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Direct Imaging of Point Defect Configurations for Au Atoms Inside Si Nanowires[1] K. VAN BENTHEM, S.H. OH, A.Y. BORISEVICH, W. LUO, Oak Ridge National Laboratory, P. WERNER, N.D. ZAKHAROV, MPI for Microstructure Physics, S.T. PANTELIDES, Vanderbilt University, S.J. PENNYCOOK, Oak Ridge National Laboratory — Aberration-corrected scanning transmission electron microscopy (STEM) was used to directly image individual Au atom configurations inside Si nanowires grown by Au-catalyzed vapor-liquid-solid molecular beam epitaxy. A three-dimensional analysis of the nanowire microstructure revealed Au atom concentrations five orders of magnitude higher than equilibrium values in bulk silicon. Three distinct interstitial Au atom configurations were identified in addition to the substitutional configuration. The stability of the observed point defect configurations was further investigated by density-functional theory. The observed configurations are in excellent agreement with theory. However, a comparison of the number densities of the various configurations with the calculated formation energies indicates an effective temperature of approximately 1000 degrees centigrade suggesting significant beam-induced atomic diffusion.

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