Model of √3x√3 phases of silicene and its multilayers

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Abstract Silicene, a monolayer of silicon atoms arranged in a honeycomb structure, received an enormous interest for being a candidate two-dimensional material that could bring the exotic electronic structure of graphene to the well-developed silicon-based technology.[1-2] Experiments have shown that silicene synthesized on Ag substrates can acquire various reconstructions. In particular, structures having √3x√3 reconstruction have been frequently observed but yet poorly understood.[3-5] Here we provide a compelling high-resolution angle resolved photoemission (ARPES) study together with first-principles calculations and scanning tunneling microscopy (STM), which unambiguously prove the existence of a particular two-dimensional arrangement of silicon atoms that, gives rise to two different phases with √3x√3 periodicity. We propose a new mechanism for explaining the spontaneous and consequential formation of both phases. We show that unlike others the √3x√3 reconstruction is intrinsic and is not dictated by the interaction with the Ag substrate.[3] The proposed mechanism opens the path to the understanding of multilayer silicon.[3,5]

References

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