

# COMPUTATIONAL MODELING OF DEFORMATION AND DAMAGE IN PARTICLE-REINFORCED COMPOSITES

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Summary The micromechanisms of deformation and fracture in particle-reinforced composites are studied through the finite element simulation of 3D multiparticle cubic cells. The simulations provided new insights on the role played by reinforcement clustering and damage (particle fracture, interface decohesion, ductile matrix failure) on the overall composite tensile response as well as on the micromechanisms of damage nucleation and growth.

## INTRODUCTION

The optimization of composite properties requires the use of sophisticated simulation tools to understand the relationship between the microstructural factors and the overall properties. This has been achieved by the development of micromechanical models, which initially considered only the matrix and reinforcement properties and their respective volume fractions. It was soon evident that this information was not sufficient for accurate prediction of many properties, and more refined models, which included the effect of particle shape, size and orientation, were elaborated. There is, however, unmistakable experimental evidence that the spatial distribution of particles and the onset of damage in regions with high local volume fraction of reinforcements determine critical important mechanical properties such as the yield strength, the ductility, the fracture toughness, etc. but the current micromechanics tools are not able to handle properly both problems. On the one hand, homogenization techniques deal with random and homogeneous descriptions of the microstructure and cannot take into account the presence of reinforcement clusters. Moreover, damage is triggered by the extremal values of stresses and strains while homogenization techniques deal with volume-average quantities. On the other hand, periodic descriptions of the composite based in a simple unit cells (FCC, BCC, etc.) cannot include the strain localization which takes place after the onset of damage. These limitations are overcome with a new analysis technique based on the three-dimensional finite element simulation of multiparticle cells. This technique provides unique information on the effect of reinforcement spatial distribution on the nucleation and growth of damage in composites as well as on the effect of damage on the overall composite properties.

## SIMULATION STRATEGY

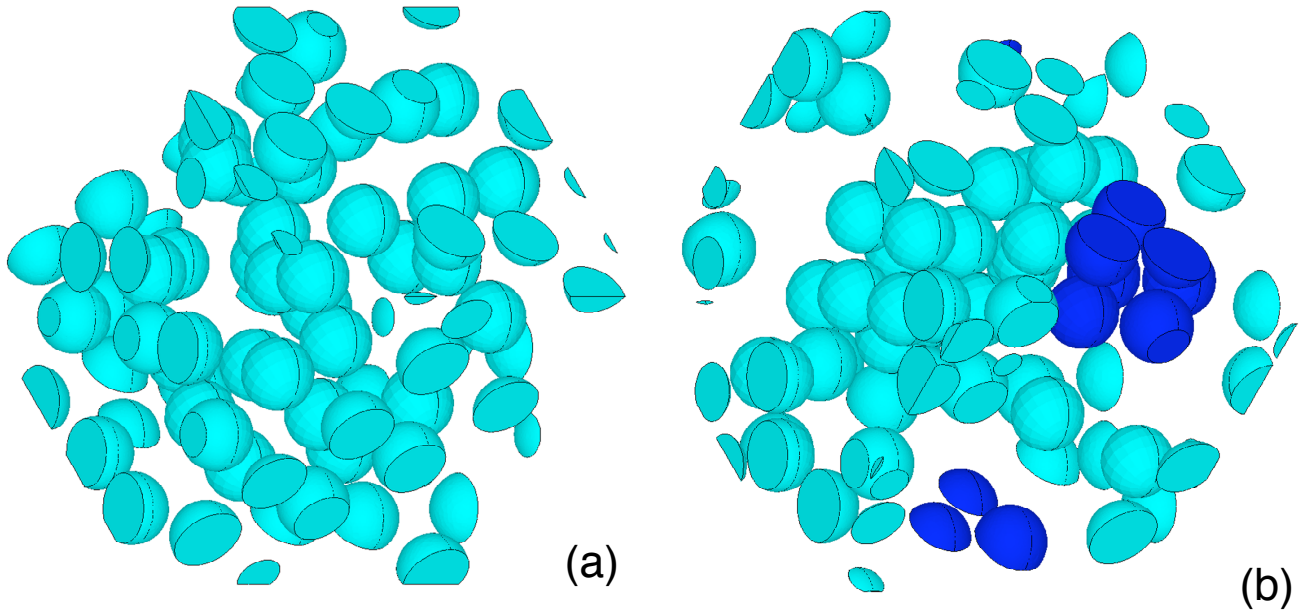
The composite mechanical behavior was studied from the finite element simulation of a three-dimensional cubic cell representative of the microstructure. The size of the cubic cell and the computer time to solve the problem increased with the number of particles in the cubic cell, and the actual figure (30 to 50, depending on the problem) was dictated by a compromise between the two factors. Moreover, the accuracy of the solution was improved by averaging the results obtained with different cells.

