	Experiment title: Structure of epitaxial silicene on diboride thin films	**Experiment number**: HC-1160
Beamline: ID03	**Date of experiment**: from: 23-04-2014 to: 29-04-2014	**Date of report**: 22-08-2014
Shifts: 18	**Local contact(s)**: Francesco Carla	*Received at ESRF:*

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Report:

Graphene is probably the hottest material currently being investigated, but other 2-dimensional materials are also of interest. Silicon is right below carbon in the periodic table, but its orbitals do not hybridize as easily into sp^2 as carbon. Although it is difficult to form, freestanding silicene has been predicted to be stable [1]. Compared to carbon, the silicene layer is expected to be more buckled and, depending on the amount of buckling and its lattice constant, silicene may exhibit a range of electronic properties. Freestanding silicene has not been made up to now, but epitaxial silicene sheets have been found on Ag(110) [2], Ag(111) [3] and on zirconium diboride (ZrB_2) [4]. The aim of this experiment was to determine the structure of silicene on ZrB_2

A silicene layer was prepared at the ESRF in the ID3 UHV chamber by annealing a sample of zirconium diboride on a silicon substrate at 800^{o}C. Several shifts were used to find the optimum sample preparation and measurement conditions. The intensity of the (0.5 0.5 0.3) reflection of the (2x2) reconstructed silicene was monitored to obtain an indication of the surface coverage and after 2.5 hours an optimum had been reached. A large dataset was subsequently measured (173 non-equivalent reflections), containing fractional-order reflections as well as integer-order reflections. The data has been fully processed (see figure), but a feasible model that fits this data has not yet been found.

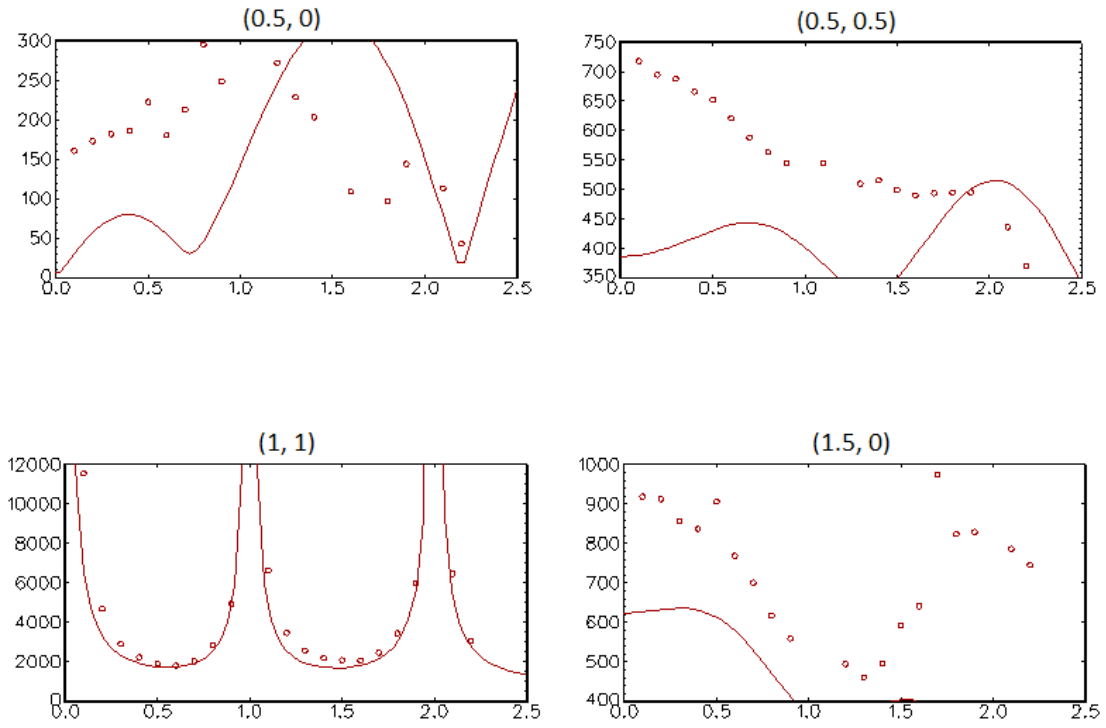

Figure 1 Some of the obtained data (dots) with a fit using the model from C-C Lee et al. [1] (line). The vertical axis depicts the measured structure factor, the horizontal axis shows the l-value, indicated on top are the (h, k) of the measured CTR.

C-C Lee et al. [5] proposed a structure for silicene on ZrB_2 where the topmost Zr monolayer is situated slightly shifted with respect to the bulk positons and the silicene itself is slightly buckled. This configuration seems to be incorrect as it does not account for the trends observed in the fractional order data (see figure). Efforts to fit the data with only the first Zr monolayer and the silicene layer as movable atoms did not yield a credible explanation for the measured data. Therefore, currently the focus is on including the subsequent boron layer as a movable layer.

In conclusion this was a successful experiment in which a good data set for the silicene-ZrB_2 system has been obtained. Data analysis is in progress and has already shown that existing models do not fit the data.

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[5] Lee, C. C.; Fleurence, A.; Friedlein, R.; Yamada-Takamura, Y.; Ozaki, T., *First-principles study on competing phases of silicene: Effect of substrate and strain*. *Phys. Rev. B* **2013,** *88* (16), 10