Anomalous growth of 2D epitaxial Si

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The initially promising deposition of Si on a metallic substrate such as Ag(111) has revealed unexpected growth modes where Si is inserted at the beginning of the growth in the first atomic plane of the substrate. In order to rationalize this anomalous growth mode, we develop an out-of-equilibrium description of a lattice-based epitaxial growth model, which growth dynamics are analyzed via kinetic Monte-Carlo simulations. This model incorporates several effects revealed by the experiments such as the intermixing between Si and Ag, and surface effects. It is parametrized thanks to an approach in which we show that relatively precise estimates of energy barriers can be deduced by meticulous analysis of atomic microscopy images. This analysis enables us to reproduce both qualitatively and quantitatively the anomalous growth patterns of Si on Ag(111). We show that the dynamics results in two modes, a classical sub-monolayer growth mode at low temperature, and an inserted growth mode at higher temperatures, where the deposited Si atoms insert in the first layer of the substrate by replacing Ag atoms. Furthermore, we reproduce the nonstandard Λ shape of the experimental plot of the island density as a function of temperature, with a shift in island density variation during the transition between the submonoloyer and inserted growth modes.

As regards the growth of Si on graphene, experiments revealed the possible growth of large silicene flakes over 100nm in size, surrounded by a ring and coexisting with three-dimensional dendritic islands, 3 to 4 monolayers thick. This anomalous growth mode is not described by conventional epitaxial growth models. Again, we have derived a model incorporating the essential atomic processes at step edges and between different layers. We solved the far-from-equilibrium many-body dynamics by kinetic Monte Carlo simulations. In particular, we have revisited the classical modeling of dewetting thermodynamics, incorporating adsorption energies on the different islands layers. We have been able to reproduce the flakes growth mode, main morphological characteristics, densities, but also the long-time evolution resulting in non-coalescent dendritic pyramids for large deposits. The

ringed 2D flakes appear as a metastable state resulting from the dewetting dynamics of a system evolving towards more energetically stable dendritic pyramids. The present modeling and understanding of the mechanisms at work in this system are the first building blocks for future systematic studies aimed at controlling and growing large silicene flake.