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MULTISCALE MODELING OF A NANOPARTICLE REINFORCED EPOXY RESIN

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The assessment of the mechanical properties of nanocomposites, e.g., nanoparticle reinforced polymers, usually requires a large amount of material tests. As the filler-matrix interphase at the nanoscale influences the macroscopic mechanical properties, it is often not only interesting to analyze different particle weight fractions, but also surface modifications, particle shapes and size distributions, to determine optimal configurations.

Numerical methods comprise (ab initio) molecular dynamics, monte carlo methods, coarse-grained molecular dynamics as well as analytical and numerical micromechanical models that are extended to the nanoscale. In atomistic simulations, the numerical effort typically rises with the size of the system, while micromechanical models require a special effort to include the effects of physical and chemical bonds at the interface of nanoscale filler particles.

In this work, we propose a multiscale algorithm that focuses on the important role of the interphases in nanoparticle reinforced polymers. Figure 1 shows a representative volume element (RVE, center) of a nanocomposite with spherical nanoparticles (red) and a polymer matrix (blue). The interphase is modeled as an atomic region while less important areas such as the particle core and the surrounding matrix are modeled as continuum regions. The simulation method is the Molecular Dynamic Finite Element Method (MDFEM) [1]. It describes how to embed the force fields of the classical molecular dynamics into commercial finite element software. In contrast to standard beam elements, which are often used in the literature [2], the results obtained with the special MD elements comply exactly with force field reference. In the transition areas between particle and

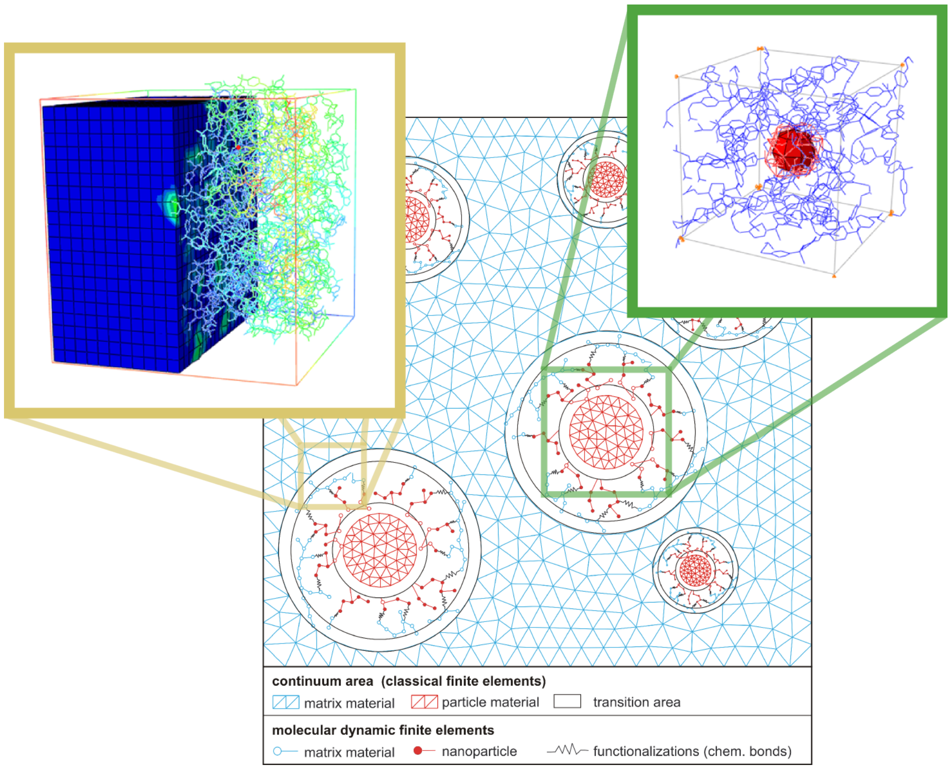

Figure 1: MDFEM multiscale simulation, center: RVE nanoparticle reinforced epoxy resin, scale transition from continuum region to atomistic region left: matrix, right: particle

matrix (left magnifier) a scale coupling technique based on the bridging domain method (BDM) [3] that was derived from the Arlequin Method [4] has been implemented. Within the particle core (right magnifier) BDM as well as a rigid coupling technique is used. As a numerical example, an epoxy resin with spherical aluminum oxide nanoparticles is analyzed. Results include the elastic properties of nanocomposites with different weight fractions, sizes and surface functionalizations as well as physical properties such as the density in the vicinity of the particles. The results are compared with chosen experiments.

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