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MULTI-SCALE MODELING OF NANOCOMPOSITES: ENHANCED MEAN-FIELD HOMOGENIZATION AND FINITE ELEMENT ANALYSIS

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ABSTRACT

INTRODUCTION: NANOCOMPOSITE MODELING

With "nanocomposite" we indicate a composite material where the size of the inclusions is less than one micron. Due to this small size, the inclusion's surface becomes an important factor determining the overall behavior and properties of the composite. For "microcomposites" (composites with inclusions larger than one micron) it is often sufficient to consider the bulk properties of the phases, while for nanocomposites some enhancement of the model is needed to capture this surface effect, or other "nano-effects". Due to these nano-effects, it is possible to obtain a given improvement of matrix properties (mechanical, electrical, thermal, ...) with a smaller weight fraction of filler, raising the interest of material manufacturers in the design of nanocomposites.

The nano-scale inclusions (or nano-filler) are usually provided as a powder of particles (average size 5–150nm). During production, the nano-filler is dispersed in the matrix. Full dispersion is rarely reached, and the nano-filler appears in the composite in the form of clusters. Clustering can give an advantageous nano-effect when the cluster of densely packed nano-particles (with voids in between) has the same size and stiffness as a solid micron-sized inclusion, while using less filler material. This beneficial use of voids in between particles is also the reason for the great property enhancements in nano-clays, where one nano-inclusion is a stack of nano-sized clay sheets [1].

MEAN-FIELD HOMOGENIZATION

Mean-field (MF) homogenization techniques describe the rheological state of a composite material based on the average value of stress and strain in each phase of the composite. These analytical formulae are then applied in a numerical simulation (incremental loading), stand-alone or interfacing with finite element (FE) software. This semi-analytical, size-independent MF approach is successful for a wide range of composites and can also handle coated inclusions. The coating option is relevant for

nanocomposites because, due to their active surface, the nano-particles interact with other nano-particles and/or with the surrounding matrix. In the case of matrix-particle interaction, the coating represents a real, new phase (called "interphase"), e.g. matrix material with density and/or stiffness variations due to polymer chain rearrangement [2]. In the case of particle-particle interaction, the coating properties are chosen as to emulate the force action between particles. Both coating applications will be illustrated in the presentation: particle-particle interaction, and reverse-engineering the properties of the matrix-particle interphase. While MF analysis is size-independent, it is possible by "design of experiment" to obtain curves representing the size-effect, i.e. the effect of coating thickness for a given particle size, as will be presented. If the inclusion is coated, then the inclusion's properties are first homogenized with the coating's properties, and this result is then homogenized with the matrix properties. A similar, two-level approach is used for densely packed clusters: in a first step the nano-filler is homogenized with the voids in the cluster, and the resulting "effective cluster material" is homogenized with the matrix. As will be presented, the resulting effect on composite level is greater than would be expected based on filler weight fraction alone.

FINITE ELEMENT ANALYSIS OF MICROSTRUCTURES

To verify the MF predictions, FE models are constructed (semi-automatically) to accurately represent the real microstructure geometry. Models and results will be presented for uniaxial traction on a polymer matrix with mono- and polydisperse nano-filler, including coating, clustering (Figure 1) and using the cluster size distribution (as determined from image analysis), as well as combining individual particles with large clusters. The MF results, obtained in seconds, are less than 5% off the FE results, obtained in days. FE analysis allows more detailed post-processing, revealing that clustering of particles may increase the maximum stress in the matrix with 25%.

CONCLUSION

Several semi-analytical and numerical techniques are applied to nanocomposite modeling (nano-effects) and compared w.r.t. accuracy, functionality and CPU time.

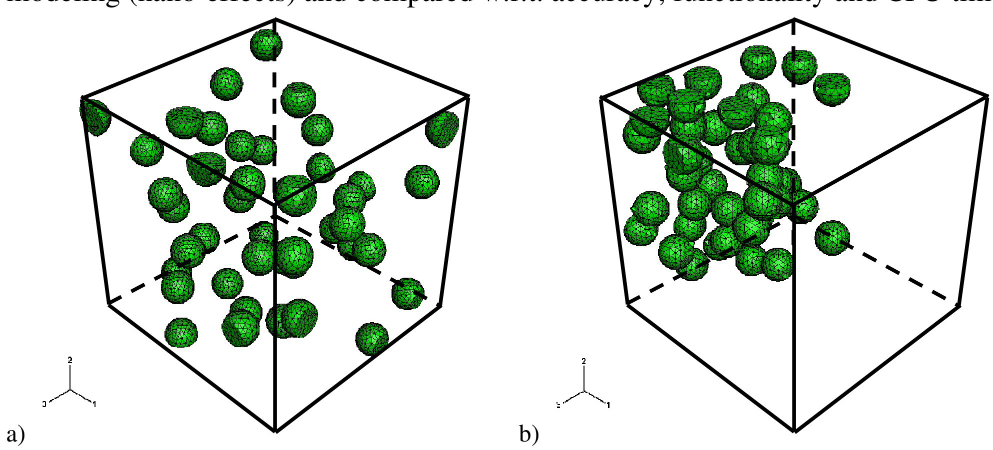

Figure 1. Finite element model of matrix with 40 spherical inclusions: a) dispersed, b) clustered.

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