COMPUTATIONAL MICROMECHANICS OF SPHERE-REINFORCED COMPOSITES

Javier Segurado, Carlos González and Javier LLorca
Department of Materials Science. Polytechnic University of Madrid. Spain

ABSTRACT

The spatial distribution of particles and the development of damage underlie some important mechanical properties of composites. New algorithms were developed to generate composite microstructures with homogeneous and randomly clustered particle distributions, and the statistical parameters which characterize the reinforcement spatial distribution (radial distribution function, average nearest-neighbor distance, etc.) were determined. Cubic 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. 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 for this purpose, the interface and/or particle strength and toughness being given by the constitutive equation of the cohesive crack.

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 microstructure. 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. Particle clustering, however, modified significantly the composite behavior when damage (as particle fracture, interface decohesion or ductile matrix failure) was included in the simulations. The simulations provided new insights into the role played by reinforcement clustering and damage (particle fracture, interface decohesion, ductile matrix failure) in the overall composite tensile response as well as on the micromechanisms of damage nucleation and growth.

1. INTRODUCTION

The optimization of composite properties requires the use of sophisticated simulation tools to clarify 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 important mechanical properties such as the yield strength, the ductility, the fracture toughness, etc., but the current micromechanic tools are not able to deal adequately with these problems. On the one hand, homogenization techniques deal with random and homogeneous descriptions of the microstructure but 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 on a simple unit cell (FCC, BCC, etc.) cannot include the strain localization which takes place after the onset of damage.

These limitations are overcome by a new analysis technique based on the three-dimensional finite element simulation of cubic cells containing an adequate number of particles to represent the composite microstructure. 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.

2. SIMULATION STRATEGY

The composite microstructure was represented by a cubic cell containing a dispersion of spherical particles, and various algorithms were developed to generate composites with different spatial distribution of the spheres in the continuous matrix [1]. The cubic cells were discretized and their mechanical response was 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 by using three-dimensional interface elements especially developed for this purpose, the interface and/or particle strength and toughness being given by the constitutive equation of the cohesive crack [2]. 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 [2].

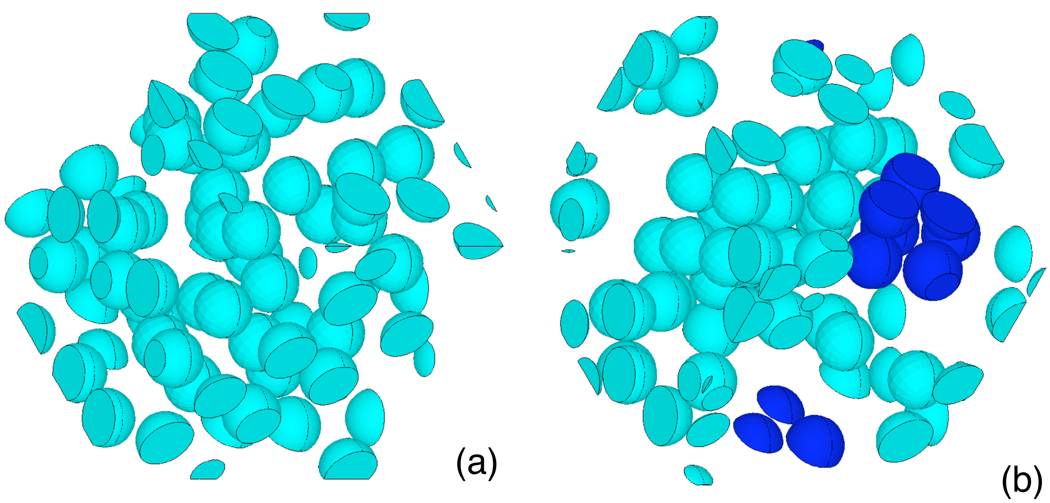

Figure 1. Sphere spatial distribution of the spheres within the cubic cell, which represents the composite microstructure. (a) Homogeneous sphere distribution. (b) Inhomogeneous (clustered) sphere distribution. Spheres belonging to the same cluster are shaded.

3. RESULTS

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 in the composite response with and without damage.

Cubic cells representative of homogeneous and highly clustered composites were generated (Figure 1). Homogeneous microstructures were made up of a random dispersion of spheres. The inhomogeneous ones were idealized as an isotropic random dispersion of spherical regions -which represent the clusters- with the spherical reinforcements concentrated around the cluster center. The average sphere volume fraction in the composites was held constant at 15% in both materials. The local volume fraction of spheres in the clustered regions of the inhomogeneous material was 40%, leading to matrix-rich and particle-rich regions within the cubic cell, Figure 1(b). 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 number (49 corresponding to 7 clusters containing 7 spheres) was dictated by a compromise between the two factors.

