STOCHASTIC MODELING OF INTERPHASE EFFECTS FOR NANOREINFORCED HETEROGENEOUS MATERIALS

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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 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 aforementioned results in order to assess some stochastic features associated with random fields of physical properties in the interphase region. These mechanical and statistical properties

![Simulation snapshot of a polymer chain near the nanoscopic inclusion.](image)
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

