Molecular dynamics study of the Cu/graphene and Ni/graphene composite under tension

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Abstract

To date, studies of the interaction of graphene with nanoparticles of various metals, such as copper, aluminum, nickel, titanium, etc., are being actively conducted. Graphene-metal structures are very interesting since they can demonstrate not only individual properties of graphene or metal, but will have qualitatively new complex properties. In this work, the deformation behaviour of composites based on graphene and Ni (or Cu) nanoparticles is studied by molecular dynamics. Composite is a crumpled graphene filled with Ni (Cu) nanoparticles of small size is obtained by hydrostatic compression at 1000 K.

The simulation results show that the Cu/graphene composite demonstrates better mechanical properties under tension than the composite with Ni nanoparticles. The highest value of the Young's modulus was obtained for the Cu/graphene composite (E = 284 GPa), since for this structure, due to the melting of Cu nanoparticles during high-temperature hydrostatic compression, the formation of new chemical bonds between the individual elements of the composite is easier. For Ni/graphene composite the Young's modulus is E = 235 GPa and the strength of the composite lower. However, it is important to note that both composites withstand large deformation under uniaxial tension and show both ductility and strength. The results obtained contribute to a better understanding of the fabrication processes, deformation behaviour, and mechanical properties of composites based on graphene and metal nanoparticles.