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The Structure and Evolution of Ge Nanoscale Structures on Si(111) – Observations and Theory SANWU WANG, Vanderbilt University, H.F. MA, Z.H. QIN, D.X. SHI, Y.L. WANG, H.M. GUO, H.-J. GAO, S.T. PANTELIDES, Vanderbilt University and Oak Ridge National Laboratory — We report scanning tunneling microscopy (STM) observations and first-principles calculations for the evolution of self-organized Ge nanostructures formed on Si(111)-7×7 for Ge coverages up to 0.5 ML and operating temperatures from room temperature to 300°C. STM measurements show that, depending on coverage and temperature, Ge atoms form various structures ranging from single-atom correlated patterns, 2-D ordered nanoscale domains, and 3-D disordered and ordered nanoclusters. First-principles theory focuses on the single-atom patterns and 2-D ordered nanostructures. We show that Ge atoms replace the Si adatoms in the initial adsorption stage. We also show that annealing of the Ge/Si(111) surface results in a partial transformation of (7×7) reconstructed unit cells to unreconstructed Si(111) configurations on which the Ge adatoms reside at the T_4 sites and form a $(\sqrt{3}\times\sqrt{3})R30^\circ$ reconstruction.

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