Accepted Manuscript

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

Jiaoyan Li , Bo Ni , Teng Zhang , Huajian Gao

PII: S0022-5096(17)30794-9
DOI: 10.1016/j.jmps.2017.12.013
Reference: MPS 3255

To appear in: *Journal of the Mechanics and Physics of Solids*

Received date: 7 September 2017
Revised date: 11 December 2017
Accepted date: 29 December 2017

Please cite this article as: Jiaoyan Li , Bo Ni , Teng Zhang , Huajian Gao , Phase Field Crystal Modeling of Grain Boundary Structures and Growth in Polycrystalline Graphene, *Journal of the Mechanics and Physics of Solids* (2017), doi: 10.1016/j.jmps.2017.12.013

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

Jiaoyan Li[1], *Bo Ni*[1], *Teng Zhang*[2], *and Huajian Gao*[1,*]

[1]School of Engineering, Brown University, Providence, RI 02912, USA

[2]Department of Mechanical and Aerospace Engineering, Syracuse University, Syracuse, NY 13244, USA

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.

[*]Corresponding author. E-mail: Huajian_Gao@brown.edu (H. Gao)