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Structural phase transformation mechanism of α-Fe under tensile loading at high strain rate: molecular dynamics study

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Abstract

One of the most significant properties of metals is their ability to undergo phase transformations and structural changes in response to external forces, temperature variations, and other environmental factors. In this study, molecular dynamics (MD) simulations are employed to investigate phase transformation mechanisms and deformation behavior in a pristine and defect-free α-Fe specimen subjected to high strain rate tensile loading. The results reveal that, during the loading process, the microstructural transformation initiates from a body-centered cubic (bcc) structure to a face-centered cubic (fcc) structure, followed by a subsequent transition from fcc to a hexagonal close-packed (hcp) configuration. Furthermore, the critical stress levels follow the order $\sigma_{hcp} > \sigma_{fcc} > \sigma_{unknown} > \sigma_{bcc}$, indicating that the hcp structure requires the highest stress to initiate transformation. Consequently, bond rupture and fracture nucleation are most likely to occur in the vicinity of this phase.

Keywords: Phase Transformation, Molecular Dynamics Simulation, Tensile Loading, High Strain Rate

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