

Multiscale nanocomposites analysis and design considering MD model and filler geometric uncertainties

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In this study, statistical multiscale homogenization approach which reflects model inherent uncertainty of molecular dynamics (MD) and filler geometric uncertainty is proposed. In molecular dynamics approach, the initial ensemble velocities are randomly distributed by Boltzmann random distribution. However, nonlinear dynamics such as molecular dynamics are sensitive to the initial location and initial velocity. Therefore, MD model inherent uncertainty of predicting elastic moduli occurs due to randomness of initial velocity. MD model inherent uncertainty is reflected in this study. Meanwhile, filler dispersion is also a critical issue. However, molecular dynamics simulation is not easy to be applied to the multi-particulate nanocomposites system because of computational resource and computing time limitations. Therefore, multiscale approach from MD to continuum homogenization model has been developed and employed in this study. Geometric uncertainties of filler radius and filler location are considered in this study at continuum-scale level. The proposed statistical multiscale scheme could be employed in the design of polymer nanocomposites.

Keywords: Multiscale analysis, Statistical approach, Model uncertainty, Polymer nanocomposites, Molecular dynamics simulation