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Molecular dynamics simulation of the recrystallization of amorphous Si layers: Comprehensive study of the dependence of the recrystallization velocity on the interatomic potential

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The molecular dynamics method is applied to simulate the recrystallization of an amorphous/crystalline silicon interface. The atomic structure of the amorphous material is constructed with the method of Wooten, Winer, and Weaire. The amorphous on crystalline stack is annealed afterward on a wide range of temperature and time using five different interatomic potentials: Stillinger-Weber, Tersoff, EDIP, SW115, and Lenosky. The simulations are exploited to systematically extract the recrystallization velocity. A strong dependency of the results on the interatomic potential is evidenced and explained by the capability of some potentials (Tersoff and SW115) to correctly handle the amorphous structure, while other potentials (Stillinger-Weber, EDIP, and Lenosky) lead to the melting of the amorphous. Consequently, the interatomic potentials are classified according to their ability to simulate the solid or the liquid phase epitaxy.

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