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# Phase Field Crystal Modeling of Grain Boundary Structures and Growth in Polycrystalline Graphene

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Abstract: A key challenge in large-scale graphene fabrication and application is controlling the grain boundaries (GBs) in polycrystalline graphene grown by chemical vapor deposition (CVD). Here, we adopt a phase field crystal (PFC) model to predict equilibrium structures as well as the dynamic formation of GBs in CVD-grown graphene. The results demonstrate that GBs consisting of clustered 5|7|5|7 dislocation dipoles, as predicted from the conventional coincidence site lattice (CSL) theory, are not energetically favorable, and should be replaced by dispersed 5|7 dislocations predicted from the PFC model. The PFC modeling also demonstrates possible routes of engineering GBs in two-dimensional (2D) materials by controlling grain orientations in pre-patterned growing seeds and suggests a simple geometric rule that explains the predominant existence of curved grain boundaries in graphene. As a prominent example of potential applications of our method, we show how to grow triple-junction-free polycrystalline graphene that exhibits enhanced mechanical strength and defy the traditional Hall-Petch relation.

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