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Comparison of Interatomic Potentials for Modeling Defects in Graphene Using Molecular Dynamics

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Abstract. In this work, we tested the ability of classical interatomic potentials to describe the energy characteristics of defects of various dimensionality in graphene crystals. Brenner's Reactive Empirical Bond Order potentials (second generation REBO, AIREBO, AIREBO-M), Tersoff potentials, as well as BOP and LCBOP potentials were considered. The data obtained in this work using the molecular dynamics method was compared with literature data obtained using the density functional theory. It is noted that when modeling point and linear defects, the potentials of the REBO family and the LCBOP potential demonstrate the best agreement with the literature data. For modeling pseudo-graphene crystals, the best fit is demonstrated by the Tersoff B-N-C potential, which shows slightly overestimated energy values for linear and point defects, but most accurately describes the geometry of the crystal lattice. The potential of BOP demonstrates its inability to correctly model defect configurations with high densities of eight-member defect rings. When simulating four-member carbon defect rings, most potentials exhibit distortions in the crystal lattice that are not observed in the density functional theory calculations.

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