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Atomistic view in the initial stages of growth of epitaxial graphene on metal substrates¹

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For both fundamental studies and potential development of graphene electronics, it is pressing to search for reliable methods for mass production of quality graphene. Epitaxial growth of graphene on catalytic metal substrates combined with post-growth transfer has become a promising route towards this goal [1,2]. However, to better control the quality and yield of graphene, a comprehensive understanding of the growth kinetics is essential. In particular, how the carbon atoms adsorbed on the metal surface (or dissolved into the metal) meet to nucleate into stable carbon islands will greatly influence both the growth rate and quality of larger carbon entities such as graphene sheets. In this talk, we first show that the delicate competition between carbon-carbon bonding and carbon-metal bonding dictates the initial nucleation sites of graphene on metal surfaces [3]. These results are discussed in connection with the experimental findings that on Ir(111) and Ru(0001) substrates graphene nucleates from the step edges [4,5]. We also predict that on Cu(111) nucleation should take place everywhere on a terrace [3]. Next we study larger carbon clusters on Cu(111) and explicitly compare the stability of linear and compact structures. We find that the linear carbon “nanoarches” are more stable than compact islands consisting of up to 13 carbon atoms, and these nanoarched structures may serve as the missing bridge between carbon dimers and larger graphene nanodomains. Based on this improved understanding of the atomistic rate processes involved, we propose a few kinetic pathways that may lead to better growth control of bilayer graphene and graphene nanoribbons as elemental building blocks for developing graphene electronics.

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