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Keynote Paper

Statistical Multiscale Approach on the Analysis and Design of Nanocomposites

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ABSTRACT

In this study, statistical multiscale approach reflecting MD model inherent uncertainty and filler geometric uncertainty is proposed. Molecular dynamics approach needs randomly distributed initial ensemble velocities such as Boltzmann random distribution. However, nonlinear dynamics simulation is very sensitive to the initial condition such as initial location and velocity. Therefore, MD model inherent uncertainty is a critical issue in predicting elastic properties and thermal characteristics and reliability-based analysis. Meanwhile, filler dispersion is also a critical issue in the process of polymer nanocomposites. Filler agglomeration from van der Waals interaction between reinforced fillers makes dispersion of fillers worse. In this study, an integrated multiscale analysis framework considering MD model inherent uncertainty and filler geometric uncertainty all together is proposed.

1. INTRODUCTION

Polymer nanocomposites have been widely used due to their weight advantage and multifunctionality. As the reinforced filler size in polymer nanocomposites decreases to nanometer scale, the surface-to-volume ratio of the fillers highly increases. For the analysis of filler size effect, molecular dynamics (MD) approach has been widely used. However, MD simulation needs high computational time and resources. Therefore, MD simulation is not appropriate for analyzing the reliability-based design approach and material/structure design optimization.

In manufacturing field, there are critical issues about filler dispersion in order to avoid filler agglomeration. As the degree of filler dispersion decreases, the overall physical properties are also degraded. For the reliable analysis of polymer nanocomposites, the manufacturing uncertainties should be considered in the analysis model. In this study, the statistical multiscale framework is proposed to cover the

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manufacturing uncertainties.

Meanwhile, there are model inherent uncertainties in MD analysis. Nonlinear dynamics simulation such as MD simulation is very sensitive to initial conditions such as initial position and velocities. Initial velocities are randomly determined by Boltzmann random distribution which satisfies the given unit cell temperature. Therefore, in spite of the same initial molecular morphologies, the predicted physical properties such as elastic modulus and thermal characteristics could be scattered due to randomness of initial velocities. Therefore, in this study, MD model inherent uncertainties are considered as well as manufacturing uncertainties.

2. Quantification of MD model inherent uncertainty

In this study, SiC/Epoxy polymer nanocomposites are considered and curing ratio of epoxy network is 61%. Filler volume fraction is fixed as 5.8% in three different unit cell model. Elastic modulus of polymer nanocomposites is predicted by Parrinello-Rahman fluctuation method (Cho 2011). In order to quantify the model inherent uncertainty, 32 trial MD simulations were conducted for each unit cell. Molecular unit cell structure is constructed as shown in Fig. 1 (a).

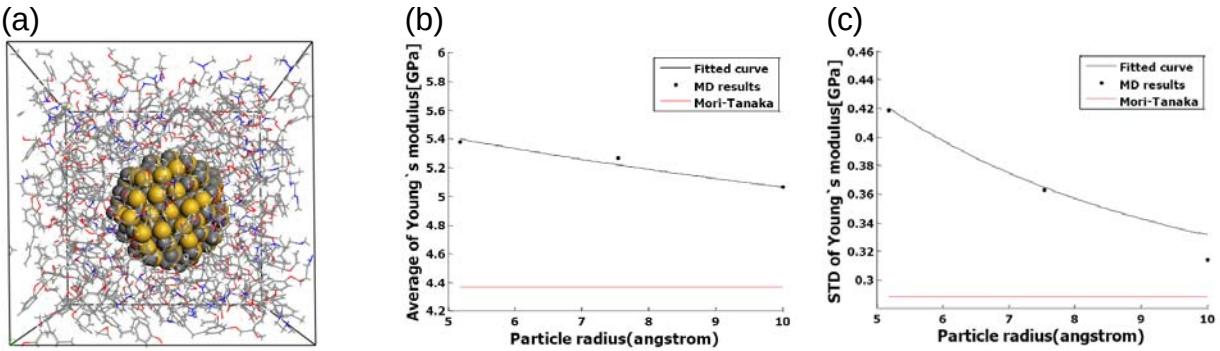

Fig. 1 Quantified MD model uncertainty about various radii: (a) molecular structure, (b) average, and (c) standard deviation.

