عنوان مقاله:

Molecular Dynamics Simulation of Functional and Hybrid Epoxy Based Nanocomposites

محل انتشار:

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خلاصه مقاله:

In this paper, the effects of filler type, filler content, functionalization, and the use of hybrid nanofillers on nanocomposite mechanical properties are investigated. For this purpose, several nanocomposite types were modeled and analyzed using Molecular Dynamics method. In the molecular dynamic's simulations, crosslinking and nanofiller/matrix interface effects were considered. First thermoset epoxy resin with 75% crosslinking ratio between DGEBA resin and DETA hardener were simulated to determine pure resin properties. Then nanocomposites consisting of single walled carbon nanotubes (SWCNT), nanographene (NG), carbon nanoparticle (CNP), functional single walled carbon nanotubes (SWCNT-COOH), and functional nanographene (nanographene oxide) in thermoset epoxy were modeled and analyzed using Materials Studio software. In addition, filler weight fraction was increased from 2.5 to 10 percent in order to investigate the effects of filler content on nanocomposite mechanical properties. The results indicated that increasing nanofiller weight fraction from 0 to 7.5% resulted in an increase in nanocomposite elastic modulus for three non-functional nanofiller types. Moreover, functionalization improving nanocomposite properties as the highest increase in resin elastic modulus were obtained for the SWCNT-COOH reinforced epoxy for filler contents up to 7.5 weight percent. Also, agglomeration occurred at filler contents higher than 7.5 weight percent in the NG/epoxy, SWCNT/epoxy nanocomposites. Finally, the use of hybrid nanofillers reduced/prevented agglomeration for filler contents even up to 10 weight percent.

کلمات کلیدی:

Molecular Dynamics, Mechanical properties, Nanocomposite, functional nanofiller, Hybrid