doi:10.1017/S1431927620022047
Microsc. Microanal. 26 (Suppl 2), 2020

Mapping Dopant Defect Complexes at the Nano and Atomic Scale for Quantum Computing

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While quantum information systems have the potential to revolutionize computing , numerous materials science problems remain before this vision becomes reality.[1] In particular, deep-level defects that are traditionally undesirable for devices can serve as the basis of solid-state quantum bits (qubits), such as the nitrogen-vacancy center.[2] From a characterization standpoint, optical spectroscopy and NMR have been the primary tools employed to study qubits. These tools, however, lack the spatial resolution necessary to directly probe their structural environments. As the local structure of the qubit has a strong effect on the properties, the application of scanning transmission electron microscopy (STEM) to these systems offers the potential to directly quantify the local environment around dopant atoms and defect complexes to aid theoretical modeling and materials synthesis.

In this presentation, we will highlight the application of STEM applied to study qubits in SiC and point defect complexes in aluminum nitride (AlN). In particular, implanted dopants in silicon carbide will be discussed, which are being developed as qubits for quantum sensing, computation, and communication applications. As an example, we will explore Er-doped SiC systems, where previous STEM imaging of Er-doped SiC has found aggregation and phase-separation in the regime of high Er concentration.[3] The local structural distortion of SiC around a single Er dopant atoms and influence on the SiC microstructure are not well understood. We will show how Er atoms can be readily located in STEM images along the < 0001 > direction using differences in contrast (Figure 1). We will discuss how along the zone, quantitative information such as the preferred lattice site (h or k in 4H crystal structure) and shifts in the surrounding atoms can be extracted. These insights yield fundamental knowledge about how implantation affects the surrounding lattice.

In the AlN system, we will explore Silicon dopant-vacancy complexes that are thought to form in this material for high-power electronics and deep UV LED/laser applications. Although finding individual, substitutional dopant Si atoms directly in STEM can be challenging due to minimal Z-contrast difference, we will show how cathodoluminescence can be employed to connect nanoscale structure from HAADF STEM (Figure 2A) to the optical properties of the defect complexes. For example, the Si-Vacancy defect complex emission red-shifts by 0.1 eV at threading dislocations, and the emission spectra can be deconstructed into the summation of two gaussians, suggesting emission from a higher and lower energy defect complexes at these locations. Coloring each pixel according to the integrated intensity of emission from the lower energy and higher energy emission reveals a greater fraction of the emission coming from the lower energy defect complex at the threading dislocation. (Figure 2B and C). We will discuss how the local strain at the threading dislocation has changed the formation energy landscape, potentially favoring different dopant complexes.

Acknowledgements

This work was supported by the Air Force Office of Scientific Research FA9550-17-1-0225. We acknowledge Gatan and David Stowe for help with the cathodoluminescence data collection. Erbium-implanted SiC samples were prepared by Gary Wolfowicz and Chris Anderson.