As shown in Fig. 1 (b) and (c), both average and standard deviation of elastic properties show size effect. As shown in Fig. 1 (b), average of elastic constants converges to those of Mori-Tanaka solution because the surface-to-volume ratio of particle increases dramatically as particle radius decreases to nano-meter scale. Initial random seed assigned to allocate the initial temperature of individual atoms cause the deviation of the calculated elasticitic constants as shown in Eq. (1).

$$f(v) = \sqrt{\left(\frac{m}{2\pi kT}\right)^3} 4\pi v^2 \exp\left(-\frac{mv^2}{2kT}\right), \tag{1}$$

where m is atomic mass, k is Boltzmann constant, v is atomic velocity and T is absolute temperature of unit cell. As shown in Fig. 1 (c), standard deviation of elastic properties decreases as particle radius increases because the individual atoms effects are canceled out in computing the elastic stiffness of unit cell. 99.7 % confidence level (2σ range) of Young's modulus is (4.7, 6.2) GPa when the average of Young's modulus

is 5.4 GPa. The length of 99.7 % confidence level of Young's modulus divided by average is about 28 %.

3. Statistical multiscale analysis framework of polymer nanocomposites

3.1. Statistical multiscale analysis framework with MD model inherent uncertainty

In order to predict the probability density distribution of composite elastic properties about various radii, the statistical multiscale analysis framework is proposed. Fig. 2 shows an iterative inverse algorithm for predicting the probability density distribution of interphase elastic properties. Probability density distribution of matrix elastic properties is determined by molecular dynamics simulation. Overall elastic properties are computed by 3 phase multi-inclusion micromechanics model. This iterative inverse algorithm is computed repetitively until average and standard deviation of multi-inclusion model is the same as those of molecular dynamics model. From the predicted interphase elastic properties distribution, the composite elastic properties distribution could be predicted explicitly by multi-inclusion model.

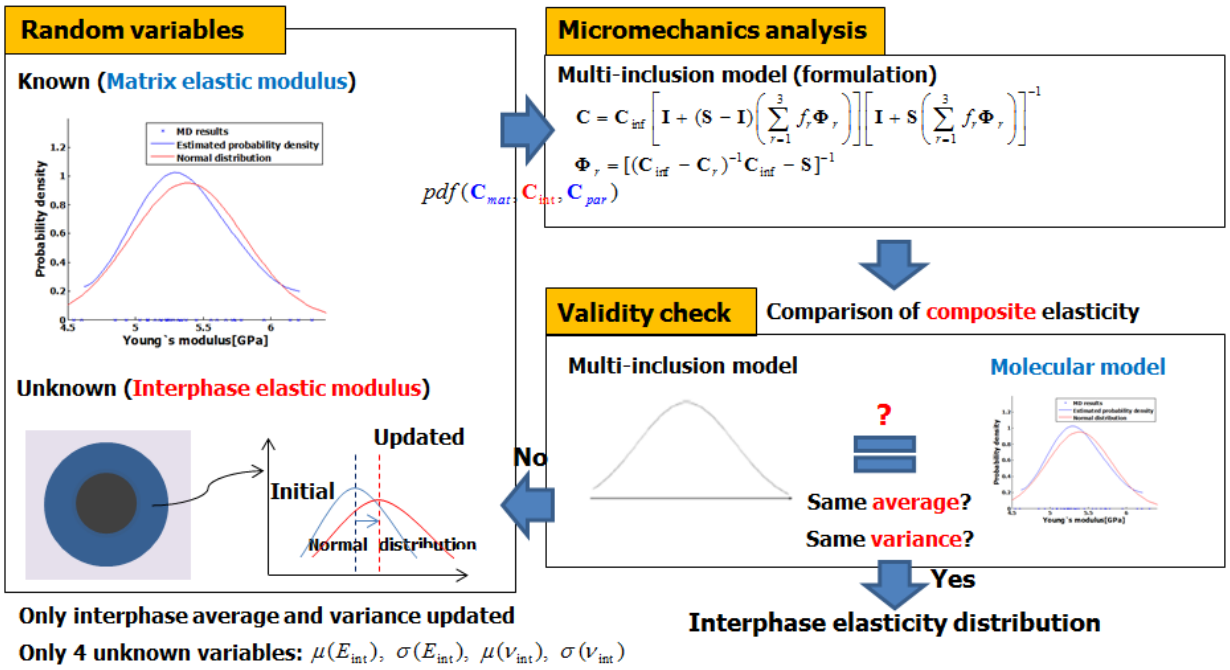

Fig. 2 Statistical multiscale framework for reflecting MD model inherent uncertainties

