Single-Dopant Arrays using Tip-assisted Incorporation Process

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For dopant-based atomic-scale devices such as the 'single atom transistor' [1] and 2D Quantum Metamaterials, single isolated dopant atoms need to be incorporated into the surface at a particular distance from other dopants. For desired device properties, certainty over both the number of dopants placed and their positions is required.

The current thermal incorporation process for P involves the deposition of three PH_3 molecules into a 3-dimer pattern. A thermal anneal drives off two PH_3 molecules and the third one incorporates. However, the yield of single P atoms is only 70% for a 3-dimer pattern, and for 4-dimer or larger patterns, there is a possibility to adsorb two P atoms[2], which would have different properties.

A proposed process to achieve a higher yield of adsorbed P and remove the possibility of adsorbing two P atoms is to use an STM tip to remove the H from a PH_2 adsorbed species, thereby closing the redesorption pathway[3]. A schematic pathway is shown in Figure 1.

We are developing tip-based incorporation processes for P and Al dopants. First, Feedback Controlled Lithography is used to create single dimer patterns. Single molecules are adsorbed into these patterns. The tip then removes H locally from the adsorbed fragments and the background Si. A short room-temperature deposition of Si is used to bury the P fragments in a locking layer before low-temperature overgrowth, to minimise the diffusion of the P during encapsulation.

For Al dopants, we are using Trimethyl Al (TMAl) as a precursor, which shows strong selectivity to the created patterns, and exploring AlH_3[4]. In this case, single dimer patterns do not appear to be reactive to single TMAl molecules; 2-dimer patterns are required for adsorption of a single molecule, and steric hindrance blocks adsorption of a second dimer, as seen in Figure 2.

1: M. Fuechsle, J. A. Miwa, S. Mahapatra, H. Ryu, S. Lee, O. Warschkow, L. C. L. Hollenberg, G. Klimeck, and M. Y. Simmons *Nat Nano* **7** 242-246 (2012) DOI: 10.1038/nnano.2012.21

2: J. G. Keizer, S. Koelling, P. M. Koenraad, and M. Y. Simmons *ACS Nano* **9** 12537-12541 (2015) DOI: 10.1021/acsnano.5b06299

3: Q. Liu, Y. Lei, X. Shao, F. Ming, H. Xu, K. Wang, and X. Xiao, *Nanotechnology*, **27**(13), 135704, (2016). DOI: 10.1088/0957-4484/27/13/135704

4: R. Smith and D. R. Bowler, Arxiv: 1711.08401, Nov. 2017.

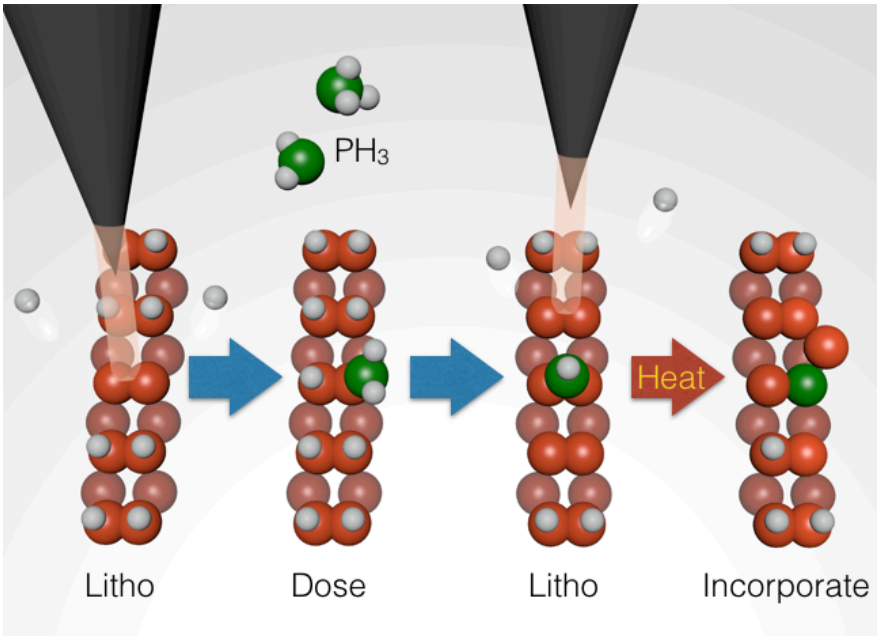

Figure 1: Proposed Tip-based Process for P dopant incorporation. A single dimer pattern is created using STM Lithography. PH3 is adsorbed, A second round of Lithography removes H from the PH2. An incorporation anneal causes exchange of the P atom with a Si dimer atom. The dopant can then be encapsulated.

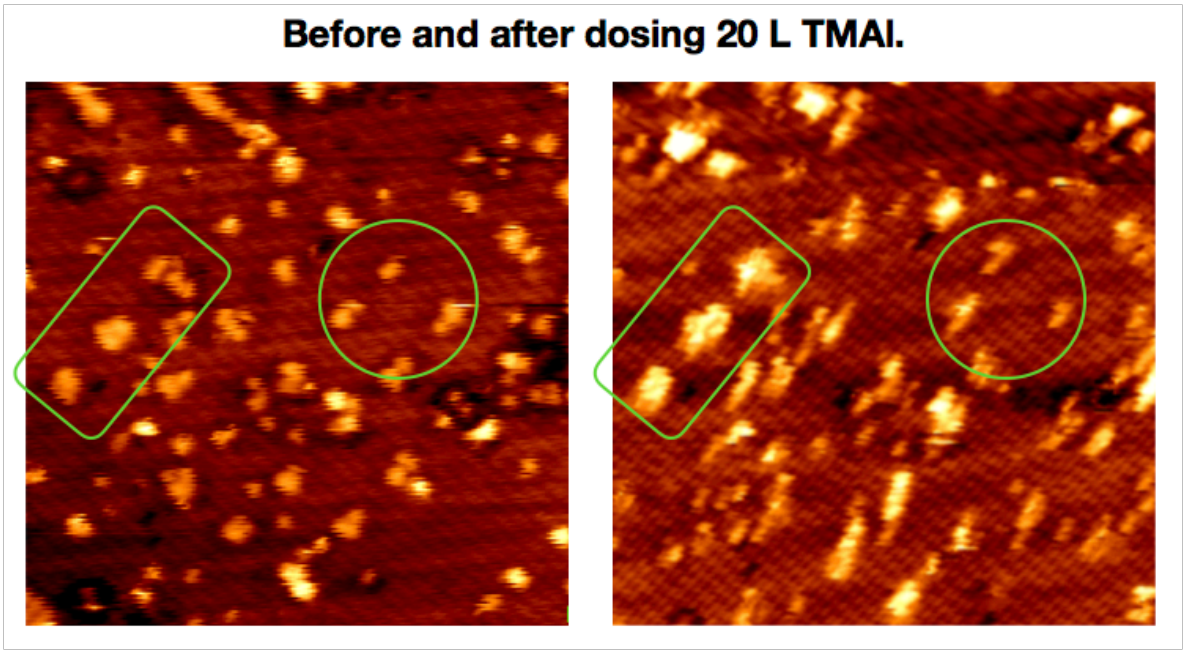

Figure 2: Array of few-dimer patterns before and after adsorption of 20L TMAl. Most of the patterns have adsorbed single TMAl molecules [rectangle]. The smallest 1-dimer-wide patterns (circled), however, show no adsorption, indicating that the minimum size pattern for TMAl adsorption is two dimers.