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Development of an Analytical Bond Order Potential for C-H-Cu Systems

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Abstract— Carbon nanostructures (nanotubes, nanoribbons, and ordered sheets) continue to attract widespread attention due to their unique properties and use in next-generation electronics. The performance of these materials is critically affected by the defects. Unfortunately, the detailed mechanisms of defect formation during nanostructure growth are either unknown or very poorly characterized. Direct molecular dynamics simulation of nanostructure growth provides powerful means to study defect formation from theories without any prior assumptions regarding the defect formation mechanisms. Such simulations, however, are extremely difficult to achieve requiring the interatomic potential used in the simulations to be transferrable, at least qualitatively, to any configurations that can possibly form on the growth surface. Here we describe our recent efforts on developing an analytical order potential for C-H-Cu systems aiming at enabling direct molecular dynamics simulations of graphene growth on Cu substrate through chemical reactions (i.e., the vapor fluxes are composed of various C-H molecules).

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