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Simulations of Phase Transitions in Silicon with the Environment-Dependent Interatomic Potential MARTIN Z. BAZANT, EFTHIMIOS KAXIRAS, Department of Physics, Harvard University, J. F. JUSTO, Instituto de Fisica da Universidade de São Paulo, Brazil — The recently developed Environment-Dependent Interatomic Potential (EDIP) holds the promise of a new degree of transferability in describing bulk phases and defects of elemental covalent solids with a simple, theoretically motivated functional form [1]. A version of EDIP fitted for bulk Si with only 13 parameters accurately reproduces bulk crystal and point defect properties as well as reconstructions of partial dislocation cores. Here we further explore the transferability of EDIP-Si for disordered structures and phase transitions, which involve local configurations quite different from those used in fitting. We report that EDIP-Si reliably simulates a direct quench from the liquid to the amorphous phase (unlike any other potential), and the resulting structure is more realistic than with previous empirical preparation methods. We also present simulations showing how EDIP-Si predicts premelting of the (100) surface well below the bulk melting point and other interesting features of melting. We conclude with prospects for extending EDIP to other covalent materials using *ab initio* theoretical calculations.

[1]M. Z. Bazant, E. Kaxiras, J. F. Justo, Phys. Rev. B **56**, 8542 (1997).

Martin Z. Bazant
bazant@cmt.harvard.edu
Department of Physics, Harvard University

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