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**Suppression of Grain Boundaries in Graphene Growth on Superstructured Mn-Cu(111) Surface**[1] WEI CHEN, Univ. of Tennessee, Univ. of Sci. & Tech. of China, HUA CHEN, Univ. of Tennessee, Univ. of Texas at Austin, HAIPING LAN, PING CUI, Univ. of Sci. & Tech. of China, TIM SCHULZE, Univ. of Tennessee, WENGUANG ZHU, Univ. of Tennessee, Oak Ridge National Lab, ZHENYU ZHANG, Univ. of Sci. & Tech. of China, Harvard University — A standing obstacle in epitaxial graphene growth on metal substrates is the prevalence of undesirable grain boundaries (GB) that severely degrade the electronic, transport and mechanical properties of graphene. Employing density functional theory calculations, we demonstrate that the inherent multi-orientational degeneracy of the graphene islands on Cu(111) is the underlying reason for the prevalence of GB. We propose a possible solution, by invoking a functionalized Cu(111) surface to lift the orientational degeneracy of graphene islands and consequently suppress the creation of GB. We have identified the candidate substrate—a superstructured Mn-Cu(111) alloyed surface, which is experimentally achievable and ensures a single orientation for the graphene islands. The proposed approach promises to drastically improve the quality of epitaxial graphene without compromising on efficiency and yield.

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