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# SIMULATING SIZE-DEPENDENCY OF THE TENSILE MODULUS OF ALUMINA/EPOXY NANOCOMPOSITES USING THE MOLECULAR DYNAMIC FINITE ELEMENT METHOD

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**Summary.** *Nanoparticles can be used to enhance the mechanical properties of polymer matrices. To reduce the number of costly experiments, a simulation strategy based on the Molecular Dynamic Finite Element Method is proposed to analyze the influence of $\gamma$-$Al_2O_3$ nanoparticles on the tensile response of epoxy resin.*

## 1 INTRODUCTION

A promising approach to enhance the properties of materials is to incorporate nanoscale fillers in order to benefit from their high specific surface. Fiber composite structures, when e.g. manufactured using liquid composite molding technologies exhibit residual stresses caused by resin shrinkage. As a consequence, inferior material performance is observed as compared to prepregs. By adding spherical nanoparticles to the matrix, residual stresses can be reduced and subsequently the overall mechanical properties improve significantly [1]. Nanoparticle type, shape, surface modification and weight fraction determine the mechanical properties of the nanocomposites. Hence a large number of experiments are necessary to identify optimal configurations.

Based on the Molecular Dynamic Finite Element Method, a simulation methodology for the prediction of epoxy resin (DGEBA) with $\gamma$-$Al_2O_3$ nanoparticles is proposed, that allows for the prediction of mechanical properties such as the tensile modulus. Being physically motivated, the simulation models can further be analyzed to gain insights on the reinforcing mechanisms of the particles.

## 2 SIMULATION METHODOLOGY

The Molecular Dynamic Finite Element Method (MDFEM) is a framework for the simulation of atomic structures within commercial finite element codes such as Abaqus, Ansys and MSC Nastran/Marc. Special 2-, 3- and 4-node MDFEM elements corresponding to the force field potentials of classical molecular dynamics are superimposed to approximate nanostructures and may subsequently also be combined with continuum elements to enable efficient multiscale simulations. For further details, see [2].

A special preprocessor has been implemented to generate MDFEM unit cells comprising epoxy resin and one nanoparticle (see Fig. 1 (left)). Parameters for particle size, weight fraction, surface functionalization and particle/matrix interaction have been introduced. Each analysis starts with a relaxation step to determine the atomic equilibrium configuration, followed by a loading step, in which the simulation cell is subjected to tensile strain. In both cases, periodic boundary conditions are applied.

## 3 RESULTS

A parametric study has been carried out to investigate the effect of particle size-dependency on the tensile modulus. Fig. 1 (right) shows the tensile modulus for various particle sizes and particle weight fractions whereas each dot represents one simulation. The scatter of the results within one group is caused by the small size of the unit cells and the random polymer network generation. Due to the computational cost, only "small" particles can be analyzed using pure MDFEM simulations. As a result, the theoretical tensile modulus is significantly higher than the experimental bulk value. However, in agreement with the experiment the higher the particle weight fraction, the higher the tensile modulus and the so-called "nano-effect" or particle size-dependency is illustrated by the exponential trend line.

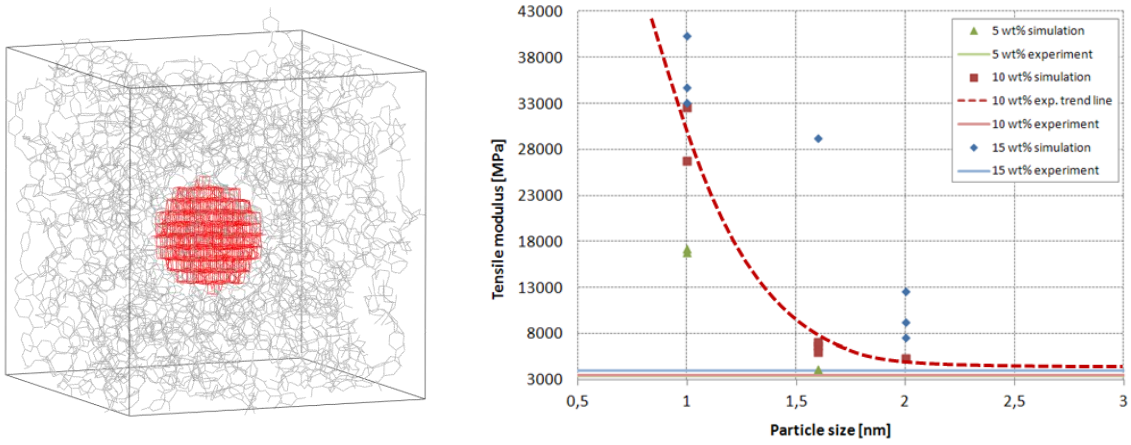


Figure 1: 2 nm particle 15 wt%, (left) tensile modulus for various weight fractions (right)

An extraction of the radial density around the particle reveals that regions of higher matrix densities occur at the interface which is the reason for the changes of the stiffness.

## REFERENCES

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