Taking Control of the Reaction: Tip-assisted Dopant Incorporation Process for P-in-Si qubit devices

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Hydrogen Depassivation Lithography (HDL) using a Scanning Tunnelling Microscope(STM) has been used to create patterns with atomic precision for Phosphorus-dopant-based quantum devices. In order to transfer the pattern into dopants, the surface is exposed to phosphine (PH_3), and then a brief anneal to 350°C or 500°C is performed to trigger the exchange of a surface P atom with a Si dimer atom. For devices such as the 'single atom transistor' [1], a single isolated P atom is incorporated into the surface at a precise distance from other electrodes. In this case, a 3-dimer pattern is created, into which three PH_3 molecules are adsorbed. The anneal process drives off two of these, and the third incorporates into the Si surface. However, three issues remain with the current process. First, the yield of single P atom incorporation is only around 70% for a 3-dimer pattern; with larger patterns, the yield increases to 100%, but it then becomes possible for 2 P atoms to be incorporated. Second, the exact position of the P atom cannot be controlled within the pattern. Finally, since the anneal process may damage the patterning, inspection of the incorporation anneal is difficult, and error correction is almost impossible.

With our ZyVector STM control system we are able to write over the same area repeatedly, as we have demonstrated using disilane to grow multiple atomic layers of Si in patterned areas of a Si(001):H surface[2]. Making use of this improved control, we have developed a tip-assisted process for P incorporation. We present STM data at elevated temperatures on PH_3-saturated Si(001) surfaces and in PH_3 patterned areas of H-terminated Si(001) surfaces, demonstrating that the P incorporation reaction can be activated by an STM tip at a temperature (ca. 200°C) where background PH_3 fragments and H are stable, as demonstrated by the formation of short Si islands similar to those obtained from a 350°C anneal process.

Scaling this down to the single P atom case, it should be possible to create a single-dimer pattern, adsorb one PH_3 molecule, remove a minimal number of H atoms around it, and thus drive adsorption into a more deterministic position. A number of other potential applications of this process can be imagined, including a double-doping process, to boost the P density past the 0.25 ML limit, and even low-temperature encapsulation using Patterned ALE to limit dopant segregation

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)
2: J. H. G. Owen, J. Ballard, J. N. Randall, J. Alexander, and J. R. Von Ehr *J. Vac. Sci. Technol.* B **29** 06F201 (2011)