Silicene formation on the Ag/Ni(111) surface

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Silicene, a silicon analogue of graphene, has attracted increasing attention during the past decade. The first theoretical prediction of the possible stability of a single sheet of Si and its band structure calculation is attributed to a 1994 paper by Takeda and Shiraishi [1] and experimentally silicene is first synthesized by Le Lay's group on the Ag surfaces [2,3]. As a counterpart of graphene and other two-dimensional materials vast studies of silicene on the atomic structure, electronic states, and the crystal growth had been conducted. Silicene is not only a new class of material for a topological insulator but it has a potential use for electronic and optoelectronic devices. Therefore controlling nucleation and growth of silicene will become a key technology for academic and industrial applications.

Because silicene can be grown on Ag surfaces in an UHV, modification of Ag sheets by means of heteroepitaxial growth on a lattice-mismatched substrate would be a possible route for controlling the silicene growth. Therefore we studied thin Ag overlayers grown on the Ni(111) surface, forming nano-sized moiré patterns in the Ag(111) surface and we would expect that the silicene growth is

affected by this moiré structure. We explored Ag thickness of 1-3 ML and temperature between RT and 473 K, and Si coverage up to 0.5 ML.

Figure 1 shows a typical STM image of silicene precursor formed on a 1 ML-Ag at 473 K. Moiré pattern can be recognized as periodic depressions on the surface, and its periodicity is $\sqrt{52} \times \sqrt{52}R13.9^{\circ}$ referring to the substrate Ni(111) unit cell [4]. The reacted region is depressed and apparently influenced by the periodic moiré pattern. In the reacted region local periodic structures with an atomic size can be recognized but they are not larger than a few unit cells.

By increasing Ag coverage to 3 ML, deposited Si is condensed to form silicene domains as shown in Fig. 2. These domains are quite similar to the previous observation [4] and 4×4 and $\sqrt{13}\times\sqrt{13}R13.9$ along with the dot structure are stabilized. Periodic moiré pattern is diminished around the reacted region although the initial surface had a moiré pattern. (not shown) This means that the moiré pattern affect the initial silicene nucleation for 1 ML-Ag but it does not play a major role for the silicene growth for thicker Ag films such as 3 ML.

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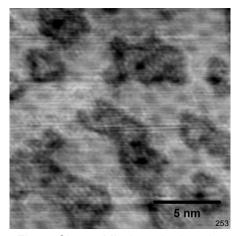


Fig. 1. Si 0.25 ML deposited on the Ag-1ML/Ni(111) surface

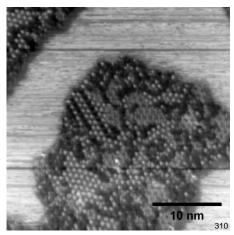


Fig. 2. Si 0.25 ML deposited on the Ag-3ML/Ni(111) surface