8th. World Congress on Computational Mechanics (WCCM8)
5th. European Congress on Computational Methods in Applied Sciences and Engineering (ECCOMAS 2008)
June 30 – July 5, 2008
Venice, Italy

Simulation of nano-particulate epoxy composites considering cross-links

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Key Words: *Nanocomposites, Molecular dynamics, Micromechanics, Multi-scale, Cross-links*

ABSTRACT

Recently, various types of multi-functional composites with nanoparticles have attracted many researchers in advanced materials science. When the size of materials decreases to nanometer scale, the ratio of its surface area to volume critically increases and enables unusual mechanical properties different from those of their macro-sized counter parts. As the ratio of area to volume is an important key factor to determine the mechanical properties in nanocomposites, the reinforcing effect of nanocomposites depends on the particle size of nanoparticles. But the relation between particle size and reinforcing effect is not fully identified and both positive and negative effects are reported in the experimental literatures[1,2]. As the special effects of interface exist in nanocomposites, simulation for confirming the effects of interface is needed. But molecular dynamics simulation which can exactly describe the interface effect is computationally expensive and not desirable in designing materials and in characterizing large scale simulation such as particles reinforced composites with particle size larger than 10nm. Conventional micromechanical method like Mori-Tanaka model does not contain the size effect of the interfaces[3]. Therefor micromechanical approach including interface size effect of nanocomposites is applied in the previous study[4]. But most of molecular dynamics simulations and related multi-scale analysis of nanocomposites are focused on the thermoplastic matrix-based composites and cross-linking effects of surrounding matrix were not considered. For example, in the case of molecular models of carbon nanotube reinforced epoxy resin composites in the previous study[5], both epoxy resin and curing agent were independently modelled and no direct cross-linking was considered. But the formation of adsorption layer critically affected by the entangled network of matrix polymers and the exclusion of cross-linking cannot exactly describes the real cured nanostructures of matrix and particle size effect at the particle-matrix interface.

Therefore, in the present study, reinforcing effect of cross-linked epoxy resin nanocomposites are studied by molecular dynamic simulation and micromechanics models. The molecular unit cell is constructed with cross-linked epoxy matrix and

alumia(Al_2O_3) nanoparticle. For cross-linked structures of matrix, Diglycidyl Ether of Bisphenol F(EPON862®) was chosen as epoxy unit monomer and curing agents Triethylenetetramine(TETA®). In order to characterize the reinforcing effects of nanoparticle, molecular dynamics simulation of pure cross-linked epoxy was accomplished. And the material properties of the simulation agree with those of the cross-linked epoxy experiments[6]. After identifying the material properties of cross-linked epoxy resin, nanocomposites of cross-linked matrix containing 5.5% of nano-particle is investigated and it showed maximum 70% increase of Young's modulus compared with pure epoxy. The molecular dynamics simulations for the size effect of nano-particles in nanocomposites under the same volume fraction are investigated. As size of particles becomes smaller, reinforcing effects of nanocomposites are more significant. In addition, multi-scale method using the effective interface model is applied to predict mechanical properties of nanocomposites.

	Results of simulation						Experiment [6]
Number of cross-linked epoxy	9	15	21	24	27	Epoxy	Epoxy
Diameter of particle [nm]	1.20	1.40	1.58	1.65	1.72	-	-
Young`s modulus [GPa]	5.80	5.63	5.27	4.88	4.51	3.36	3.43
Deviation	0.630	0.235	0.729	0.376	0.362	-	-

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