Computational Study of the Mechanical Properties of Epoxy Resins and Carbon Nanotubes Doped with SiO_2 Nanoparticles

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Composite materials have been widely used due to their high mechanical properties and great resistance, generally proven in the aeronautical industry. However, it is sought to place reinforcements of other types of particles to be useful in applications of interest such as medicine, specifically for the design of materials for a foot prosthesis. It is for this reason, that in this work a study of the mechanical properties of polymeric nanocomposites was carried out from computational techniques of semiclassical mechanics and neural networks. The GROMACS 2019.2 software and the CHARMM36 force field were used to perform molecular dynamics simulations in polymer nanocomposite systems with different polymer chain lengths and number of carbon nanotubes. In addition, a Neural Network was used to predict the mechanical properties of the nanocomposites. The most relevant results of this study include the determination of the relative energies between the studied species, which allowed us to understand at the molecular level the effectiveness of the nanocomposite assembly as a fundamental reason for the improvement that the mechanical properties could have. In addition, it was possible to obtain inferences regarding the proportions of the three studied polymer sizes suggested by the neural network, which allowed predicting the mechanical properties of the nanocomposites with an accuracy of less than 10%. Finally, it was possible to study the percentage change in the Poissons ratio according to the distortions suffered by the lengths parallel to the direction of application of the external pressure, which made it possible to compare the responses of the different systems as the size of the pipe increased. polymer or the number of Carbon Nanotubes was increased. In conclusion, this study demonstrates the utility of molecular dynamics simulations and neural networks to predict the mechanical properties of polymer nanocomposites and improve their use in industrial or scientific applications.

