Influence of Interface Quality on Stress and Strain Distribution in a Micro Cell of a Composite

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This paper presents an analysis of a composite cell at a micro level. The authors modeled the interface between a micro sphere and a polymeric matrix for two cases: an interface characterized by a strong bond between the two involved bodies and an interface with low friction between the micro sphere and the polymeric matrix. Even if these models are ideal images of actual composites, the analysis of strain and stress distributions reveals there is a big difference in the mechanical behaviour of the two micro cells. These two cases were analyzed considering a perfect elastic behaviour of involved materials. The shape and the intensity of stress distributions are different for the analyzed models. A weak interface makes the matrix to have restrained zones with high values of von Mises stresses, concentrated on top and bottom of the sphere (on the loading direction). An actual cell of a similar composite (polymeric matrix and a micro sphere as reinforcement) could not have an „extremist" behaviour as these two here presented, but an intermediate one, depending on actual properties of the materials and the nature of the interface.

Keywords: micro cell composite, strain distribution, stress distribution

The mechanical properties of composites depend on their microstructures, i.e. on the content, geometries, distribution and properties of phases and constituents in the composites [1-3]. As commented by Mishnaevsky [4], the concept of computational experiments as a basis for the numerical optimization of materials is formulated. Many specialists are interested in simulating the mechanical behaviour of composites as a sensible interpretation of the results could formulate reliable recipes for composites [4-8].

FEM (Finite Element Method) offers the opportunity for anticipating the material behaviour, especially for composites [2, 9-12]. When modeling machine elements made of polymers, the particular behaviour of these materials has to be taken into account [13], including elasto-plastic aspects.

But a reliable model of a composite has to prove by experimental research in order to be useful for designers. In order to solve a design for a composite, there are several steps to be done: designing the model geometry and defining the restrictions and the load, meshing the bodies, including the selection of the element type, identifying nodes and elements, elaborating the equations for the mesh elements, establishing the boundary conditions, solving the problem and the interpretation of the results.

Modeling the unit cell of a composite with spherical reinforcement

A composite may be modeled at three different levels: micro, mezo and macro [4]. For instance, the blade of a wind turbine from [14] is modeled at a macro scale, taking into account physical and mechanical characteristics as given by the suppliers. The optimization of the material could rely on a model elaborated at micro, mezo or macro scale, even on a combined scale model that will reduce the time necessary for the experimental stage of the material or even for the wind turbine.

The model here presented is done for a unit cell of a composite, at micro level. It is quite difficult to define a unit cell for a composite, taking into account the diversity of the involved materials, both matrix and adding material(s). Some specialists considered as the unit cell of a composite a micro volume including all materials involved in the composite, with their relevant properties for the composite behaviour, at mezo or macro scale. According to this idea, any volume including a fiber, a bead, even a cluster typical for the adding materials, could be considered a unit cell of the composite. By this analysis, the authors would like to emphasize the importance of the interface for the mechanical behaviour of a composite, even at the micro level of its unit cell. The importance of the interface properties was underlined by Medadd and Fisa [15], which proposed a model for traction fracture, that has been proved to be applicable to polymeric composites with glass beads, in a qualitative way. From figure 1, it may be noticed that the traction fracture of a composite with micro spheres depends very much on the interface quality:

a) the resistant interface is not damaged under load and the break is initially developed in the composite matrix;

b) a partially damaged interface usually depends on the elasticity modulus, the volume fraction of the adding material without damaged interfaces and the complementary volume fraction of the adding material that has a damaged interface (the ratio between these two interface categories being actually hard to be estimated);

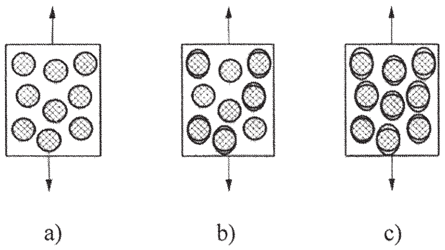
a) b) c)

Fig. 1. The deterioration models for the interface in polymeric composites with hard spherical particles

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Table 1
CHARACTERISTICS OF MATERIALS INVOLVED IN MICRO CELL DESIGN AND SIMULATION

Material	Characteristic*	Value	Unit
PBT	Density	1300	kg/m^3
	Coefficient of thermal expansion	0.0009	°C^{-1}
	Young modulus	3.3E+09	Pa
	Poisson coefficient	0.42	
	Compression modulus	6.875E+09	Pa
	Shear modulus	1.162E+09	Pa
	Traction limit at break	7.5E+07	Pa
Glass bead	Density	2180	kg/m^3
	Young modulus	6.66E+10	Pa
	Poisson coefficient	0.19	
	Compression modulus	3.5828E+10	Pa
	Shear modulus	2.8E+10	Pa

