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MD simulation of steady shock waves with bcc-to-hcp phase transition in single-crystal Iron VASILY ZHAKHOVSKY, KIRILL MIGDAL, All-Russia Research Institute of Automatics, NAIL INOGAMOV, SERGEY ANISIMOV, Landau Institute for Theoretical Physics, RAS, Russia — Overdriven shock waves propagating along the main crystallographic directions of single-crystal bcc iron were studied with moving-window molecular dynamics (MD) technique. To simulate correctly the shock-induced bcc-to-hcp phase transition a new EAM potential fitted to the cold pressure curves and pressure transition at about 13 GPa was developed for iron by the stress matching method. We demonstrate that structure of shock fronts depends on orientation of crystal. A peculiar structure of steady shock-wave front in [100] direction is observed. While a single-wave plastic shock front in [100] direction has no elastic precursor, a single two-zone elastic-plastic shock wave with highly-overcompressed elastic zone ahead of a plastic front propagates in other directions. The mechanisms and interplay of elastic-plastic transformation and bcc-to-hcp phase transition induced by steady shock waves in iron are discussed.

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