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Molecular Dynamics Simulations of Shock-Induced Defect Healing in Silicon XIANG GU, YOU LIN, IVAN OLEYNIK, Physics Department, USF, CARTER WHITE, Naval Research Laboratory — Molecular dynamics (MD) simulations of the interaction of planar shock waves with point defects (interstitials and vacancies, or Frenkel pairs) have been performed to investigate the possibility defect reduction in Si resulting from substantial mechanical stress behind the shock wave front. The MD shock experiments were run in Si samples containing Frenkel pairs of varying concentration and composition. The defect dynamics behind the shock wave front were studied as a function of the shock wave intensity and the crystallographic orientation of its propagation. We also simulated shock unloading that returns the compressed samples to their uncompressed state. The overall effectiveness of shock-induced defect healing was studied as well. Such an unusual application of the shock compression of solids might be useful in the microelectronics industry where such defects produced by ion implantation are considered a serious obstacle towards the further size reduction of Si CMOS devices.

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