STM-Fabricated Single-Dopant Boron and Phosphorus Structures in Silicon

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We present progress with STM-based single-atom fabrication of dopant structures in silicon, focusing on the extension of methods for controlled single-donor incorporation to mixed donor–acceptor systems. We deterministically pattern adsorption sites in a single atomic layer of H-Si(100) using hydrogen depassivation lithography (HDL) to enable placement of dopants with nanometer-scale precision.

We previously demonstrated[1] the use of phosphine precursors followed by STM-controlled manipulation as a means to reliably incorporate individual phosphorus donors, which can be positioned in proximity to dense HDL patterned dopant regions that function as conductive leads and electrostatic gates. To further develop this fabrication technique we are investigating single-atom boron incorporation using diborane as a precursor, with the goal of enabling atomically precise donor–acceptor architectures. We present STM observations (Figure 1) of boron-related adsorbate species and incorporated features where diborane has been dosed onto a starting surface consisting of randomly placed bare silicon dimers on H-Si(100). We compare experimental STM images to density functional theory (DFT)-simulated images to gain insight into the local bonding configurations and aid in identification of adsorbed/incorporated species.

Our results highlight STM-based atomic fabrication as a method for creation of dopant-engineered silicon devices where functionality is defined by the precise atomic geometry, providing a basis for studying the fundamental physics of dopant interactions as well as quantum-enabled nanoscale devices.

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[1] J. Wyrick, X. Wang, P. Namboodiri, R. V. Kashid, F. Fei, J. Fox, and R. Silver, Enhanced Atomic Precision Fabrication by Adsorption of Phosphine into Engineered Dangling Bonds on H–Si Using STM and DFT, ACS Nano **16**, 19114 (2022).

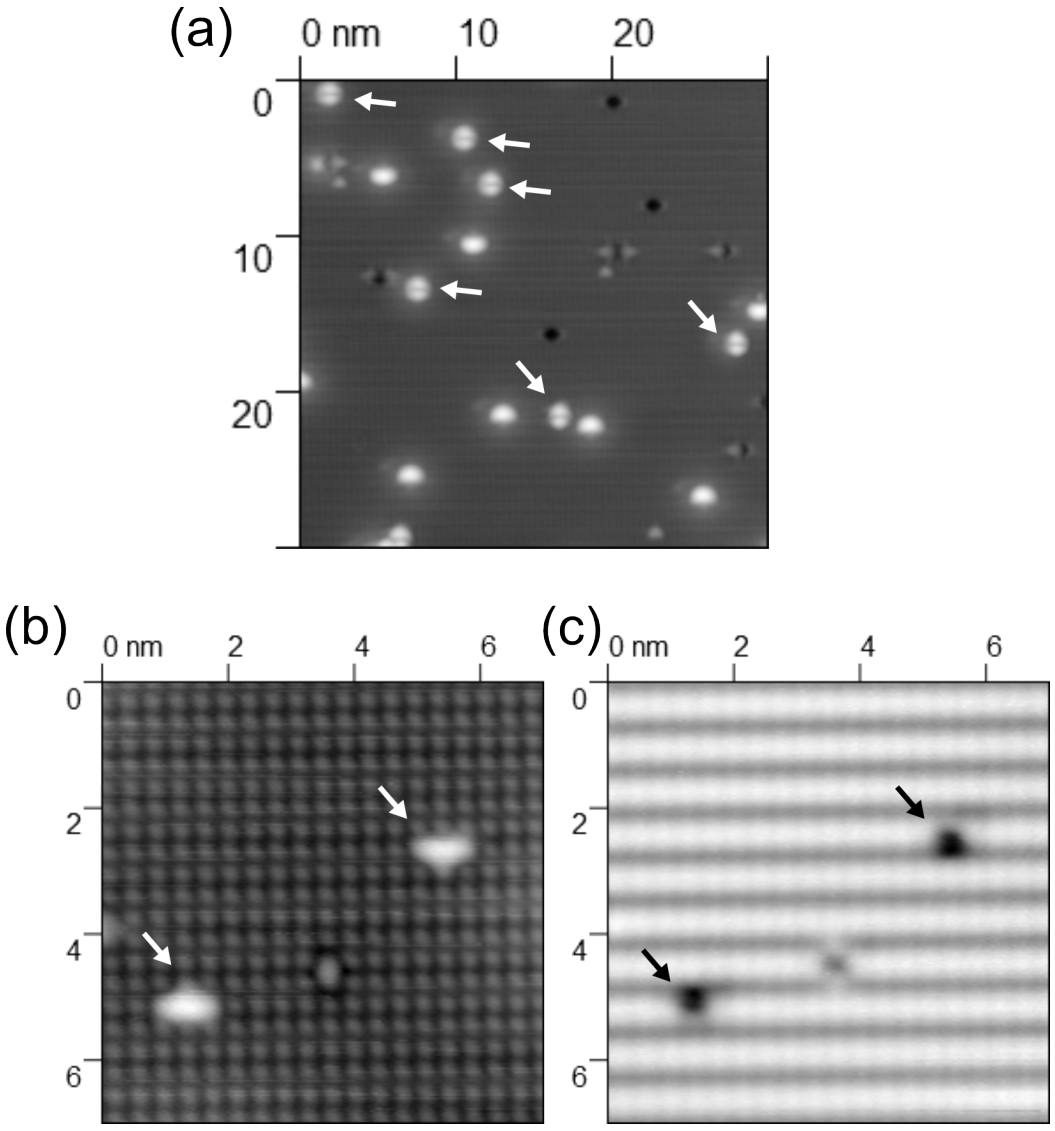

Figure 1: Constant Current STM micrographs of bare silicon dimers and adsorption species post diborane dosing. (a) H-Si(100) surface prepared at elevated temperatures to induce formation of bare silicon dimers (white arrows). Imaging conditions: 2V sample bias, 10 pA setpoint current. (b,c) H-Si(100) surface after B_2H_6 deposition. Arrows indicate adsorbed species (the other prominent feature is a siloxane dimer defect. Imaging conditions: (b) 1.6V sample bias, 100 pA setpoint current, and (c) -1.6V sample bias, 100 pA setpoint current.