Statistical multiscale homogenization modelling of polymeric nanocomposites

Maenghyo Cho[1], Hyunseong Shin[2], Seongmin Chang[3], Seunghwa Yang[4], Suyoung Yu[5], and Byeng Dong Youn[6]

[1, 2, 3, 6] School of Mechanical and Aerospace Engineering, Seoul National University, Seoul 151-742, South Korea
[4] Department of Mechanical Engineering, Dong-A University, Busan 604-714, South Korea
[5] School of Mechanical Engineering, Kyungnam University, Changwon 631-701, South Korea
[1] mhcho@snu.ac.kr

Key Words: *Multiscale analysis, Statistical approach, Model uncertainty, Polymeric nanocomposites, Molecular dynamics simulation.*

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 at continuum-scale level. The proposed statistical multiscale scheme is applied to the design of polymer nanocomposites. Figure 1 shows the schematics to quantify interphase statistic elastic stiffness.

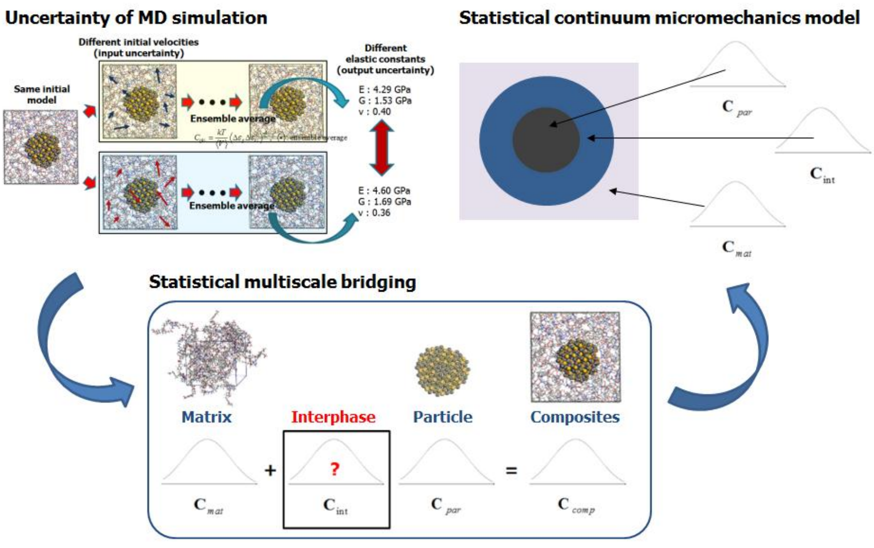

Figure 1. Schematics for characterization of interphase elastic modulus uncertainty.

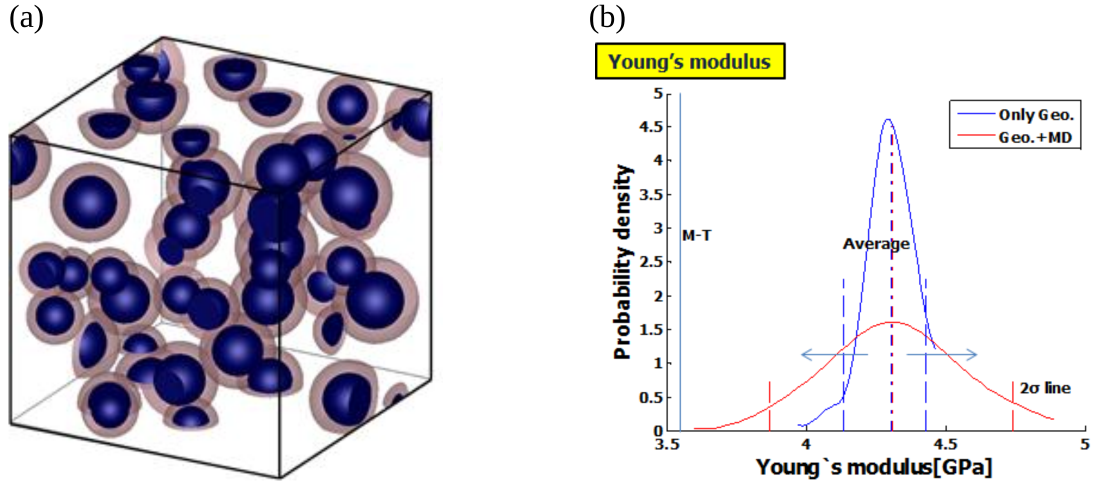

Figure 2. (a) Continuum model reflecting filler geometric uncertainties, and (b) Probability density distribution of Young's modulus.

Figure 2 (a) is the continuum model reflecting filler geometric uncertainties. Figure 2 (b) is the merged result of model uncertainty and filler geometric uncertainty. As the filler geometric uncertainty is considered, the probability density distribution of Young's modulus are more widely distributed and it is dispersed more than twice of that of geometric uncertainty only. Figure 2 (b) shows the dominant effect of model uncertainty. For the reliable estimation of stiffness and strength of the nanocomposites, continuum-based FE homogenization technique and micromechanics techniques are combined with Molecular dynamics simulation technique to extract nano scale particle filler interphase information. In the present study, within statistical approach, the multiscale analysis from molecular level to continuum level is proposed within computational homogenization method. The present approach can be extended to various reinforcing particles including graphene, CNT, metal, and semiconductive particles embedded in various polymer matrices.

REFERENCES

[1] M. Cho, S. Yang, S. Chang, and S. Yu, A study on the prediction of the mechanical properties of nanoparticulate composites using the homogenization method with the effective interface concept. *Int. J. Numer. Meth. Eng.*, Vol. 85, pp. 1564-1583, 2011.

[2] S. Yu, S. Yang, and M. Cho, Multi-scale modeling of cross-linked epoxy nanocomposites. *Polymer*, Vol. 50, pp. 945-952, 2009.

[3] H. Shin, S. Yang, S. Chang, S. Yu, and M. Cho, Multiscale homogenization modeling for thermal transport properties of polymer nanocomposites with Kapitza thermal resistance. *Polymer*, Vol. 54, pp. 1543-1554.

[4] M. P. Bendsoe, and N. Kikuchi, Generating optimal topologies in structural design using a homogenization method, *Comp. Meth. Appl. Mech. Eng.*, Vol. 71, pp. 197-224, 1988.

[5] J. M. Guedes, and N. Kikuchi, Preprocessing and postprocessing for materials based on the homogenization method with adaptive finite element methods, *Comp. Meth. Appl. Mech. Eng.*, Vol. 83, pp. 143-198, 1990.

[6] M. Parrinello, and A. Rahman, Strain fluctuations and elastic constants, *J. Chem. Phy.*, Vol. 76, pp. 2662-2666, 1982.