ESRF	Experiment title: **Atomic structure of a silicon single layer on Ag(111) and Ag(110) surfaces forming a graphene-like structure : a characterization by SXRD.**	**Experiment number**: SI-2026
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Names and affiliations of applicants (* indicates experimentalists):

(*) **Dr. AUFRAY Bernard** / CINaM / Campus Luminy, Marseille, France

(*) **Dr. BARBIER Antoine** / C.E.A./Saclay, Saclay, France

(*) **Prof. LELAY Guy** / Université Aix-Marseille, France

(*) **Dr. DE PADOVA Paola** / CNR, Rome, Italy

Experimental Report:

The experiment aimed at determining the atomic structure of one monolayer of Si deposited on Ag(111) and Ag(110). A perfect silicon monolayer arranged within a honeycomb lattice which covers the whole scanned area was previously observed in laboratory conditions. In the case of Ag(111) this surface arangement is accompagned by a $(2\sqrt{3}\times 2\sqrt{3})R30°$ superstructure as determined by LEED patterns. In order to cross check the presence of the expected reconstruction the presence of a LEED equipement, as it is the case on BM25, was very important.

Because on both faces (110) and (111), the atomic structure of one Si single layer looks like *silicene* (the counterpart of graphene for silicon) it was of prime importance to confirm and to know precisely the Si atomic structure. Especially it is very important to determine the exact distance between two Si atoms as well as the corrugation between the two Si sub-lattices since these values are closely linked to the nature of the silicon hybridization (pure sp^2 or mixed sp^2-sp^3). Furthermore the knowledge of the Si-Ag distance would be a good hint of the Ag substrate role. Indeed, if it is only a catalyst which favors the formation of the *silicene* layer, the atomic structures on both faces will be very close in terms of distance and corrugation.

To fulfill the experiment a home made Joule effect Si evaporator was installed in the UHV chamber of the surface interface grazing incidence X-ray diffraction setup of BM25. This kind of evaporator allows evaporating the deposition of Si layers of ultra-high purity. The clean Ag(111) could be prepared in good UHV conditions and sharp LEED patterns could be obtained (figure 1). The single crystal was of adequate quality with sharp diffraction peaks and a mosaic spread limited to about 0.03°.

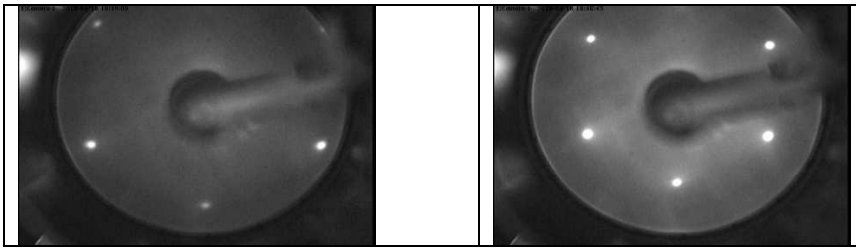

Figure 1: Sharp LEED patterns of the single cristalline Ag(111) surface as prepared during the experiment for primary electron energies of 69eV (left) and 140eV (right).

After extensive evaporator outgasing, a first deposition attempt of Si, in our usual laboratory conditions, during several hours lead to surface contamination with a negligible deposited Si thickness as check by specular X-ray reflectivity. The surface was cleaned and reprepared.

A second evaporation with higher evaporation conditions lead to a 3 monolayer thick Si layer as measured by specular X-ray diffraction. For such a thickness no clear LEED pattern could be observed and extensive in and out of plane exploration of reciprocal space showed only noisy spectra with parasitic peaks that could not be indexed within a realistic structure.

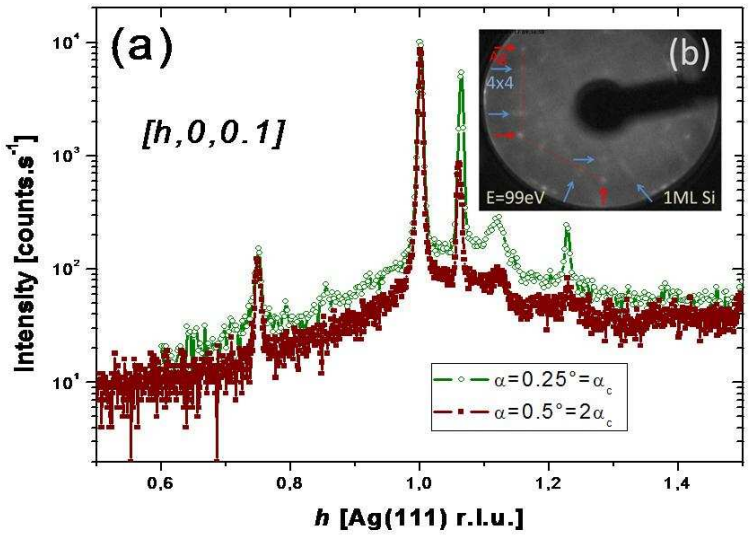

Figure 2:
For a 1 ML thick Si deposit on Ag(111):

(a) Scan along the [h,0,0.1] reciprocal space direction using critical incidence angle α_c and $2\alpha_c$.

(b) Corresponding LEED pattern showing a feint (4x4) reconstruction along with unresolved structures and high background.

The next surface preparation allowed realizing the expected 1ML thick Si monolayer on Ag(111). The thickness could be checked by reflectivity. The structure appeared to be of a feint (4×4) type and not $(2\sqrt{3}\times2\sqrt{3})R30°$ (or maybe some residual $(2\sqrt{3}\times2\sqrt{3})R30°$ could be included in the fuzzy patterns) . The high background and presence of other unresolved features in LEED (figure 2b) is confirmed in reciprocal space by extra peaks, high background and a mosaic spread as large as 0.5°. The reconstruction signal is exhalted in critical incidence condition indicating a top surface location (figure 2a). Reciprocal space exploration only revealed a total of 4 well resolved reconstruction peaks within high background which is fairly insufficiant to settle a clear cristalligraphic determination of the surface structure. The structure is understood as small (4×4) reconstructed domains within a rather desorganized layer.

Unfortunately further surface preparation could not be performed because of a leak on the evaporator.

The beamline and the setup showed to be well adapted to the topic allowing preparing high quality surfaces and adlayers. Variation around the known laboratory conditions in terms of sample – evaporator distance and actual sample temperature are likely to have prevented the preparation of the expected sample. More laboratory work is necessary to understand the conditions which favor the (4×4) and $(2\sqrt{3}\times2\sqrt{3})R30°$ structures. The Si thickness appears are being not the only critical parameter in the preparation of well organized layers.