Crystal Phase Engineering of Silicene
by Sn-modified Ag(111)

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The synthesis of silicene by direct growth on silver is characterized by the formation of multiple phases and domains, posing severe constraints on the spatial charge conduction towards a technological transfer of silicene to electronic transport devices. Here we engineer the silicene/silver interface by two schemes, namely, either through decoration by Sn atoms, forming an Ag_2Sn surface alloy, or by forming a silicene-stanene heterostructure with stanene buffering the substrate [1]. Whereas in both cases Raman spectra confirm the typical features as expected from silicene, by electron diffraction we observe that a very well-ordered single-phase 4×4 monolayer silicene is stabilized by the decorated surface, while the buffered interface exhibits a sharp √3×√3 phase at all silicon coverages. Both interfaces also stabilize the ordered growth of a √3×√3 phase in the multilayer range, featuring a single rotational domain. Theoretical ab initio models are used to investigate low-buckled silicene phases (4×4 and a competing √13×√13 one) and various √3×√3 structures, supporting the experimental findings. This study provides new and promising technology routes to manipulate the silicene structure by controlled phase selection and single-crystal silicene growth on a wafer-scale.

References

[1]   Daya Sagar Dhungana et al., Adv. Funct. Mater. 31 (2021) 2102797

Figures
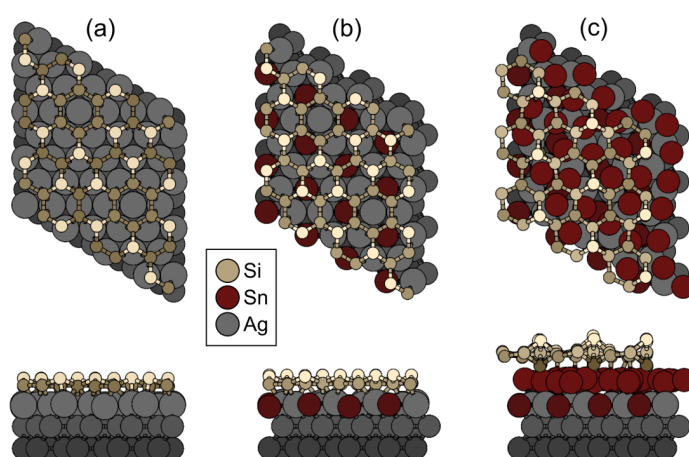
Figure 1: Structural models of silicene grown on (a) Ag(111), (b) $SnAg_2$/Ag(111), and (c) stanene/$SnAg_2$/Ag(111).