Molecular Dynamics Study on Wetting of Wrinkled Graphene

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Abstract

Graphene is a rapidly rising two-dimensional material and vast research efforts have been focused on its extraordinary mechanical, electrical, thermal, and optical properties [1]. The wettability of graphene, which is an important property regarding to its application as surface engineering, has not been fully studied. Most previous studies are focused on flat graphene sheet which revealed that graphene is a weekly hydrophobic material with a water contact angle (WCA) measured within the range of 87°-127°. But actually, wrinkling is ubiquitous existing in two-dimensional graphene due to thermodynamically unstable status. The graphene films widely used in electronics, energy storage, composites and biomedicine are all crumpled [2]. Thus, it has great significance to understand the wetting behavior of water on wrinkled graphene, which may have potential applications in novel graphene based conductive coatings and electrodes that are superhydrophobic and tunable wettability.

In this study, we characterize the wetting properties of graphene by performing classical molecular dynamics (MD) simulations using the large-scale atomic/molecular massively parallel simulator (LAMMPS). Firstly, a model of a flat graphene with a nanodroplet above is established and the WCA of the flat graphene is obtained from the droplet density profiles using atom trajectories. Then, another two models are built as graphene under uniaxial or biaxial compression. A pattern of parallel ridges forms in plane of graphene by compressing in one direction and a more complex crumpling pattern with ridges and vertices is formed by biaxial compression. The values of WCA of these two types involving wrinkled graphene with different compression magnitude are calculated.

In our simulation results, the WCA of flat graphene is about 95°, which is consistent with experiment result very well. As to the wrinkled graphene, WCA is larger than the flat one, which means that wrinkle could enhance the hydrophobic property. Furthermore, WCA increases with the increasing of compression. A relation between mechanical and wettability property has been obtained, which may support the development and application of graphene as coating materials.

Keywords: Molecular dynamics, Wetting, Graphene, Wrinkled, Contact angle.

References

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