## 2D dopant arrays using a Tip-assisted Incorporation Process

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Keywords: STM Lithography, Atomic-Precision Patterning

Hydrogen Depassivation Lithography (HDL) using an STM tip has become established as a method for atomic-precision patterning for P-dopant-based devices. For devices such as the 'single atom transistor'[1], single dopant atoms need to be placed precisely relative to other device elements, such as electrodes, gates, other single dopant atoms. Furthermore, for 2D Quantum Metamaterials[2], arrays of single dopants are required, with extreme precision and high yield.

The current thermal incorporation process is lacking in both required aspects. In this process, a 3-dimer pattern is created using HDL. Three PH<sub>3</sub> molecules adsorb into the pattern. A short thermal anneal causes two of the PH<sub>3</sub> molecules to recombine and desorb, providing the required dangling bonds to allow the third PH<sub>3</sub> to decompose to P + 3H, which then incorporates into the surface. However, the yield of single P atoms is only 70% with this process; in 30% of cases all three PH<sub>3</sub> molecules desorb[3]. Also there is uncertainty in the position of the P atom after the incorporation step. For the intended array application, the overall yield for *n* sites will be  $0.7^n$  and hence the individual yield needs to be close to 100%.

Based on previous work on isolated PH<sub>3</sub> molecules on the clean Si(001) surface [4], we are developing a tip-assisted incorporation process whereby the STM tip removes the H atoms from the adsorbed PH<sub>2</sub> group, which prevents the recombination and desorption process. As a result, we need to write single-dimer patterns to adsorb only one PH<sub>3</sub> molecule. For these small patterns, automated Feedback Controlled Lithography is used, so as to remove only 2 H atoms from the surface. We are working to improve the detection of the H atom removal, using not only the change in tunnel current, but also the resulting change in the local barrier height [5]. As shown schematically in Fig.1, single PH<sub>3</sub> molecules are adsorbed into these small patches, the H is removed from the PH<sub>2</sub>, and a brief anneal is used to drive incorporation of the atom. Moreover, since the requisite H atoms have already been removed, we can reduce the temperature of the anneal process. In preliminary experiments, the exchange occurs at temperatures between 200-250°C, at which temperature the surface H is not mobile[6]. Thus in principle, it is possible to return to the device location after the thermal anneal, and determine if the dopant atoms have incorporated, and if not, to repeat the process, and thus drive the final dopant density of the array towards 100%.

In summary, as a result of this process, we are able to reduce the position uncertainty of the P atom, but more importantly, the yield of P atoms in a 2D dopant array required for Quantum Metamaterial fabrication should rise above the 70% limit defined by the thermal process, towards 100%.

## References

[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] Workshop on 2D Quantum Metamaterials, 25<sup>th</sup> April, 2018. https://www.zyvexlabs.com/2d-workshop/
[3] J. G. Keizer, S. Koelling, P. M. Koenraad, and M. Y. Simmons ACS Nano 9 12537-12541
(2015) DOI: 10.1021/acsnano.5b06299

[4] 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

[5] F. Tajaddodianfar, S. O. R. Moheimani, J. Owen, and J. N. Randall, *Rev. Sci. Instrum.*, vol. 89, no. 1, p. 13701, 2018

[6] D. R. Bowler, J. H. G. Owen, K. Miki, and G. A. D. Briggs, "Diffusion of paired hydrogen on Si(001)," *Phys. Rev. B*, **57**(15), pp. 8790–8793, (1998). DOI: 10.1103/PhysRevB.57.8790 *This work was partly supported by DARPA, AFRL Contract FA8650-15-C-7542.* 



Figure 1: Proposed Tip-based Process for P dopant incorporation. A single dimer pattern is created using STM Lithography.  $PH_3$  is adsorbed, A second round of Lithography removes H from the  $PH_2$ . An incorporation anneal causes exchange of the P atom with a Si dimer atom. The dopant can then be encapsulated.



Figure 2: Small patterns created using automated Feedback Controlled Lithography. (a): A 3x7 grid of single dimer patches. The litho yield is low after the first pass. (b): A cluster of 3-dimer patterns written as a series of FCL dots rather than short lines.