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Multi-scale analysis of nanoparticle reinforced composites : Scale bridging method for non-dilute concentration

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ABSTRACT

With the aid of advanced nano-scale manufacturing technology, nanoparticle reinforced composites have attracted many researchers for its promising properties[1,2]. It is generally known that the evolution of new characteristics of nanocomposites originates from the increased surface to volume ratio of nanoparticles which enables strong and sensitive interaction with surrounding matrix called interface effect. In order to verify the interface effect, several analytical approaches have been attempted using molecular dynamics and multi-scale analysis [3]. But the former results are based on the dilute distribution condition and particle-particle direct interactions were not considered both in molecular dyanmics and continuum micromechanics parts.

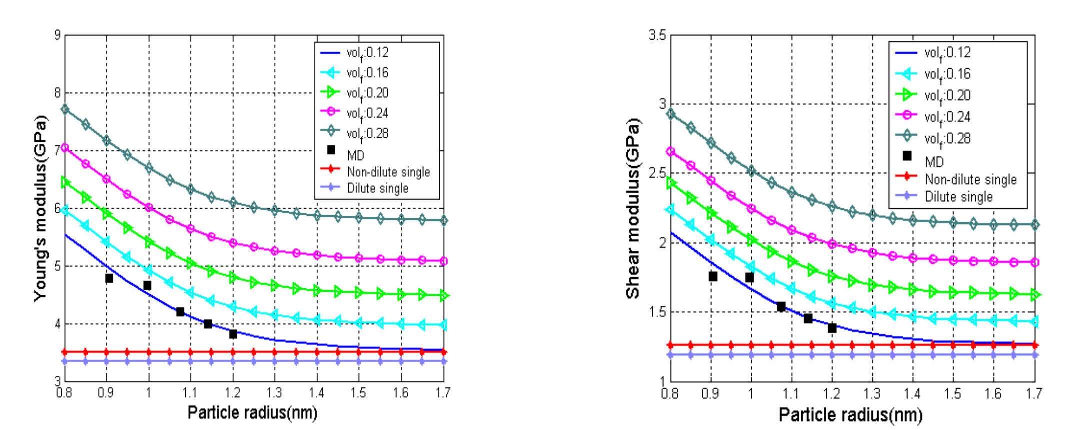
In this study, multi scale analysis of nanocomposites considering non-dilute particle concentration is developed thorough molecular dynamics simulations and continuum micromechanics. In molecular dynamics part, five sample sets having different particle sizes with the same volume fraction are considered as periodic unit cells to verify particle size effect of α-quartz/polyimide(BPDA-APB) nanocomposites. In constructing the unit cells, volume fraction of the nanoparticle is set to 12% which is enough high to narrow the particle-particle and particle-effective interface distance less than the non-bond cutoff radius of 9.5Å. All the simulations are implemented at 300K, 1bar using Andersen-Berendsen isobaric ensemble to obtain well equilibrated structures. Mechanical properties of nanocomposites are obtained from Parrinello-Rahman fluctuation method. Resultant elastic modulus obtained from molecular dynamics simulations are listed in Table I with the conventional single phase particle micromechanics estimations. As shown in Table I, both Young's and

Radius(Å)	E(Gpa)	G(Gpa)
9.06	4.78±0.21	1.76±0.08
9.97	4.66±0.10	1.74±0.04
10.74	4.20±0.53	1.54±0.20
11.41	3.99±0.26	1.45±0.11
12.01	3.81±0.22	1.38±0.09
Single phase (Non-dilute)	3.51	1.26
Mori-Tanaka (Dilute)	3.34	1.19

Table I : Elastic modulus of nanocomposites

shear modulus of nanocomposites increase as the particle size decreases and all the molecular dynamics results are higer than conventional single-phase micromechanics results.

Therefore, non-dilute periodic two-phase particle model[4] was used to describe particle-matrix interface as a second phase of particle. Expressing the eigen strain field of nanoparticle in terms of Fourier series expansions[5], effective elastic modulus of the systems were derived and rearranged with respect to the interface stiffness matrix. Assuming that the volume fraction of the interface is constant(consequently, thickness of the interface gradually increases), inteface stiffness matrix was implicitly calculated and converted into the continuous function of particle radius using least square approximation. Effective elastic modulus obatained from present multi-scale analysis are shown in Fig. 1 with the discrete molecular dynamics results. As can be seen in the discrete points(molecular dynamics results) and blue-colored solid curve, our suggested model follows very well the MD results and it shows the size effect of the nanocomposites under non-dilute distribution condition. Elastic modulus at different volume fractions were efficiently predicted by the present non-dilute multi-scale method.



(a) Young’s modulus (b) Shear modulus

Fig. 1 Elastic modulus of nanocomposites obtained from multi-scale analysis

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