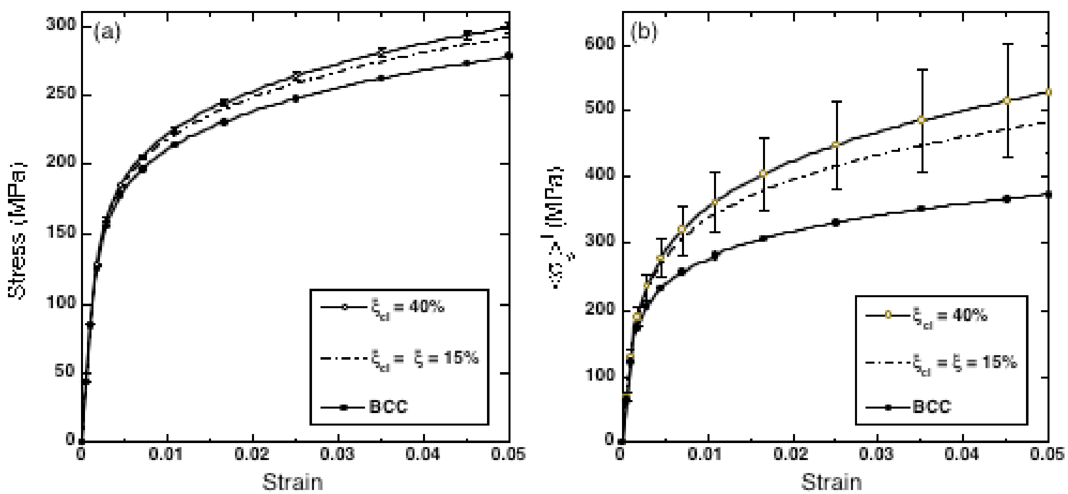

Figure 2. (a) Tensile stress-strain curve of an elasto-plastic matrix reinforced with 15 vol. % of elastic spheres as a function of the reinforcement spatial distribution. (b) Average maximum principal stress in the spheres as a function of the applied strain for the composites in (a).

The tensile stress-strain curves of three composites made up of a dispersion of elastic spheres within a metallic matrix are plotted in Figure 2(a). The sphere volume fraction was 15% in all cases and the composites differed in the reinforcement spatial distribution which included a regular BCC spatial arrangement, and two random (homogeneous and clustered) sphere distributions. Each curve plotted in Figure 2(a) for the composites containing random particle distributions (either homogeneous or clustered) is the average value of 12 different particle arrangements, and the standard deviation of the simulations is plotted for the composite with inhomogeneous microstructure. The standard deviation in the tensile curves of the homogeneous material was also very small and is not plotted. No significant differences were found in the elastic regime among the three composites, but the flow stress of the one with a BCC particle arrangement was visibly lower than that of the composites with random particle distribution. However, the differences between the stress-strain curves of the composites with homogeneous and inhomogeneous random sphere distributions were very limited, indicating that the influence of clustering on the effective composite behavior was very insignificant in the absence of damage.

The volume-averaged stress tensor in each sphere, $\langle \sigma_s \rangle$, was computed as

$$\langle \sigma_s \rangle = \sum \sigma_i V_i / \sum V_i \quad (1)$$

where σ_i and V_i stand, respectively, for the stress tensor and the volume associated with the Gauss point i in the sphere. The maximum principal stress of the volume-averaged stress tensor in the whole sphere, $\langle\sigma_i\rangle^I$, was determined from the eigenvalues of $\langle\sigma_s\rangle$, and the evolution of $\langle\sigma_i\rangle^I$ in all the spheres corresponding to one microstructure is plotted in Figure 2(b) as a function of the far-field applied strain for the three particle arrangements, where the standard deviation of $\langle\sigma_i\rangle^I$ corresponding to all the spheres in each microstructure is plotted for the composite with clustered microstructure. The deviation of $\langle\sigma_i\rangle^I$ in the homogeneous material was slightly lower and for clarity is not plotted. These curves show that the maximum principal stresses in the spheres increased with the degree of inhomogeneity and the differences between the composites with random particle distributions and those with a regular BCC arrangement were very important. Basically, the highest stress concentrations occurred in composite regions where the particles were closely packed and oriented along the loading axis, which were found in all the random microstructures but not when the spheres were arranged in a regular BCC lattice. In addition, the intensity of the stress concentration was maximum within the clusters, and the particle stresses in the inhomogeneous material were higher than in the inhomogeneous one. These findings were also valid for the interface and matrix stresses, which also were the highest within the clusters containing a high local volume fraction of spheres.

