Kinetic Monte Carlo Simulation of Epitaxal Growth of 2D Si

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The epitaxial growth of 2D Si on Ag (111) [1] and double layer Graphene/SiC substrates [2] reveals unexpected growth modes. On Ag (111), Si atoms can insert into the substrate surface, forming inserted islands at high temperature (T >=300k). On the double layer Graphene/SiC, Si forms three distinct types of islands: 3D fractal islands, 2D hexagonal flakes with a surrounding ring, and 2D irregular flakes with a surrounding ring.

To rationalize these anomalous growth modes, we develop an out-of-equilibrium description of a lattice-based epitaxial growth model, which growth dynamics are analyzed via kinetic Monte-Carlo simulations where the process rate depends on the type and number of nearest neighbor atoms. For the Ag(111) case, we use a pseudo-morphic lattice and introduce intermixing effects between Si and Ag atoms. In the double layer Graphene/SiC scenario, a height-dependent adsorption effect is incorporated to reconcile contradictions observed in experiments.

Through meticulous analysis of atomic microscopy images and island density fitting, we successfully reproduce both qualitatively and quantitatively the anomalous growth patterns of Si on Ag (111) [3]. While our research on double layer Graphene/SiC is ongoing, we have made significant strides in explaining a portion of this intriguing phenomenon.

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[2] Zouhour Ben Jabra, Mathieu Abel, Filippo Fabbri, Jean-Noel Aqua, Mathieu Koudia, Adrien Michon, Paola Castrucci, Antoine Ronda, Holger Vach, Maurizio De Crescenzi, and Isabelle Berbezier. Van der Waals Heteroepitaxy of Air-Stable Quasi-Free-Standing Silicene Layers on CVD Epitaxial Graphene/6H-SiC. ACS Nano 2022 16 (4), 5920-5931 DOI:10.1021/acsnano.1c11122

[3] Kejian Wang , Geoffroy Prévot & Jean-Noël Aqua. Anomalous intralayer growth of epitaxial Si on Ag(111). Scientific Reports | (2024) 14:2401 | https://doi.org/10.1038/s41598-024-52348-1