Silicene Ribbons: Synthesis, Electronic and Geometric Structure at the Atomic Scale

A. Costine [1], Z. Gai [2], and P. Reinke [1] #

[1] *Department of Materials Science and Engineering, University of Virginia, 385 McCormick Road, Charlottesville, VA 22904*

[2] *Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, Oak Ridge, TN 37831*

[#] Author for correspondence: Petra Reinke pr6e@virginia.edu

Silicene is a 2D material which poses significant challenges in synthesis and device integration but offers unique electronic properties which are not yet fully understood. Challenges remain in silicene synthesis on non-metallic substrates and the control of buckling. The degree of in-plane buckling is tied to the emergence of a Dirac point and intriguing quantum phases have been predicted. [1-4] In our previous work we discovered a new pathway to silicene synthesis using h-$MoSi_2$ (0001) surfaces as templates, [5] and we present here the formation of silicene nanoribbons on the same surface, and measure their geometric and electronic structure with STM and STS at 77 K. Our work promises a new pathway to create silicene layers and nanoribbons with molecular beam epitaxy directly on silicon wafers.

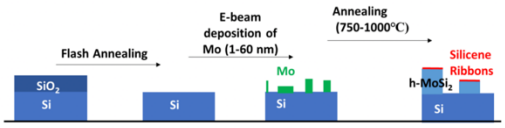

Figure 1: Schematics of synthesis method used for silicene nano-ribbons.

The h-$MoSi_2$ (0001) crystallites are synthesized on Si(100) by deposition of a thin Mo film with electron beam evaporation, and subsequent annealing to form well-defined crystallites with 15 - 120 nm in diameter. Nanoribbons cover the entire surface for all "flat top" silicide crystallites with (0001) surfaces. Several surface reconstructions present intermediate superstructures, and are precursors for the nanoribbons. The STM images in Fig. 2 illustrate the geometric structure of the nanoribbons which are 1.8 nm in width and separated by a distinct groove of roughly a single atomic row in width. Models of the nanoribbon's geometric structure will be discussed. The atoms located at the ribbon edge appear brighter which is likely due to density of states (DOS) modulation by edge states. Characteristic defects are seen in the ribbons and express identical STM. The average DOS (dI/dV) measured with STS is indicative of a Dirac type electronic signature with a V-type dip around E_F, and the position dependent DOS across the ribbons allows to identify the Dirac type regions. We will discuss all aspects of electronic and geometric structure of the nanoribbons including electronic confinement, and localized Dirac type signatures. In addition, point defects, and long range deformations induced by strain are addressed and inform our structural models.

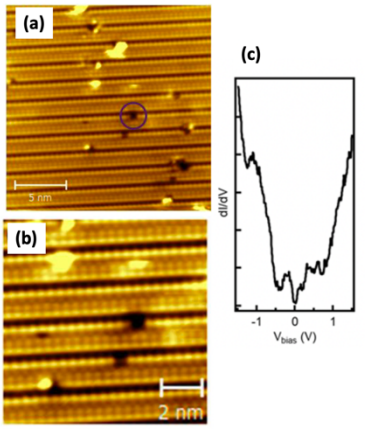

Figure 2: Ribbon-silicene on h-$MoSi_2$ crystallites (a) 20×20 nm empty state image (V_B = +1.5 V), (b) 10×10 nm zoom-in of the empty state image (V_B = +1.5 V), All images are at I_t = 0.1 nA. (c) average STS spectra across a ribbon.

[1] C. Grazianetti et al.. ACS Nano **11**, 3376-3382 (2017). [2] C.-C. Liu et al.. Physical Review Letters **107**, 076802 (2011). [3] A. Molle et al. Chemical Society Reviews **47**, 6370-6387 (2018). [4] H. J. W. Zandvliet. Nano Today **9**, 691-694 (2014). [5] C. Volders et al. Nano Letters **17**, 299-307 (2017).