Atomic Precision Advanced Manufacturing for Ultraprecise 2D Bipolar Devices

J. H. G. Owen, R. Santini, E. Fuchs and J. N. Randall
Zyvex Labs LLC, 1301 N. Plano Rd, Richardson, TX 75081, USA.

J. P. Mendez, X. Gao, D. Mamaluy and S. Misra
Sandia National Laboratories, Albuqerque, NM 87123

Atomic Precision Advanced Manufacturing (APAM)[1], the ability to fabricate 2D atomic-scale devices such as the 'single-atom transistor' [2] and dopant patch array devices [3] via the placement of *n*-type dopants such as P and As in single planes of Si(001) is being extended to bipolar devices. While the direct Gr.III equivalents of the Gr.V hydride precursors are not stable at room temperature, we have been using halide precursors, BCl_3 and $AlCl_3$ [4].

In this work, we demonstrate the ability to form bipolar atomic-scale devices using BCl_3 to place B and PH_3 to place P using a H mask. The process involves sequential patterning, dosing and incorporation steps for each dopant. The P parts of the device are patterned, dosed and incorporated first, then the surface is repassivated, and a second round of patterning is performed for the B parts. The second round of patterning must be aligned with atomic precision to the P parts. as shown in Fig.1.

Our goal is to develop the ability to produce a new class of bipolar devices with a number of advantages, including a significantly improved gain-bandwidth product, low-noise operation and cryogenic operation. An example of a pn junction device pattern after incorporation of both B and P dopants, but before burial of the complete device, is shown in Fig. 1.

To help understand the operation of these 2D bipolar devices, we leverage Sandia's open-source, TCAD (Technology Computer Aided Design) device simulator, Charon [5], and expand its capability to first understand previously published results on diborane-based 2D p-n junctions [6], as shown in Fig. 2. Once established, Charon modeling will be used to design device dimensions in the proposed bipolar devices.

(1) Bussmann, E. *et al.* Atomic - Precision Advanced Manufacturing for Si Quantum Computing. *MRS Bull.* **2021**, *46*, 1–9.
(2) Fuechsle, M. *et al.* A Single-Atom Transistor. *Nat Nano* **2012**, *7*, 242–246.
(3) Wang, X. *et al.* Atomic-Scale Control of Tunneling in Donor-Based Devices. *Commun. Phys.* **2020**, *3*, 82.
(4) Dwyer, K. J. *et al.* Area-selective deposition and B delta-doping of Si(100) with BCl_3; Radue, M. S. *et al.* $AlCl_3$-Dosed Si(100)-2x1: Adsorbates, Chlorinated Al Chains, and Incorporated Al. arxiv **(2021).**
(5) Gao, X. *et al*, Analytic band-to-trap tunneling model including band offset for heterojunction devices, J. Appl. Phys. **125**, 054503 (2019).
(6) Škereň, T. *et al.* Bipolar Device Fabrication Using a Scanning Tunnelling Microscope. *Nat. Electron.* **2020**, *3*, 524–530.

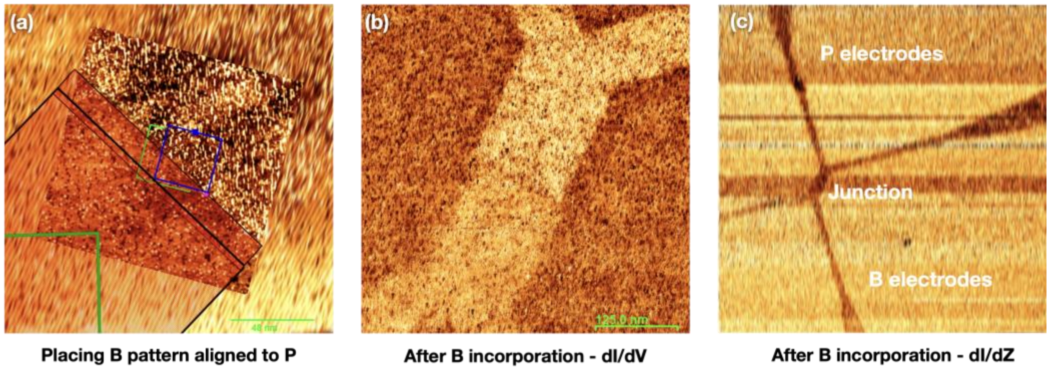

Fig. 1: (a): Aligning B pattern (red) to existing incorporated P electrode. (b) p-n junction after B patterning, dosing and incorporation. (c) Complete pn junction device.

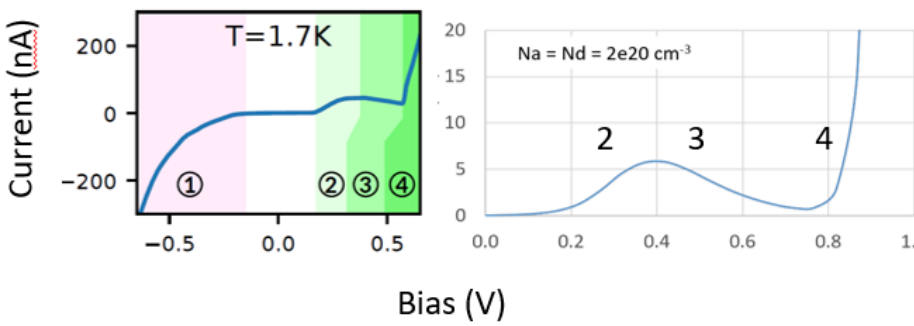

Fig. 2: Current-voltage characteristics of a p-n tunnel diode fabricated using STM lithography (left, from Ref. 6), and simulated as 4 nm thick layers of the same lateral dimensions (right). The numbers call out the tunneling (2), negative differential conductance (3) and thermionic emission (4) regimes.

This material is based upon work supported by the U.S. Department of Energy, Office of Science, Advanced Manufacturing Office, under Award Number DE-SC0020817. Sandia National Laboratories is managed and operated by NTESS under DOE NNSA contract DE-NA0003525.