Type of structural element (graphene flake) on the mechanical properties of crumpled graphene: insight from molecular dynamics

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Recently, considerable attention has been paid to graphene nanostructures with new architecture, for example, to 3D graphene consisting of monolayers of wrinkled and crumpled graphene. Such carbon structures exhibit high tensile strength, have low weight, and can be easily functionalized by other elements. The primary goal of the present work is to define the effect of structural morphologies (monodisperse and polydisperse structures) on the mechanical properties of crumpled graphene using molecular dynamics simulations.

For monodisperse structure, all graphene flakes are small with the same shape and size, while for polydisperse structure flakes are very different with the number of atoms from 80 to 500 and variously rippled. All the simulations are conducted using the LAMMPS package with the AIREBO potential [1]. Periodic boundary conditions are applied along all dimensions. The Nose–Hoover thermostat was used to control the system temperature. To study mechanical properties of the considered samples, uniaxial tension is applied.

It is revealed, that crumpled graphene with monodisperse morphology has an almost two times bigger critical strain and tensile strength. In case of monodisperse morphology, more homogeneous structure is obtained during initial compression, since this shape and size of flakes allowed to obtain much more sp^3-bonds on their edges. However, the polydisperse structure of crumpled graphene is more isotropic, which is also an important advantage [2].

REFERENCES

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