* Reference temperature: 22 °C

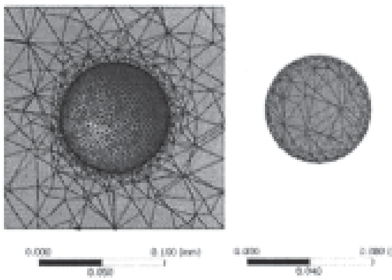
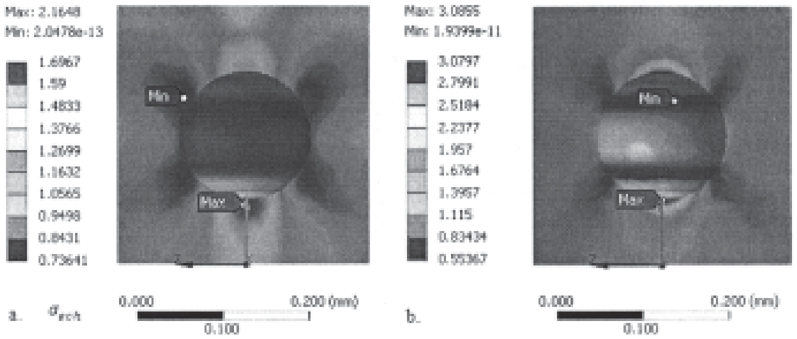


Fig. 2. The resulted mesh for the micro unit cell



a. perfectly bonded interface

b. weak interface (very low friction between the micro sphere and the matrix)

Fig. 3. Von-Mises stress distribution [MPa] (here the micro sphere is transparent)

c) a weak defective interface is easily destroyed when applying a traction load.

Taking into account models presented in [2, 15], the authors simulated the behaviour of a unit cell characterized by continuous interfaces (without detaching the polymer from micro spheres), but each one with different properties. The unit cell initially has a cubic shape; then the micro cell was loaded with a uniform pressure of 1 MPa, applied on the top face of the cub. The cell contains a micro glass bead (having a perfectly spherical shape), the centre of the sphere being in the center of the cub. It is an ideal situation. The aim of this simulation is to use the information from this unit cell to build a virtual composite with desired properties and to analyze in a future work how far the composite properties could be as compared to those of the unit cell. For this purpose, ANSYS 14.4 was used and the material characteristics are given in table 1.

This paper is a first step in a more complex study and here the materials are considered perfectly elastic (both for the sphere and the matrix). Actually, many composites, especially those with polymeric matrix, exhibit an elasto-visco-plastic behaviour.

The analyzed model of the composite cell consists of a cub of 100 μm in side, with a central sphere characterized by the radius R (here, R = 25 μm). The centres of the cub and of the sphere are overlapped. The volume left around the sphere consists of a polymer (here, PBT). Load was considered uniformly distributed on the top side of the cub as a compression load of p = 1 MPa and it was directly applied on the cub surface. Two cases are analyzed:

a.the reinforcement is perfectly bonded to the polymeric matrix; this configuration implies that interface could not be destroyed and the separation or the slipping between the two bodies are not allowed;

b.the interface allows for slipping between the two bodies, this slipping being characterized by a friction coefficient; the contact between the reinforcement and the matrix is designed as a friction contact between two solids. This paper presents only the results for a very low friction coefficient ($\mu = 5 \cdot 10^{-6}$), implying a very weak adherence between the materials of the model.

The boundary limits are:

- the micro unit cell of the composite is laying on a perfectly rigid plane solid ($y = 0, x \neq 0, z \neq 0$, the matrix material accepting lateral displacements on y, in the plane next to the bearing rigid surface);
- the load is uniformly distributed on the top face of the cub (a uniform pressure of 1 MPa).

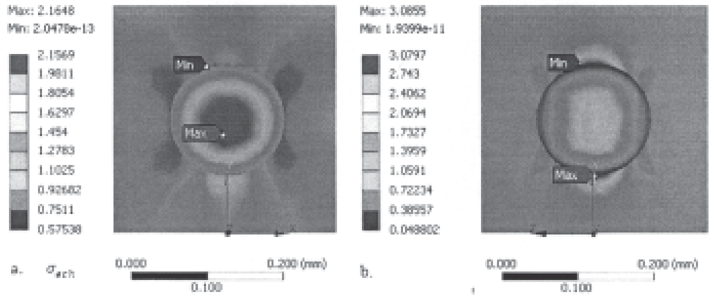
Figure 2 presents the resulted mesh for the micro unit cell. Finally, the mesh includes 38,621 interacting elements and 64,365 nodes.

