11th World Congress on Computational Mechanics (WCCM XI)
5th European Conference on Computational Mechanics (ECCM V)
6th European Conference on Computational Fluid Dynamics (ECFD VI)
July 20–25, 2014, Barcelona, Spain

STOCHASTIC MODELING OF INTERPHASE EFFECTS FOR NANOREINFORCED HETEROGENEOUS MATERIALS

Thinh LE, Johann GUILLEMINOT and Christian SOIZE

Université Paris-Est, Laboratoire Modélisation et Simulation Multi Échelle, MSME UMR 8208
CNRS, 5 bd Descartes, 77454 Marne-la-Vallée, France

Key words: *interphase; molecular dynamics; nanocomposite; polymer; probabilistic model; random fields.*

This paper is concerned with the multiscale analysis of nanoreinforced heterogeneous materials and more specifically, with the probabilistic modeling of interphase effects. The latter have been widely investigated (in a deterministic framework), either in an experimental setting (see [1], among others) or from a computational point of view (see e.g. [2] and the references therein). The aim of this work is twofold. First, we investigate, through molecular dynamics (MD) simulations performed on a nanoreinforced polymer, the local morphology (see Fig. 1) and the mechanical nonlinearities induced by the perturbation of the matrix phase surrounding the inclusion. The simulations allow typical results, such

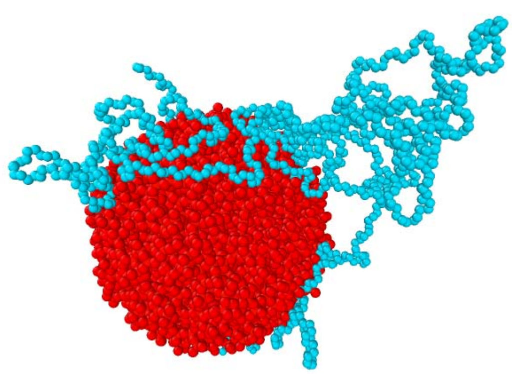

Figure 1: Simulation snapshot of a polymer chain near the nanoscopic inclusion.

as the exhibition of a reinforcing effect (see Fig. 2, left) or the local perturbation of the polymer density (see Fig. 2, right), to be recovered. Second, we make use of the aforementionned results in order to assess some stochastic features associated with random fields of physical properties in the interphase region. These mechanical and statistical properties

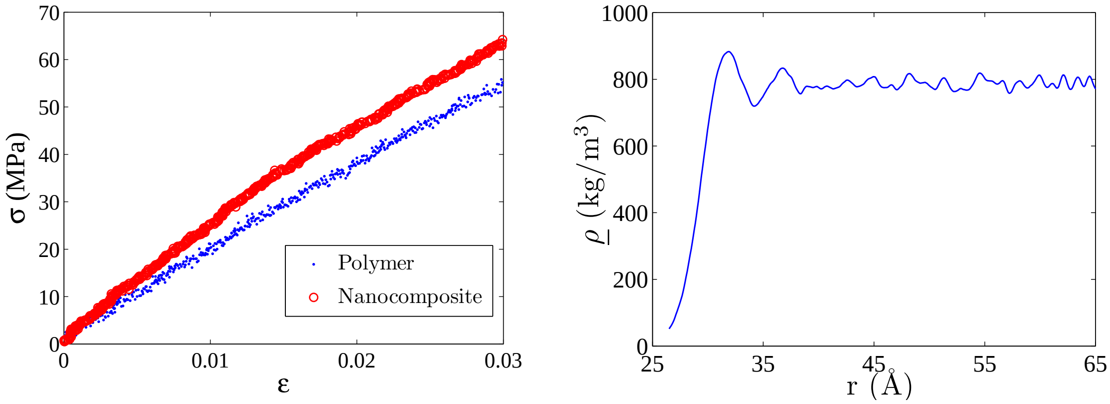

Figure 2: Left panel: loading curve of a tensile test along the x-direction for the polymer and for the nanoreinforced polymer at 100K (loading rate: 0.1MPa/2ps). Right panel: graph of the polymer radial density $r \mapsto \underline{\rho}(r)$, where r denotes the distance from the nanoparticle center of mass (at 100K).

are subsequently used in order to construct and identify a suitable probabilistic model for the interphase elasticity, in the spirit of previous works by the authors [3]. Finally, the model thus obtained serves as a theoretical basis for the definition of an equivalent asymptotic interface model.

REFERENCES

[1] J. Berriot, F. Lequeux, L. Monnerie, H. Montes, D. Long and P. Sotta. Filler-elastomer interaction in model filled rubbers, a H NMR study. *Journal of Non-Crystalline Solids*, Vol. **307-310**, 719–724, 2002.

[2] D. Brown, V. Marcadon, P. Mélé and N. D. Albérola. Effect of filler particle size on the properties of model nanocomposites. *Macromolecules*, Vol. **41**, 1499–1511, 2008.

[3] J. Guilleminot, C. Soize. Stochastic model and generator for random fields with symmetry properties: Application to the mesoscopic modeling of elastic random media. *SIAM Multiscale Mod. Simul.*, Vol. **11(3)**, 840–870, 2013.