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Shock waves and recovery in polycrystalline iron NINA GUNKELMANN, Physics Department and Research Center OPTIMAS, University Kaiserslautern, DIEGO R. TRAMONTINA, EDUARDO M. BRINGA, Instituto de Ciencias Básicas, Universidad Nacional de Cuyo, Mendoza, HERBERT M. URBASSEK, Physics Department and Research Center OPTIMAS, University Kaiserslautern —
It is well known that shocks create not only plasticity in Fe, but also phase transform the material from its bcc phase to the high-pressure hcp phase. These two mechanisms were recently examined in several simulation studies. However, there are still important questions that are not answered in our current understanding of shocks in Fe. In particular, the morphological properties of shock recovered samples have not been extensively explored in experiments, and are still unexplored in atomistic simulations. In this work, we study shocks and recovery of large polycrystalline iron samples by molecular dynamics simulations. With increasing shock strength, we find a transition from a 2-wave structure (elastic and plastic wave) to a 3-wave structure (an additional phase-transformation wave), in agreement with experiments. The phase transformation is preceded by dislocation generation at grain boundaries. Our analysis shows that recovery leads to twinning inside the recovered bcc grains. The structure of the twins is in good agreement with experimental results and a semi-analytical model which assumes a critical shear stress for twinning.

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