Figures 3 to 10 present comparative results for a uniform load of 1 MPa, directly applied on the top surface of the cub.

The shape and the intensity of stress distributions are different.

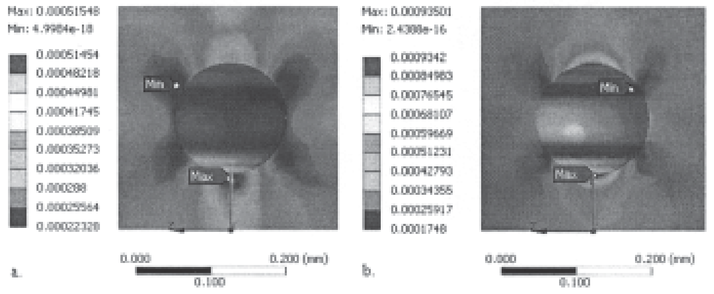
A weak interface makes the matrix to have restrained zones, with high values of von Mises stresses, concentrated on top and bottom of the sphere (on the loading direction). figure 4 presents the Von-Mises stress distribution in the polymeric matrix and in the glass bead. When the interface is bonded to the sphere, a stress concentration is noticed into the reinforcement body, the values of von Mises stresses into the matrix being lower as compared to the values obtained in the micro glass bead. The advantage is that the matrix is less loaded and its durability could be longer, implicitly that of the composite.

Figure 3.b presents the distribution of von Mises stresses for the second case, when the slipping between the matrix and the reinforcement is allowed. The maximum values are higher (3 MPa), but they are concentrated on the loading direction and the volume affected by this high stress is smaller as compared to the first case. This high stress concentration increases the risk of material failure, especially for the matrix. In actual cases, the matrix begins to yield around the more rigid body or the matrix is even



a. perfectly bonded interface; b. weak interface

Fig. 4. Von-Mises stress distribution in the vertical section containing the micro sphere and the cub centre [MPa]



a. perfectly bonded interface; b. weak interface

Fig. 5. Equivalent elastic strain distribution [MPa] (matrix made of PBT and the sphere is transparent)

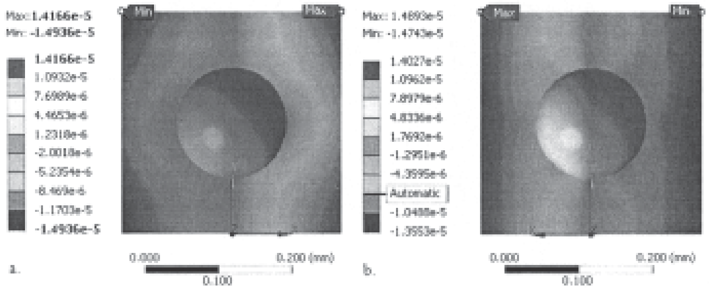
detached from the micro-sphere, the entire strength of the system being damaged.

Figure 5 presents the elastic equivalent strain distribution for each of the two cases. This characteristic has also high values for the second case, meaning a weak interface is not recommended for a composite.

Figures 6 and 7 present the strain distribution along the main direction of the reference system, Ox, Oy (that for Oz being similar to that for Ox). For the first case of the bonded interface, the polymer has an obvious tendency to creep near the cub corners (where the material has poor properties - those of the matrix). The harder micro sphere does not allow for the material to be deformed near the interface due to the strongly bonded interface.

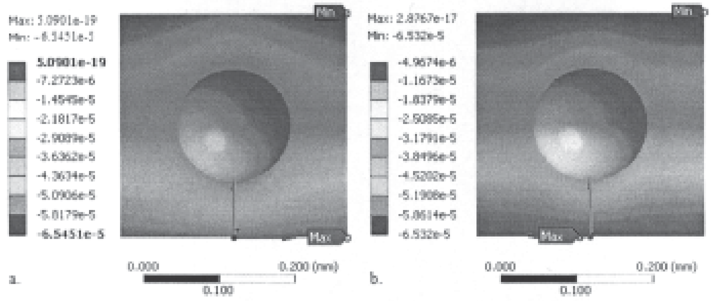
For the second case, the polymeric material is deformed in almost all its volume, due to the weak interface, characterized by a very small friction coefficient ($\mu = 5 \cdot 10^{-6}$), but the values of the maximum strains are similar on x direction. Differences are noticeable on y direction, but they are very small. Even if the directional strains have different distributions for the two analyzed cases, their maximum values are close (figs. 6 and 7).

