

Movement and Imaging of Single-Atom Dopants in Silicon

Bethany M. Hudak¹, Jiaming Song¹, Paul C. Snijders¹, and Andrew R. Lupini¹

¹ Materials Science and Technology Division, Oak Ridge National Laboratory, Oak Ridge, TN, USA

Theoretical predictions show that quantum computers should be able to perform beyond the capabilities of the most powerful current supercomputers, making the realization of quantum computing of interest to both civilian and government institutions. One quantum computing architecture that is particularly appealing consists of individual atoms doped into a semiconductor, where the spin states of these dopant atoms provide a method to encode the qubits [1]. The widespread application of silicon in electronics makes it an ideal material for quantum computing due to existing infrastructure for the production, study, and use of Si-based devices. Group V elements are promising candidates for use as single-atom qubit dopants in Si [1,2]. Atoms with a similar atomic number (Z) to Si, such as phosphorous, are difficult to observe through conventional single-atom imaging techniques such as scanning transmission electron microscopy (STEM), making approaches to accurate single atom positioning challenging. Pnictogens other than phosphorous, particularly the heavier Group V elements, are potential candidates to function as qubits and overcome these obstacles. Bismuth – with large spin-orbit coupling, strong clock transitions [3], and a greater potential to be imaged by STEM – is very promising. Bi in Si has been shown theoretically to allow gates operating in the MHz regime [4]. It has also been suggested that Bi may allow qubit operation at liquid nitrogen temperature, an important aspect of practical device operation.

However, the accurate placement of single atom dopants within a solid with control and understanding of their local environment has not yet been realized with the necessary degree of accuracy for quantum computing applications. Here we demonstrate the ability to image and move single Bi atoms within Si. Samples of Bi-doped Si films were grown using molecular beam epitaxy (MBE) and imaged at a variety of accelerating voltages. The dopant atoms can be imaged with atomic-resolution at low voltages, and at higher voltages we intentionally induce the motion of single Bi dopants inside the film. Figure 1 shows a selection of frames from a sequence of images taken at 200 kV demonstrating that under these conditions we can observe the movement of a single Bi dopant. Image sequences acquired at lower accelerating voltages show less dopant movement.

Electron beam interactions with the sample are well known. Recently, it has been shown that the electron beam can be used for atomic-level sculpting [5] of oxide lattices. While this phenomenon may be somewhat expected, the mechanism by which it occurs needs to be understood so that the process can be controlled and exploited. Due to the dopant behavior above and below the knock-on damage threshold of Si, and with the use of density functional theory (DFT) calculations, we have determined some of the factors that are necessary to produce dopant movement. By fully understanding the mechanism by which the dopant atoms move and developing this mechanism for directed atom movement, we can begin to build atomic-scale architectures for quantum computing. [6]

References:

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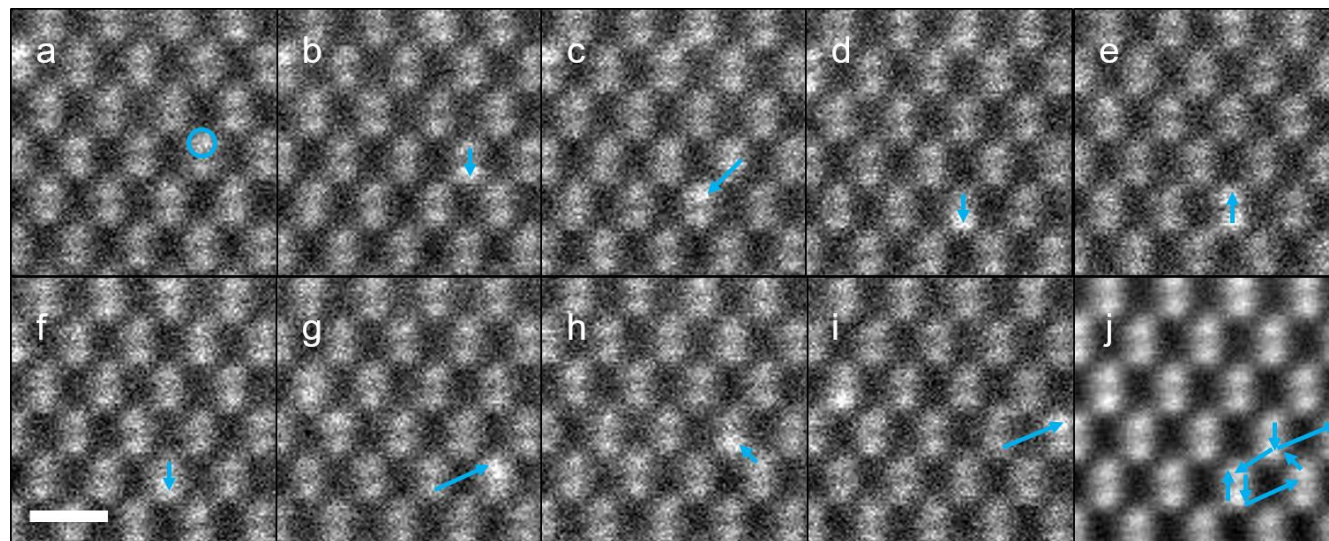


Figure 1. Electron beam-induced movement of a single Bi atom. (a-i) Extract from 20 sequential frames acquired at 200 kV. (a-i) The random motion of one Bi atom is followed, as indicated by arrows. (j) Overlaid images showing the path covered by the Bi atom during this acquisition. Beam current was about 140 pA with an 8 nm field of view at 4 μ S/pixel. Scale bar = 0.5 nm