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Multiscale modeling of polycrystalline graphene PETRI HIRVONEN, MIKKO ERVASTI, ZHEYONG FAN, Aalto University, MORTEZA JALALVAND, University of Tehran, KHATEREH AZIZI, Aalto University; University of Tehran, MATTHEW SEYMOUR, McGill University, S. MEHDI VAEZ ALLAEI, University of Tehran, NIKOLAS PROVATAS, McGill University, ARI HARJU, Aalto University, KEN ELDER, Oakland University, TAPIO ALA-NISSILA, Aalto University; Brown University — 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 [Elder et al., Phys. Rev. Lett. 88, 245701 (2002)] 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. [Hirvonen et al., Phys. Rev. B 94, 035414 (2016)] 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.

Petri Hirvonen
Aalto University

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