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Silicon under mechanical shear: molecular dynamics study ALI KERRACHE, NORMAND MOUSSEAU, LAURENT J. LEWIS, Univ. of Montreal — Relaxation processes and defect behavior in amorphous silicon (a-Si) under shear are investigated by molecular dynamics simulations using the empirical Environment Dependent Inter-atomic Potential. Shear deformations allow us to reproduce a vast range of interesting dynamics in disordered materials. For example, it has been shown recently that high-energy ion irradiation deforms plastically a-Si samples, following a pattern similar to the application of a shear. While large shear reproduce high-irradiation effects, moderate one can accelerate defect diffusion. A controlled application of shear can therefore help us to understand better the nature of defect diffusion in a-Si, in addition to generating new defects that could be placed with the appropriate external field at critical positions or even lead, in some cases, to crystallization of the a-Si. The properties of a-Si under shear are analyzed as a function of imposed shear velocity and as a function of the distance from the wall.

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