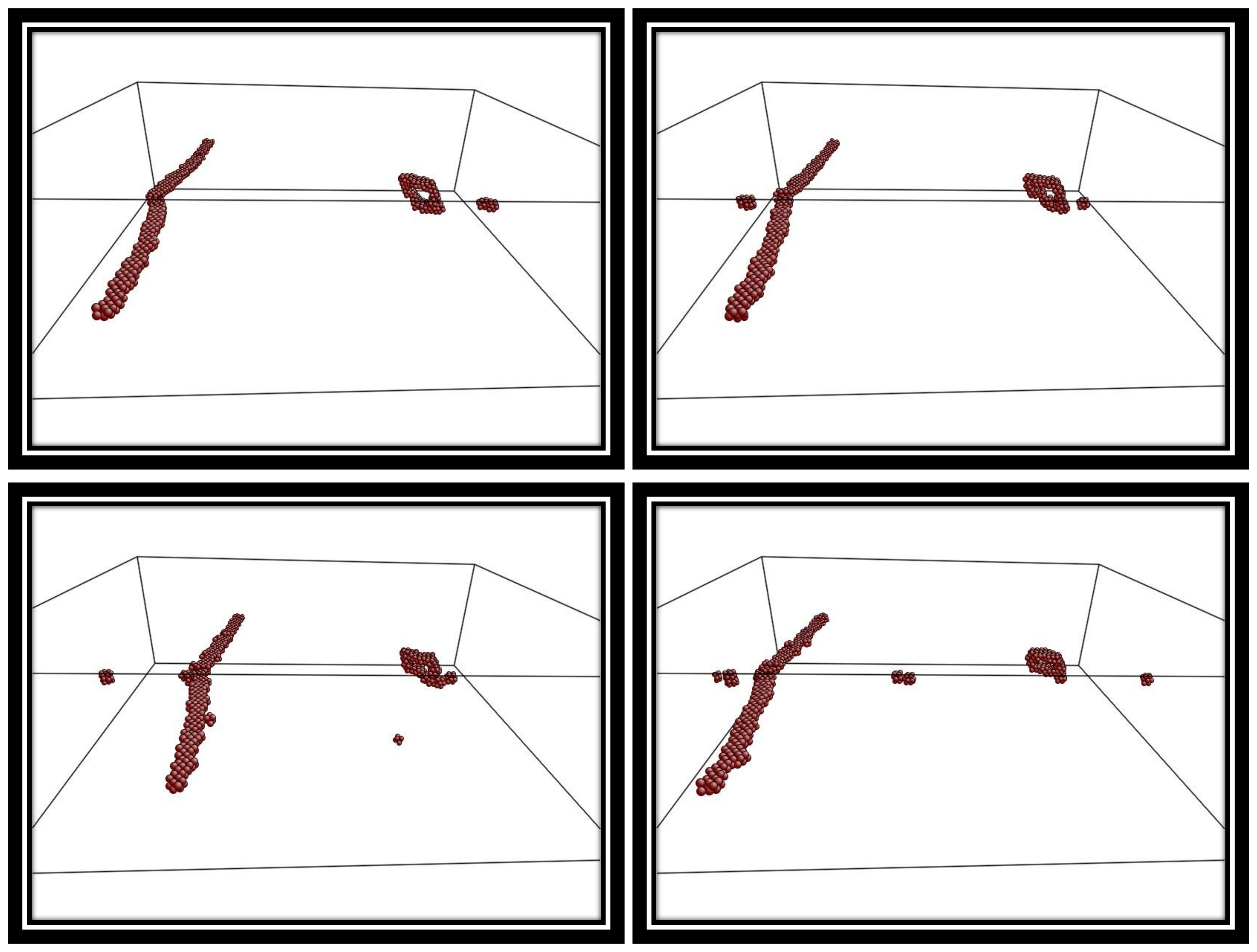
•A prismatic loop or a void is generated by removing atoms from the structure. The prismatic loop is of [100] type.