The shear stress distributions reveal greater differences between the maximum values of the two models. Thus, the maximum value for τ_{xy} is much greater (almost 4 times) for the weak interface and the maximum values for τ_{yz} and τ_{zx} are almost double. The conclusion is that a weak interface generates greater shear stress and actual polymer materials could yield or be detached from the harder bodies (figs. 9 and 10). Figure 8 presents the elastic shear strain in xOy plane. For the weak interface, the maximum values are almost three times greater as compared to the bonded interface and they are situated on the load direction, near the rigid body.



a. perfectly bonded interface; b. weak interface

Fig. 6. Strain distribution along Ox axis [mm] (similar to those along Oz axis)



a. perfectly bonded interface; b. weak interface

Fig. 7. Strain distribution along Oy axis [mm]

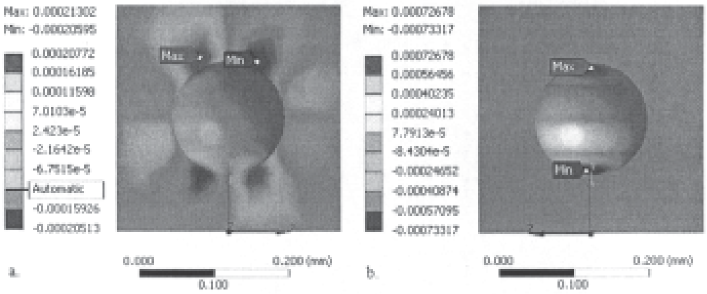
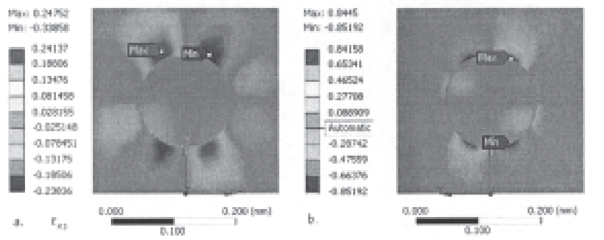


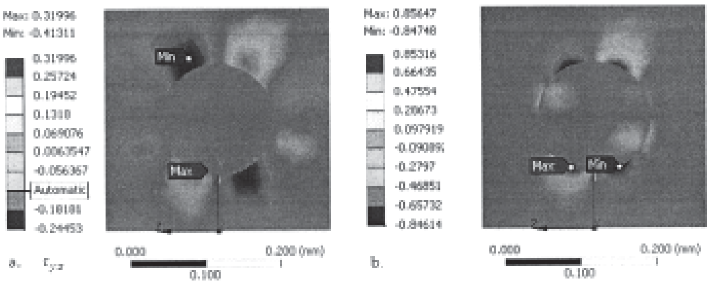
Fig. 8. Shear stress deformation in plane xOy for the matrix [mm/m] (transparent glass bead)

a. perfectly bonded interface; b. weak interface



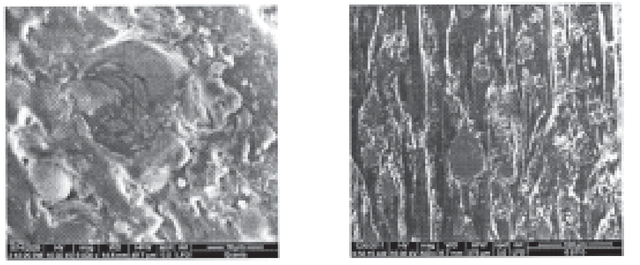
a. perfectly bonded interface; b. weak interface

Fig. 9. Shear stress distribution in xOy plane [MPa]



a. perfectly bonded interface; b. weak interface

Fig. 10. Shear stress distribution in yOz plane [MPa]



a) composite polyamide + 50% glass beads, with weak interface, tribotester pin-on-disk, v = 1.5 m/s, p = 3 MPa, L = 10,500 m [16]

b) composite PBT + 20% glass beads, tribotester block-on-ring, v = 0.25 m/s, F = 5 N, L = 7,500 m [17]

Fig. 11. Different interfaces for polymeric composites with glass beads

Conclusions

The results of these simulations differentiated only by the interface properties. The properties of the polymeric matrix and those of the reinforcement were kept constant. The two analyzed models are not easy to be found in practice, but they represent two extremes, actual cases being between them. In order to give examples of actual behaviour of two different interfaces, Figure 11.a presents a composite polyamide + glass beads that behaves as a composite with weak interface [16] (one may see that the glass beads could rotate into the matrix, the micro spheres having high mobility within the polymeric matrix of the superficial layers), this composite being nearer the model with weak interface and figure 11.b presents a composite with the same glass beads, but the matrix is made of PBT [17] (one may see fragmented beads and all beads did not seem to be moved into the matrix, this material being closer to the model with bonded interface).

The results underline that the mechanical behaviour of a micro unit cell for a composite is strongly influenced by the interface quality.

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