Imaging Rare-Earth Dopant Clusters in SiC in 3D using Multislice Electron Ptychography

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There has been a long-standing interest in exploring rare-earth dopants and clusters within wide-bandgap materials as a platform for quantum computing [1]. Atomic-scale characterization of these dopants is crucial for understanding activation mechanisms and optimizing doping strategies. Multislice electron ptychography (MEP) is a new approach capable of imaging the atomic distribution of dopants inside a material, offering sub-Ångstrom lateral resolution and a few nanometers depth resolution, making it possible to visualize atomic-scale vibration envelopes and single dopants [2, 3]. Here, we use MEP to image the effects of implanting Sm and Co atoms in SiC, a prototypical host whose rare-earth-doped defect centers display promising photonic and spintronic functionality [4].

Figure 1 presents a region of SiC containing Sm dopant clusters, comparing MEP with conventional Annular Dark Field (ADF) imaging. The MEP reconstruction reveals depth dependent features showing that the Sm atoms occupy Si positions inside the sample and displace nearby C and Si atoms, even whole columns (yellow arrow) – details that ADF fails to capture. This new capability to study atomic defects in 3D not only deepens our understanding of defect behavior in complex materials but also allows us to tackle such problems in the actual device structures needed for optoelectronic and quantum computing.



Figure 1 Experimentally imaged Sm dopants in SiC matrix. (a) MEP reconstruction showing the SiC lattice with the buried Sm columns inside it and displaced Si and C columns. (b) ADF image of the same region only showing the Sm columns. Scale bars are 5 Å.

- [1] G. Wolfowicz et al., Nat Rev Mater 6, 906 (2021).
- [2] Z. Chen et al., Science **372**, 826 (2021).
- [3] Z. Chen et al., *arXiv preprint arXiv:2407.18063* (2024).
- [4] U. Kaiser, D. A. Muller, J. L. Grazul, A. Chuvilin, and M. Kawasaki, Nature Materials 1, 102 (2002).

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