3.2. Integrated multiscale analysis framework with filler geometric uncertainties

In this study, filler size and location are accounted for filler geometric uncertainties. Filler radius distribution is assumed to follow normal distribution and filler location is uniformly randomly distributed. Elastic properties of continuum model are computed by asymptotic homogenization method (Cho 2011). In the representative volume element (RVE), about 30 reinforced particles are considered. 99.7% confidence level(2σ range) of filler radius is (5.5, 10)Å. Computed homogenized elastic properties distribution

shows the dominant effect of MD uncertainty. Without MD uncertainty, the length of 99.7 % confidence level for Young's modulus is about 1 GPa when the average of Young's modulus is 5.25 GPa. However, the length of 99.7 % confidence level for Young's modulus increases more than twice when MD uncertainty is accounted for additionally as shown in red line of Fig. 3.

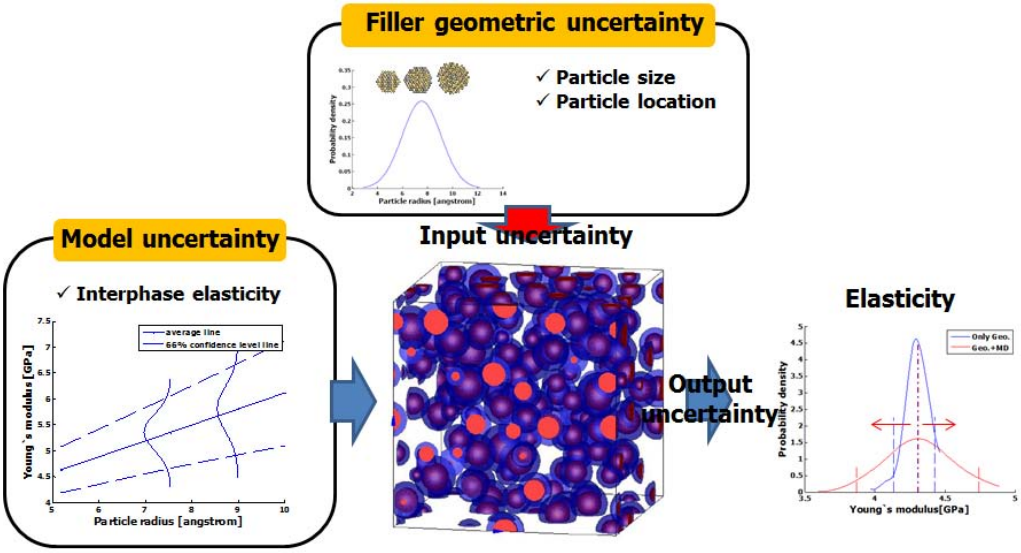

Fig. 3 Integrated multiscale analysis framework merging filler geometric uncertainty with MD model inherent uncertainty

4. Conclusion

In this study, an integrated statistical multiscale analysis framework is proposed. Statistical approach is essential to design polymer nanocomposite materials with reliability. In molecular dynamics model, there is an inherent uncertainty due to initial velocities of atoms which follows Boltzmann random velocity distribution. The contribution of MD uncertainty on homogenized elastic modulus was investigated as well as the effect of geometric uncertainty such as random filler size and filler location. The propagated MD uncertainty occurs to the substantial variation of homogenized elastic properties more than the case when the geometric uncertainty is accounted for only. The proposed statistical multiscale analysis could be applied to optimal design and reliability-based analysis. This proposed statistical multiscale framework could be extended to various simulation of thermo-mechanical behavior of nanocomposites such as thermoelastic problem and nonlinear mechanical problem. An extension of the proposed multiscale problem is currently in process.

REFERENCES

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