•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

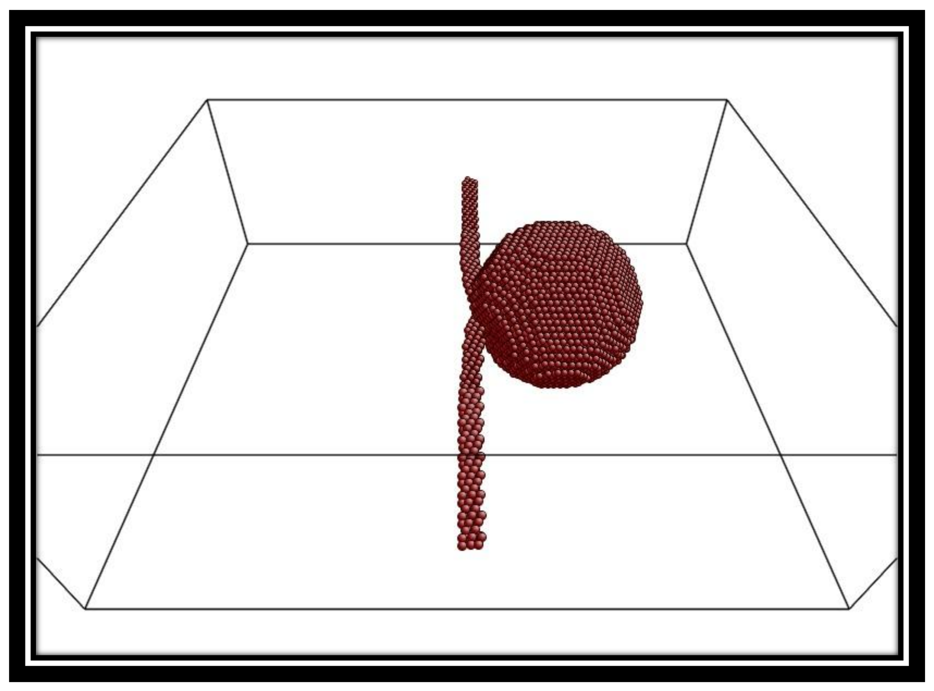
I. Dislocation - prismatic loop interaction



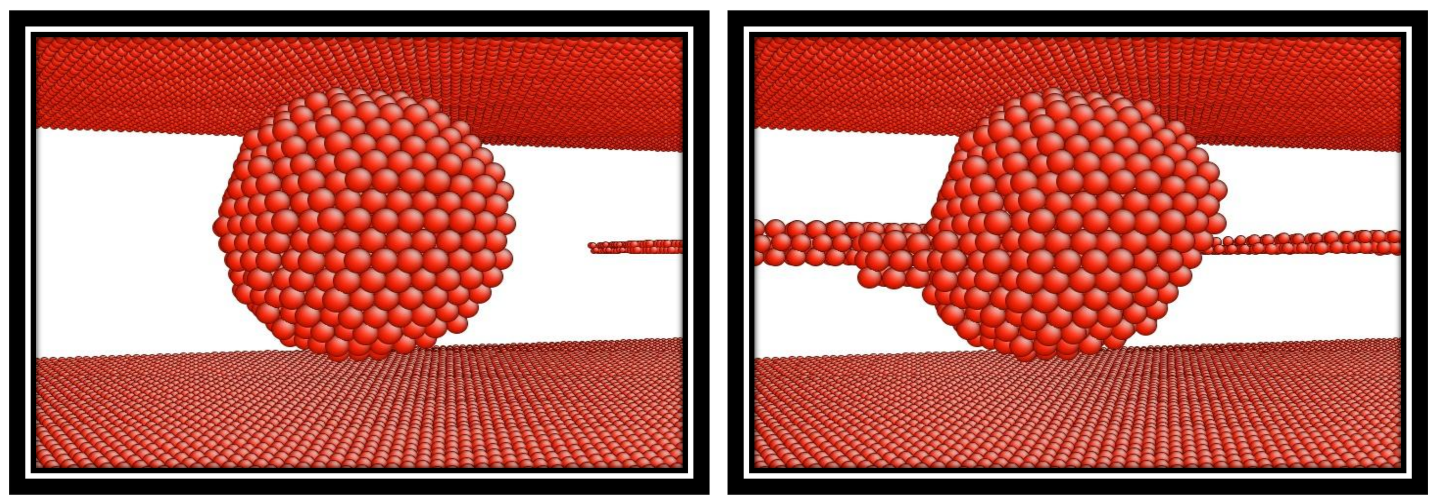
•Temperature: 350K Diameter of loop: 4 nm

