Structure and Growth Mechanisms of Silicene Layers †

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Abstract:
The synthesis of bidimensional silicon films that would display electronic properties analog to those of graphene attracts today a considerable interest, in particular for applications in microelectronics. Since the theoretical prediction of the metastability of free-standing silicene, a buckled hexagonal Si plane presenting a Dirac cone in its electronic structure, silicene layers have been claimed to grow on various substrates such as MoS_2, ZrB_2, graphite or Ir(111). Up to now, most of the studies have been performed on Ag(110) and Ag(111) substrates where hexagonal structures presenting electronic band structure expected from silicene have been deduced from scanning tunneling microscopy (STM) and photoemission (ARPES) experiments.
Using scanning tunneling microscopy, grazing incidence X-ray diffraction, and DFT calculations, we have real-time followed up the growth of silicene single layers and multilayers on silver substrates and elucidated the structure of several phases. Whereas the silicene single layers grown on Ag(111) truly correspond to hexagonal buckled planes, Si/Ag(110) forms alternate rows of Si pentamers. We evidence an unexpected growth mechanism. During Si deposition, Ag atoms are expelled from the substrate, leading to missing rows on Ag(110), and to the formation of inserted Si domains on Ag(111).
On this surface, further growth leads to the formation of thick Si islands, instead of multilayer silicene, that are partially inserted in the Ag substrate: during their formation, Ag atoms are expelled from the substrate. Nearly half of them form the honeycomb chain triangle Ag/Si structure on top of the islands, the other half intercalate between the remaining single silicene layer and the substrate, as evidenced by STM. This is the signature of an unforeseen "surfacting competition" between Ag and silicene: the silver surface remains covered by silicene during this additional Ag growth, and the surface of Si islands remains covered by Ag atoms during Si growth.

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