New algorithms were developed to generate composites with homogeneous and inhomogeneous (clustered) particle distributions, and the statistical parameters which characterize the reinforcement spatial distribution (radial distribution function, average nearest-neighbor distance, etc.) were determined. Representative volume elements of the microstructures were discretized and analyzed by the finite element method. Particles were assumed to behave as linear elastic solids, while the matrix was modeled as an elasto-plastic solid with isotropic hardening. The simulations took into account the various damage mechanisms experimentally observed. Damage in the matrix was introduced by the modified Gurson model while reinforcement fracture and interface decohesion at the matrix/reinforcement interface were included using three-dimensional interface elements especially developed to this purpose, the interface and/or particle strength and toughness being given by the constitutive equation of the cohesive crack. The new interface element, made up of two triangular surfaces compatible with the faces of the ten-node tetrahedra, was developed using a large displacement formulation, necessary to account for the large voids formed at the interface and within the particles during fracture. In addition, a new control technique was presented to obtain the whole load-displacement response in a simulation at a reasonable computational cost because the nucleation of damage in the microstructure often leads to numerical instabilities, which delay (or even impede) the convergence.

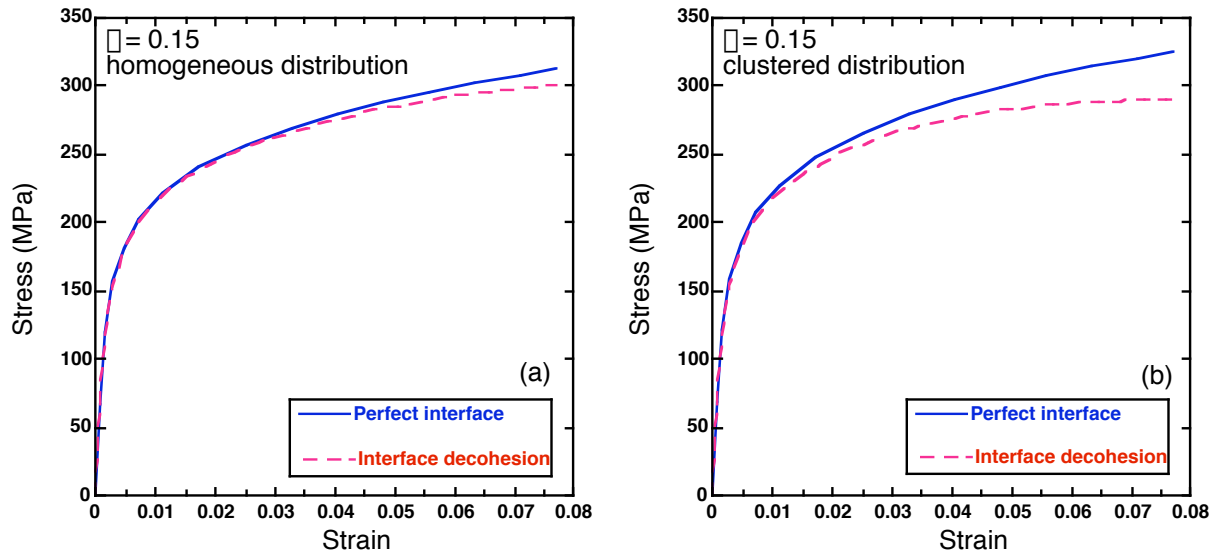
## RESULTS AND CONCLUSIONS

The numerical results provided the macroscopic composite response as a function of the reinforcement volume fraction and spatial distribution, and showed how the details of the local particle arrangement controlled the nucleation and growth of

damage in the composite throughout the three-dimensional microstructure. In particular, the simulations were aimed at elucidating the role of the spatial particle distribution on the composite response with and without damage. Cubic cells representative of homogeneous and highly clustered composites were generated (Fig. 1) and the composite behavior in tension was obtained by the finite element method. It was found that the overall composite response was weakly influenced by the reinforcement particle distribution in the absence of damage, although the maximum principal stresses in the particles at the local level were significantly higher in the clustered microstructures. This difference did influence the composite behavior when damage (as particle fracture, interface decohesion or ductile matrix failure) was included in the simulations. This is shown in the tensile stress-strain curve of a composite containing 15 vol. % of spherical particles embedded in an elasto-plastic matrix presented in Fig. 2. Four curves corresponding to two different microstructures (homogeneous and clustered) with two particle/matrix interfaces (perfect bonding or interfacial decohesion) are plotted. They show the synergistic contribution of an inhomogeneous particle distribution and interfacial fracture to the composite strain hardening capacity, and the results were more marked when other damage mechanisms were included. As a conclusion of the simulations, the influence of the statistical parameters which describe the microstructure on the mechanical properties was obtained as a function of the dominant damage mechanism.



**Figure 1.** Particle distribution within the cubic cell. (a) Homogeneous. (b) Clustered.



**Figure 2.** Tensile stress-strain curve of the composite. (a) Homogeneous. (b) Clustered microstructure.