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Theory and hierarchical calculations of [0001] tilt grain boundaries in graphene JOHAN CARLSSON, Accelrys Ltd, Cambridge (UK) and Fritz-Haber-Institut, D-14195, Berlin, LUCA M. GHIRINGHELLI, Fritz-Haber-Institut der MPG, D-14195, Berlin, A. FASOLINO, Institute for Molecules and Materials, Radboud University Nijmegen, The Netherlands — Several experiments have revealed the presence of grain boundaries in graphene that may change its electronic and elastic properties. Here, we present a general theory for the structure of [0001] tilt grain boundaries in graphene based on the coincidence site lattice (CSL) theory. We show that the CSL theory uniquely classifies the grain boundaries in terms of the misorientation angle θ and periodicity d. The structure and formation energy of a large set of grain boundaries generated by the CSL theory for $0^\circ < \theta < 60^\circ$ (up to 15 608 atoms) were optimized by a hierarchical methodology and validated by density functional calculations. We find that low-energy grain boundaries in graphene can be identified as dislocation arrays. In contrast to three-dimensional materials, the strain created by the grain boundary can be released via out-of-plane distortions that imply to an effective attractive interaction between dislocation cores. This leads to a (secondary) minimum structure at $\theta = 32.2^\circ$, where the grain boundary is made of a flat zigzag array of only 5– and 7–rings. We discuss the importance of these findings for the interpretation of recent experimental results.

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