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Effect of nano-void on the phase transformation of single crystal iron under shock compression[1] XINLIN CUI, WENJUN ZHU, HONGLIANG HE, YINGJUN LI — Shock-induced phase transformation (body-centered cubic α phase to hexagonal close-packed ε phase) in single crystal iron has been investigated by means of the molecular dynamics (MD) simulation using an embedded atom method (EAM) potential. By introducing a nano-void in the single crystal iron, the nucleation velocity and the nucleation sites are observed to be different from the ideal single crystal iron. The simulation results show that the void accelerates the nucleation velocity, which induces the new phase to nucleate easier. At the same time, the void affects the nucleation sites, the initial homogeneous nucleation is observed near to the leading front of the shock wave in the ideal single crystal iron, but they firstly occur around the edge of the void, and finally form a butterfly shaped transformation zone in the defect single crystal iron. By calculating the distribution of the resolved shear stress along the slip plane, the reason why the nucleation sites are different has been explained.

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Xinlin Cui

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