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The effect of graphene oxide nanosheet size and initial temperature on the mechanical and thermal properties of epoxy/graphene oxide structure using molecular dynamics simulation

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Abstract

This study investigated the effect of graphene oxide nanosheet (GON) size, and initial temperature (IT) on the mechanical properties (MP), and thermal properties (TP) of epoxy/GO structure using the molecular dynamics simulation (MDS). The stress-strain curve, Young's modulus (YM), the atomic order parameter (AOP), and the thermal expansion coefficient (length changes) of simulated structures were studied. The results show that increasing GO length improved the simulated structure's MP. As the GO length increased to 20Å, YM increased from 2.96 to 4.04GPa. Furthermore, by changing the length of simulated GONs, the amount of van der Waals force applied from each plate to the atoms present in the atomic matrix changes; so, as the size of GONs increased, AOP in the structures increased. Increasing the size of simulated GONs reduced the expansion of structure. This behavior showed higher thermal resistance, and consequently, atomic stability in the samples as the nanosheets became larger. In general, increasing IT led to increasing the atomic fluctuations. Consequently, the attraction energy among the atoms decreased by increasing the atomic oscillations. Therefore, increasing the IT to 350K led to a decrease in the YM of samples. Therefore, the MP of samples was reduced by increasing IT. Moreover, increasing IT decreased the amount of AOP in the samples. Finally, increasing IT increased the oscillation amplitude, and the distance of atoms from each other, which caused the expansion in the structure under study.