•After each pass the prismatic loop shrinks in size and the dislocation leaves a new defect behind.

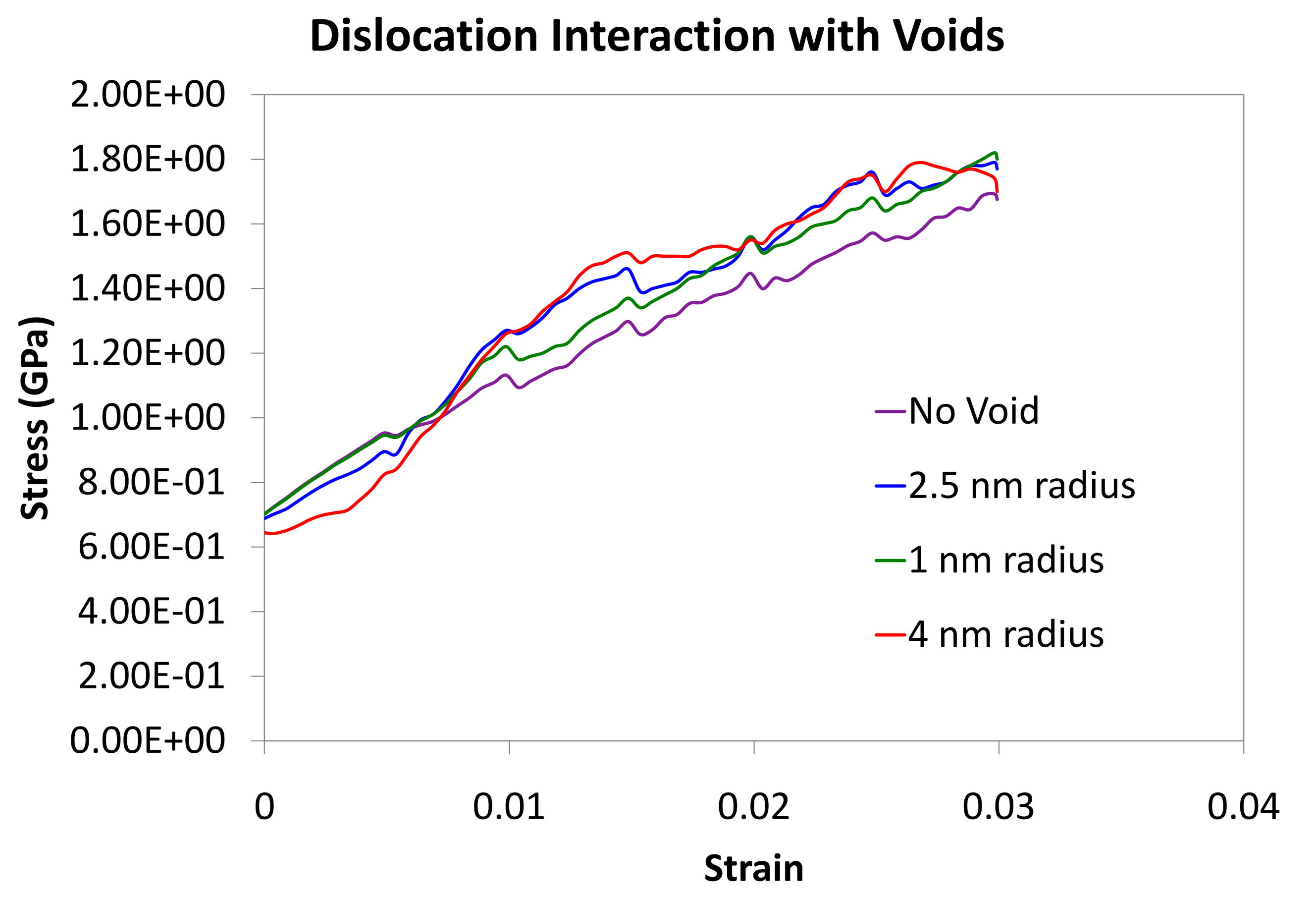
II. Dislocation – void interaction



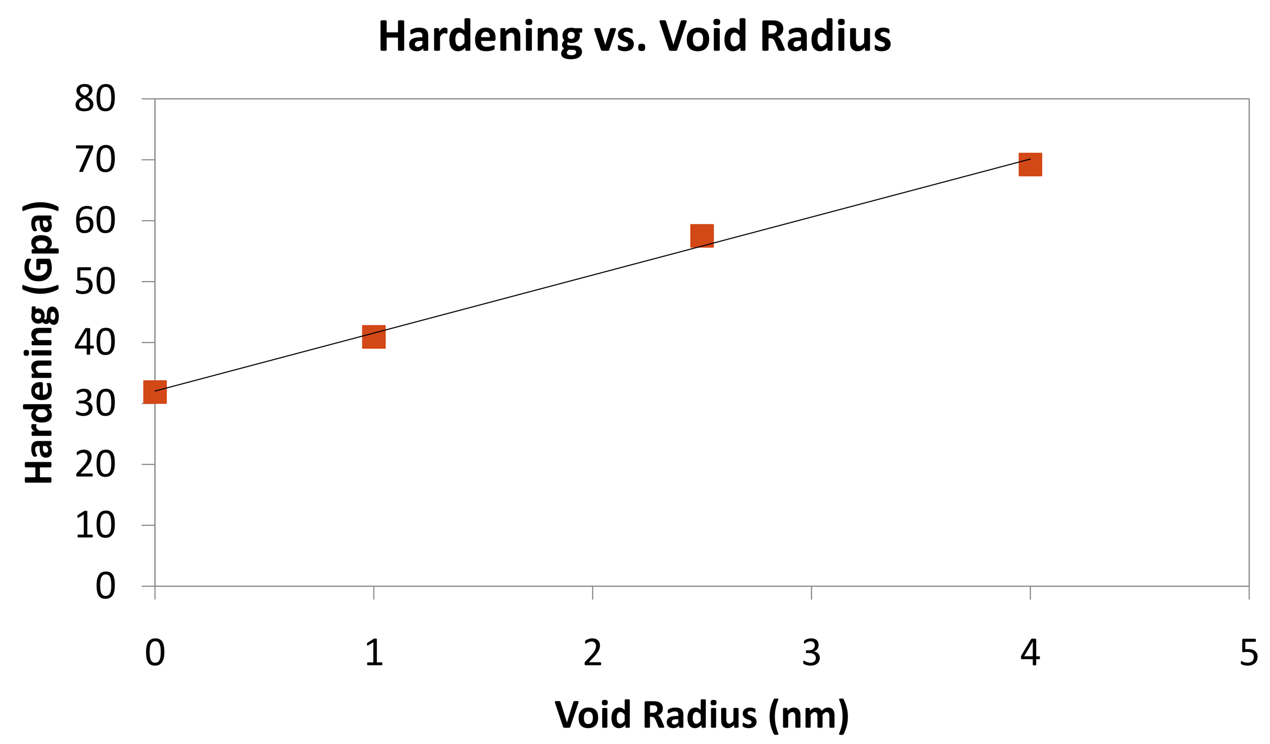
•As the dislocation moves closer to the void, the void's free surface attracts the dislocation. The radius of the void is 3 nm.



• 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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