

Nanoscale dynamic response of the structural transition in single crystal iron: ramp wave and pressure-shear wave loading

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ABSTRACT

Most metal crystals may experience a polymorphic transition under compression. A comprehensive understanding of the polymorphic transition is of great significance in basic and applied research. Iron is a prototypical metal of polymorphic transition, which will undergo the BCC-HCP structural transition when compressed to the high pressure of ~13 GPa. This report mainly introduces our recent researches on the mechanism and dynamic properties of structural transition in iron based on atomistic simulations. Firstly, the ramp wave loading along different crystal directions of single crystal iron was simulated, and the stress threshold of HCP nucleation, grain size of new phase, and the sliding path of atoms under extreme strain rate were all discussed. Then, the compression-shear wave loading was also simulated, and the effect of shear wave on the HCP nucleation, the strain localization, and the twin formation were all discussed.

Keywords: Iron; Structural transition; Ramp wave; Shear wave; Atomistic simulation