The microscopic deformation mechanism and energy dissipative mechanism of graphene foam materials

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Abstract

Recent experiments have shown that graphene foam materials exhibit a rubber-like constitutive behavior under uniaxial compression and a good energy dissipative capability under cyclic load. Coarse grain molecular dynamics simulations are carried out in this work in order to disclose the micro-mechanisms of the two phenomena. It is found that the rubber-like constitutive behavior is mainly attributed to the microstructure deformation, rearrangement and compaction in three stages, respectively. The elastic deformation of microstructures leads to the initial linear behavior of the graphene foam material. Microstructure rearrangement, including bending, self-folding and flake-rotation, should be responsible for the second stage with a good performance of deformation but with a low bearing capacity. Microstructure compaction leads to a high bearing capacity at the last stage. As for the micro-mechanism of energy dissipation, the typical stress-strain relationship found in experiments under large-strain loading-unloading and small-strain cyclic load are first reproduced by coarse grain molecular dynamics simulations, respectively. Based on the microstructure analysis, three major energy dissipative mechanisms in the scale of flakes, i.e., rippling, sliding and impacting, are uncovered. The influencing effects of the cycle number, strain magnitude and loading rate on energy dissipation are further investigated. It is found that the much higher dissipative energy in the first loading cycle is essentially due to the drastic flake rearrangement, which decreases to a smaller one in the subsequent cycles. In addition, the dissipative energy increases almost linearly with the strain magnitude in the first cycle, while it increases with a reduced slope in the subsequent cycles due to the stacking structures formed by flake assembly. For a given strain magnitude, the dissipative energy will be enhanced as the loading rate increases. All the results would deepen our understanding on the energy absorptive and dissipative mechanisms of graphene foams and should be helpful for the development of novel multi-functional graphene-based composites.

Keywords

Graphene foam material, rubber-like behavior, energy dissipative mechanism, microstructural evolution, micro-mechanism,

Reference

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