

## Buckling of epitaxial silicene from Si 2p photoelectron diffraction experiments

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### Introduction

As the counterpart of graphene, silicene is an atom-thick honeycomb layer of silicon. Different to graphene, however, it is considered to be stable in its slightly buckled form [1,2]. While two-dimensional silicene is discussed only theoretically, previously, silicene ribbons formed on the Ag(110) surface have been well characterized by surface science techniques [3,4]. In yet unpublished work, we demonstrate that two-dimensional silicene forms spontaneously on the surface of zirconium diboride, ZrB<sub>2</sub>(0001), grown on Si (111) wafers [5]. Determined by the epitaxial relation with the substrate, scanning tunnelling microscopy (STM) images reveal the  $\sqrt{3} \times \sqrt{3}$  structural motif.

### Experimental

Surface-sensitive Si 2p core-level photoelectron spectroscopy has been performed at BL18A using a photon energy of 130 eV. A high resolution of better than 130 meV is obtained by employing third-order light. Samples are prepared by annealing at a temperature of about 800 °C *in situ* such that the native oxide is removed.

### Results

The Si 2p spectrum obtained at normal emission is shown in Fig. 1(A). As quantified by a peak fitting, the spectrum is composed of three components in a ratio of about 2:3:1, labeled A, B and C that proof the existence of Si ad-atoms in three distinct chemical states. This ratio is consistent with a structure model derived from the STM images where Si<sub>A</sub> atoms are located at hollow sites of the hexagonal Zr lattice, Si<sub>B</sub> atoms at intermediate positions between top and bridge sites, and Si<sub>C</sub> atoms on top of Zr atoms. When varying the polar photoelectron emission angle  $\theta$  with respect to normal, perpendicular to the Si-Si nearest-neighbor direction, the intensity ratios A/B and C/B remain constant up to  $\theta=60^\circ$  (Fig. 1(B)), while along the nearest-neighbor direction, A/B decreases by about 30 % indicating diffraction of Si<sub>A</sub> photoelectrons on Si<sub>B</sub> atoms. This shows that electron-rich Si<sub>A</sub> atoms are in a lower position than Si<sub>B</sub> atoms providing decisive experimental evidence for an atomic scale buckling of the silicene layer which is imprinted by interactions with the diboride substrate.

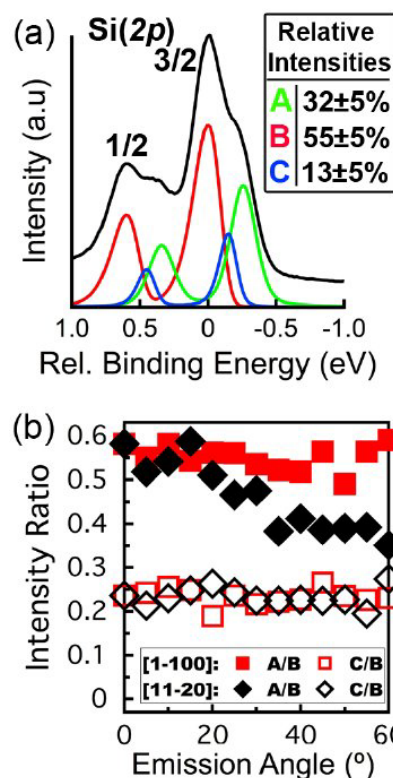


Fig. 1: (a) Si 2p photoelectron spectrum in normal emission. The inset shows a table containing the intensities of three chemical states obtained by a peak fitting procedure. (b) Intensity ratios A/B and C/B as a function of the polar photoelectron emission angle  $\theta$ , along the two high-symmetry directions.

### References

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