Abstract Submitted
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Atomistic mechanisms for bilayer growth of graphene on metal substrates[1] WEI CHEN, PING CUI, WENGUANG ZHU, University of Science and Technology of China, EFTHIMIOS KAXIRAS, Harvard University, YANFEI GAO, University of Tennessee, ZHENYU ZHANG, University of Science and Technology of China — Epitaxial growth on metal substrates has been shown to be the most powerful approach in producing large-scale high-quality monolayer graphene, yet it remains a major challenge to realize uniform bilayer graphene growth. Here we carry out a comparative study of the atomistic mechanisms for bilayer graphene growth on the (111) surfaces of Cu and Ni, using multi-scale approaches combining first-principles calculations and rate equation analysis. We first show that the relatively weak graphene-Cu interaction enhances the lateral diffusion and effective nucleation of C atoms underneath the graphene island, thereby making it more feasible to grow bilayer graphene on Cu. In contrast, the stronger graphene-Ni interaction suppresses the lateral mobility and dimerization of C atoms underneath the graphene, making it unlikely to achieve controlled growth of bilayer graphene on Ni. We then determine the critical graphene island size beyond which nucleation of the second layer will take place. Intriguingly, the critical size exhibits an effective inverse "Ehrlich-Schwoebel barrier" effect. These findings allow us to propose a novel alternating growth scheme to realize mass production of bilayer graphene.

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