Model of $\sqrt{3}x\sqrt{3}$ 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.\cite{1,2} Experiments have shown that silicene synthesized on Ag substrates can acquire various reconstructions. In particular, structures having $\sqrt{3}x\sqrt{3}$ reconstruction have been frequently observed but yet poorly understood.\cite{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 $\sqrt{3}x\sqrt{3}$ periodicity. We propose a new mechanism for explaining the spontaneous and consequential formation of both phases. We show that unlike others the $\sqrt{3}x\sqrt{3}$ reconstruction is intrinsic and is not dictated by the interaction with the Ag substrate.\cite{3} The proposed mechanism opens the path to the understanding of multilayer silicon.\cite{3,5}

References