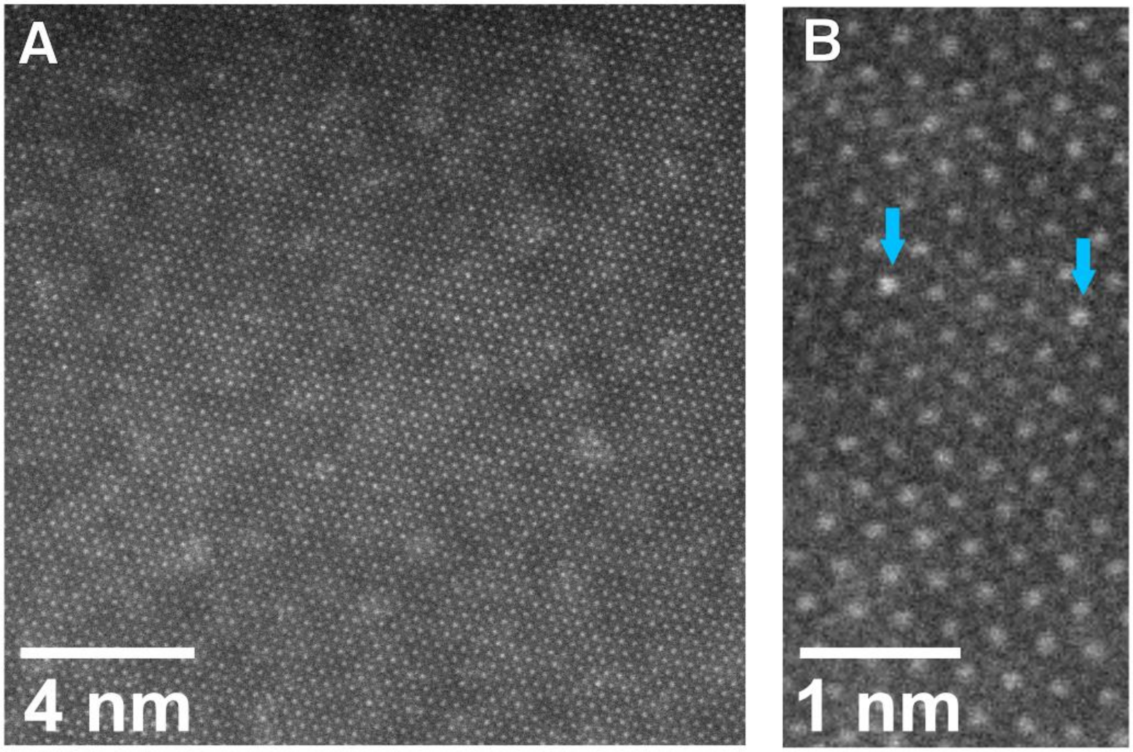

Figure 1. (A) HAADF-STEM image of Erbium-implanted 4H-SiC down the [0001] zone axis (B) Zoomed image of two atom columns with significant contrast increase-suggesting the presence of Er.

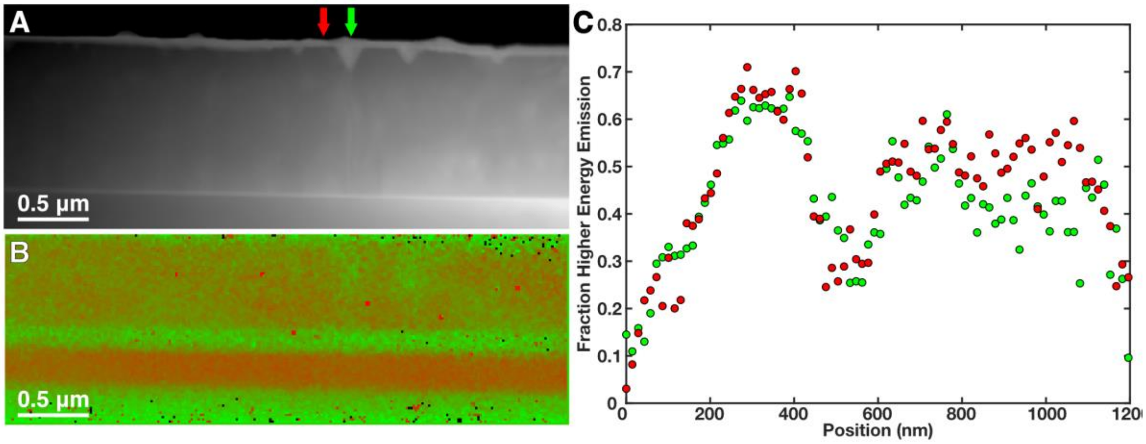

Figure 2. Correlating structure and emission of Silicon-doped Aluminum Nitride A) HAADF STEM image of Si-doped AlN sample with visible threading dislocations (green arrow). B) From cathodoluminescence collection, the emission spectra of each pixel can be fit using the summation of two gaussians. Each pixel is color coded by the integrated intensity of emission from the higher energy (red) and lower energy (green) defect complex. C) Line scans of the fractional integrated intensity from the higher energy emission complex at the threading dislocation (green, corresponding to green arrow in A)) and a region without defects (red, corresponding to red arrow in A)).

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