

Abstract

In this study, firstly, the graphene foam (GF) and polymer composite structure have been produced in the laboratory. Raman spectroscopy and scanning electron microscope (SEM) images characterized the synthesized GFs structures. Then, using the results of SEM images, the polymer matrix and GF structure were simulated in the nanoscale by a new four-step method. Particularly, four types of GF with increasing mass density and decreasing porosity and three groups of polymers with different chain unit sizes have been investigated. Mechanical and thermal properties of GFs and polymer matrices have been calculated using molecular dynamics (MD) and developed codes. By simulating the tensile test by introducing different strain rates to the GFs, it was found that changes in the strain rate do not affect the value of their Young modulus. Non-equilibrium molecular dynamics (NEMD) method has been used to compute the thermal properties of GF groups and polymer matrices. The thermal conductivity (TC) amount has been investigated by defining the hot source and the cold sink on both sides of the simulation boxes. Thermoelastic properties were calculated as temperature dependent for all GF groups by MD platforms. Generally, GFs' coefficient of thermal expansion (CTE) increased with temperature and porosity percentage. By calculating the specific heat of GFs, it was discovered that the specific heat also increased as the temperature increased. By a slight change in mass density and percentage of porosity at the nanometer scale, significant changes occur in the Young modulus of GF samples, resulting in their mechanical and thermoelastic properties acting differently from each other. Furthermore, it was found that GFs with the highest porosity have the most significant specific surface area. The specific surface area decreases with decreasing porosity percentage. On the other hand, the TC of the PDMS matrix increased with the increasing number of chain units. Also, by reducing the percentage of porosity, GF's TC has improved significantly. It was found that two main factors affect the TC of GFs, the first factor being the number of foam connections and the second one being the presence

of defects. In fact, the groups of GF in this study with different connectivity and various defects show different TC values. Therefore, we can argue that the mass density (or pore size) and the number of defects in determining the TC almost cover each other. The effect of different potentials and the similarity of their results with experimental works were also investigated. It should be mentioned that although the simulated GFs with Tersoff potential have shown higher TC, the accuracy of Airebo potential was more elevated in considering all interatomic interactions in carbon atoms, so, Airebo's potential is preferred. Overall, GF's network structure creates an excellent TC while being lightweight and low-density, causing satisfactory heat transfer. A multiscale method has been used to calculate the mechanical and thermal properties of GF/Polymer composites. By considering repeating unit cells (RUC), for the first time, mechanics of structure genome (MSG) based on Carrera unified formulation (CUF) was used to calculate the effective properties of GF/polymer composites by using the properties of their components in the MD platform. Tensile testing highlights the effect of GF drying percentage on the composite and shows a 138% and 48% increase in the Young modulus and tensile strength compared to the neat polymer. After comparing the effective mechanical properties of composites with the multiscale method used in the present study, the method's accuracy was ensured. It was uncovered that the composite consisting of GF with the highest density and the lowest porosity has the lowest CTE. Also, the heat capacity of the composite depends not only on the heat capacity of the components but also on the Young modulus, CTE, and geometry. The effective TC of the composite is increased by expanding the chains of the polymer matrix and decreasing the porosity of the three-dimensional network of GF. It must be mentioned that GF's density can directly control the volume percentage of reinforcement in the composite. In GFs, due to lack of agglomeration, the TC increases with increasing volume fraction.