

MULTISCALE MODELING OF POLYCRYSTALLINE GRAPHENE

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Defects and grain boundaries greatly influence the properties of graphene but modeling their formation is challenging due to the multiple length and time scales involved. We extend the Phase field crystal (PFC) approach [1] to quantitative modeling of defected graphene microstructures. We assess four PFC models by studying grain boundary structures and their formation energies. We compare PFC results to density functional theory (DFT) and molecular dynamics (MD). The one-mode PFC model is found to produce realistic defect topologies, whereas the three-mode model predicts quantitatively correct grain boundary energies. [2] PFC models are able to capture the dynamics of large (poly)crystalline systems on diffusive time scales while retaining atomic resolution. We exploit these multiscale characteristics by demonstrating the preparation of large polycrystalline PFC graphene systems whose sizes and formation time scales are beyond the reach of DFT calculations and MD simulations, respectively. We use these systems as the starting point of MD simulations for investigating the heat and charge transport properties of polycrystalline graphene.

- [1] K.R. Elder, M. Katakowski, M. Haataja and M. Grant, Physical Review Letters 88 (2002) 245701.
- [2] P. Hirvonen, M.M. Ervasti, Z. Fan, M. Jalalvand, M. Seymour, S.M. Vaez Allaei, N. Provatas, A. Harju, K. Elder and T. Ala-Nissila, Physical Review B 94 (2016) 035414.