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A study on the hierarchical multiscale modeling on polymer nanocomposites with elastoplastic behavior

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In this study, a hierarchical multiscale modeling approach to characterize the elastoplastic behavior of polymer nanocomposites is proposed through molecular dynamics simulations and a continuum nonlinear asymptotic homogenization method. The characterization of the condensed interphase zone between nanoparticle such as silica and carbon materials and polymer matrix is still an open issue. The interphase mechanical behavior is estimated by multiscale bridging method which has been employed to demonstrate many other related studies for mechanical problems.

Nonlinear mechanical behavior of polymer nanocomposites has been identified by molecular dynamics simulation. The elastoplastic mechanical behavior by using molecular dynamics simulation of polymer materials has been investigated in our previous study (*Yang et al.*, 2012). The stress-strain curve of polymer follows the Ludwik's model as shown in Fig. 1. The Ludwik's model is as follows:

$$\sigma_e = \sigma_Y + h(\varepsilon^p)^n \tag{1}$$

where σ_Y, h and n are the yield strength, strength coefficient, and hardening exponent, and σ_e and ε^p are the von Mises' effective stress and the effective plastic strain of the matrix, respectively. In this study, only small deformation is considered and nanoparticle is assumed to follow linear elastic model. The elastoplastic behavior of effective interphase will be considered by iterative inverse algorithm based on the nonlinear asymptotic homogenization method. The effective interphase is assumed to be a homogeneous and isotropic single phase.

Deformation field of macroscopic simple structure with periodic microstructures will be computed and demonstrated. From the microscopic homogenized tangential moduli, the macroscopic deformation field is computed where the microscopic self-equilibrium condition is satisfied. In order to do this kind of macro-scale analysis, Newton-Raphson iteration algorithm is employed for every loading step. In this study, this type of computational scheme is called the hierarchical multiscale modeling. In order to simplify the complex microscopic deformation behavior, proper orthogonal decomposition (POD) is employed for efficient extraction of microscopic behaviors.

It is too heavy computation to solve macroscopic equilibrium equation and microscopic equilibrium equation simultaneously. POD is very powerful mathematical tool for reduction of large data analysis. The proposed multiscale approach faciliates the analysis of polymer nanocomposites materials more practically.

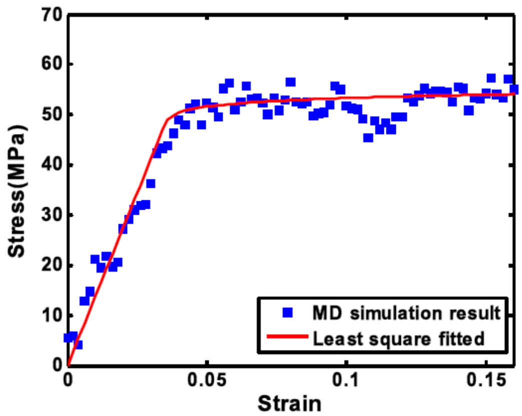

Figure 1. Stress-strain curve of pure PP matrix obtained from MD simulations at 200 K and 1 atm (*Yang et al.*, 2012).

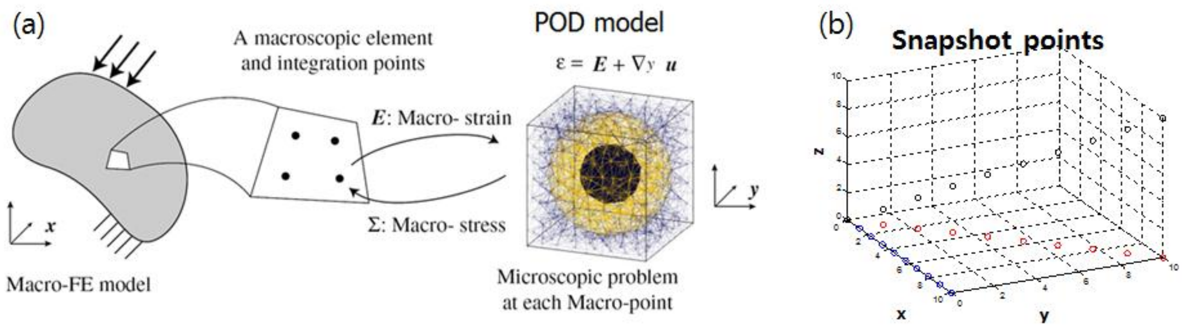

Figure 2. Schematic of hierarchical multiscale modeling. (a) Coupled mechanical problem of macroscopic equilibrium and microscopic equilibrium, and (b) Snapshot macroscopic strain points for construction of POD.

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