

Abstract Submitted
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Phase-field theory for phase transition dynamics of reconstructed semiconductor surfaces BANG-GUI LIU, Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China — We propose a natural two-speed model for the phase dynamics of Si(111) 7×7 phase transition to unreconstructed phase. Our simulated results show that a 7×7 island decays with its shape kept unchanged, and its area decay rate is a constant increasing with its initial area. LEEM experiments concerned are explained, which confirms that the dimer chains and corner holes are broken first, and then the stacking fault is remedied slowly. We also propose a phase-field-crystal model for the (2×1) - (1×1) phase transitions of Si(001) and Ge(001) surfaces. Simulated periodic arrays of dimerization is consistent with STM images. Calculated temperature dependence of the dimerization indicates that normal dimers and broken ones coexist between T_L and T_H , and a first-order phase transition takes place in between. This phase-field method is a reliable approach to phase dynamics of surface phase transitions. Phys. Rev. Lett. 100, 056103 (2008).

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