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Stochastic continuum modeling of random interphases from atomistic simulations. Application to a polymer nanocomposite

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Abstract

This paper is concerned with the probabilistic multiscale analysis of polymeric materials reinforced by nanoscopic fillers. More precisely, this work is devoted to the stochastic modeling and inverse identification of the random field associated with the elastic properties in the so-called interphase region. For illustration purposes, a prototypical polymer system reinforced by a Silica nanoscopic inclusion is considered. Molecular Dynamics (MD) simulations are first performed and used to characterize the conformational properties of the polymer chains in the neighborhood of the inclusion. It is shown that these chains are characterized by a specific tangential orientation which, together with the density profile and variations in chain mobility, allows for the geometric definition of the interphase region. Mechanical virtual testing is next completed on a set of initial configurations, hence providing a simulated database for model calibration. The results thus obtained are subsequently used to construct a random field model for the interphase stiffness. An inverse calibration procedure is finally proposed and relies on a stated equivalence between the apparent properties obtained from MD simulations and those computed by numerical homogenization in the continuum mechanics formulation. The interphase elasticity random field is seen to exhibit nonnegligible fluctuations, and the estimates of parameters related to spatial correlation are shown to be consistent with characteristic lengths of the atomistic model, such as the interphase thickness.

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