Crystal Phase Engineering of Silicene on Ag(111) by Molecular Beam Epitaxy Via Interface Engineering

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The debut of graphene-like two dimensional (2D) silicon, i.e. Silicene, in the past decade has opened the path for a variety of potential applications in the field of like nanoelectronics, energy and nano-optics. Although the silicene fabrication process is well established in the literature, few existing bottlenecks need to be vanquished to preserve and transfer their peculiar properties to devices. First, the monolayer silicene that is grown on pristine Ag(111) by Molecular Beam Epitaxy (MBE) appears as a mixture of 4×4, $\sqrt{13} \times \sqrt{13}$ R13˚ type-I and II, and other reconstructions. Second, when multilayer silicene is realized by piling additional atomic silicene layers on the first monolayer, the silicene superstructures show single $\sqrt{3} \times \sqrt{3}$R30˚ reconstructions but are with multiple rotational domains.[1,2]

A possible and viable solution to address these issues is the substrate modification. Indeed in our recent work, we showed that 2D silicene-stanene heterostructure is an appealing way to tailor the Xenes growth.[3,4] In this work, inspired by the silicene-stanene heterostructure concept, we will present in detail the interface engineering of Ag(111) substrate that we pioneered with complete convergence between theoretical *ab- initio* calculation and experimental dataset. On the Sn engineered Ag(111) substrates we are able to select single phase silicene on demand for both mono and multilayer silicene. On one hand, we demonstrate that when the growth template is Ag_2Sn-Ag(111) , silicene superstructures show single phase 4×4 reconstruction. On the other hand, when the template is modified as Sn-Ag_2Sn-Ag(111) by varying the Sn coverage, $\sqrt{3} \times \sqrt{3}$ R30˚ silicene phase was found to get stable even at low coverage. Equally interesting are the domains of multilayer silicene realized on these Sn engineered Ag(111) surfaces which show single orientation of $\sqrt{3} \times \sqrt{3}$ R30˚ silicene superstructures. All these outcomes be presented and discussed in detail with various *in-situ* and *ex- situ* characterizations and in terms of theoretical studies.

References

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