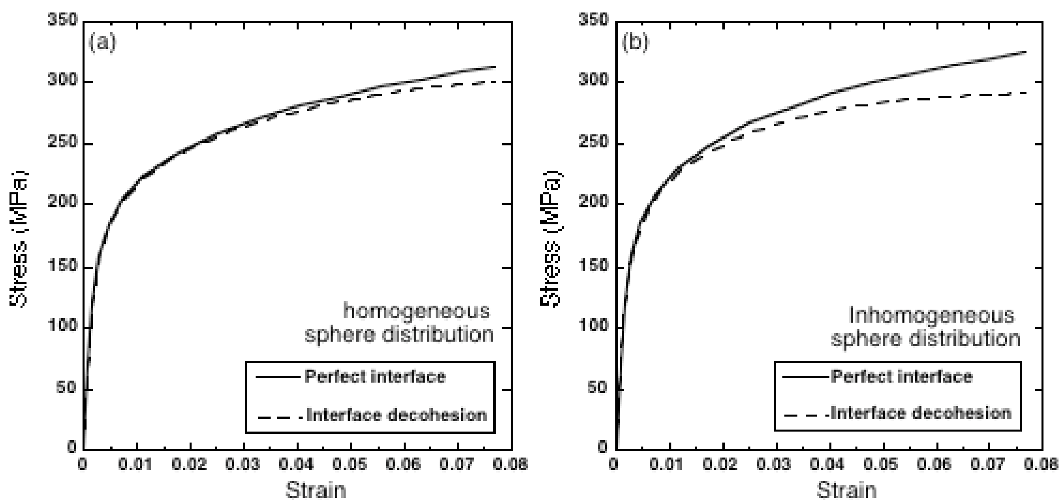

Figure 3. Influence of interface decohesion on the tensile stress-strain curve of an elasto-plastic matrix reinforced with 15 vol. % of elastic spheres. (a) Homogeneous sphere distribution. (b) Inhomogeneous sphere distribution.

These differences in the local values of stresses (and strains) did influence the composite behavior when damage (in the form of particle fracture, interface decohesion or ductile matrix failure) was included in the simulations, and this is shown in Figure 3, which presents the tensile stress-strain curve of a composite containing 15 vol. % of spherical particles embedded in an elasto-plastic matrix. Four curves corresponding to two different microstructures (homogeneous and clustered) with two particle/matrix interfaces (perfect bonding or interfacial decohesion) are plotted. In the absence of damage, the composites with homogeneous and inhomogeneous particle distributions showed very similar behavior, as indicated in the previous paragraph. Damage by interface decohesion reduced the composite flow stress in both types of microstructure but the influence was much more marked in the composite with a clustered particle distribution. The final outcome was that the flow stress of the inhomogeneous composite was lower than that of the homogeneous one because of the early nucleation of interface damage.

Similar results were obtained when other damage mechanisms (particle fracture or matrix void grow) were included in the simulations, and they showed that the nucleation and growth of damage in these composites was very sensitive to the spatial distribution of the reinforcements. The strain and stress concentrations within the clusters triggered the nucleation of damage at low strains and reduced markedly the composite flow stress as well as strain at the onset of plastic instability, which controls the tensile ductility of these composites. Of course, the damage pattern was very different from the one found in the composite with a regular sphere arrangement, where the distance between the reinforcements is constant and the local stress concentration due to the presence of closely packed particles is not found.

4. CONCLUSIONS

The tensile deformation of sphere-reinforced composites was studied by the finite element simulation of three-dimensional multiparticle unit cells. It was found that the particle spatial distribution did not modify significantly the composite stress-strain curve in the absence of damage, although the local stresses in the matrix and the particles increased with the degree of inhomogeneity. The scenario changed completely if damage (either by particle fracture, interface decohesion or matrix void grow) was included in the simulations. Damage always nucleated earlier in the composites with inhomogeneous particle distributions and was localized in regions where the particles were closely packed and oriented along the loading axis. As a result, the flow stress and the ductility of composites with inhomogeneous particle distribution were significantly lower than in those with a homogeneous distribution.

4. REFERENCES

[1] J. Segurado, C. González and J. LLorca, A Numerical Investigation of the Effect of Particle Clustering on the Mechanical Properties of Composites. Acta Materialia, 51, 2355 – 2369, 2003.
[2] J. Segurado and J. LLorca. A New Three-Dimensional Interface Finite Element to Simulate Fracture in Composites. International Journal of Solids and Structures, 41, 2977-2993, 2004.