

Investigating Nitrogen Diffusion in Silicon through Scanning Tunneling Microscopy

Thomas R. Sheridan, DeAnna M. Campbell, Christopher R. Allemang, Jeffrey A. Ivie, Ezra Bussmann, Shashank Misra.
Sandia National Laboratories, 1515 Eubank Blvd, Albuquerque, NM 87123
trsheri@sandia.gov

The movement of dopants in silicon is a critical field of study for the fabrication of novel electronic devices. This movement of dopants is particularly concerning for atomically precise advanced manufacturing (APAM)-based devices¹, as the small number of dopants and nanometer-scale areas of interest mean that the movement of even one dopant atom may change the intended device properties dramatically.

Diffusion of commonly-used APAM-compatible dopants like phosphorous and boron has been previously studied, but nitrogen has generally been overlooked. While nitrogen has difficulties in achieving high electrical activity, the fact that ammonia (NH₃) readily dissociates onto Si (100) and the potential advantages of nitrogen for nanoscale devices² makes the study of its diffusion highly interesting. Nitrogen also has similar issues of complexation as has been proposed for boron and phosphorous³, and thus studies of its diffusion may provide insights into the movement of currently used donors. While general diffusion coefficients have been extracted for annealed N in Si⁴, detailed imaging of chemical changes and their relation to N diffusion would be valuable.

We have combined scanning tunneling microscope (STM) observations of the dissociation of NH₃ with TOF-SIMS depth profiles to further elucidate the relation between the structure of N and its ability to diffuse in Si. STM images of ammonia-dosed surfaces annealed at 450°C and 700°C show both substitutional and interstitial N. However, up to an anneal temperature of ~600°C and regardless of molecular structure, N does not diffuse long distances in silicon during annealing or cap growth. The data presented may help to explain diffusion patterns in common dopants and help in targeting future APAM-compatible donors.

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² Yadav, P.; Arora, H.; Samanta, A. *Appl. Phys. Lett.*, 122, 083502, **2023**.

³ Dwyer, K. J.; Baek, S.; Farzaneh, A.; Dreyer, M.; Williams, J. R.; Butera, R. E. *ACS Appl. Mater. Interfaces*, 13, 41275-41286, **2021**.

⁴ Itoh, T.; Abe, T. *Appl. Phys. Lett.*, 53, 39-41, **1988**.

Sandia National Laboratories is managed and operated by NTESS under DOE NNSA contract DE-NA0003525.