A NUMERICAL SIMULATION OF MECHANICAL PROPERTIES OF SMART POLYMER COMPOSITE WITH MICROCAPSULES FOR DAMAGE SENSING APPLICATIONS

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Abstract

The mechanical behaviour of polymer composites with polyvinyl acetate matrix filled with melamine-formaldehyde resin microcapsules was investigated. Such composites as self-sensing materials could be used for damage sensing applications as damaged zones with ruptured microcapsules can be seen due to a spill of dyes. These microcapsules contained the solution of colourless leuco dyes. In this investigation using experimentally obtained mechanical properties of both the polymer matrix and microcapsule shell material, representative volume elements (RVE) of polymer composite microstructure were generated on the basis of verified finite element model of capsule material. As the diameter of microcapsules varies the influence of this diameter upon plastic strain both in the matrix and capsule was investigated.

1. Introduction

Recently microcapsules are applied in many advanced materials and composites [1-3]. The concept of the use of microcapsules as sensors for controlled release of high performance polymeric coatings is one of the most relevant. This concept is based on the combination of the active protection with sensing functionalities that indicate when the protective coating is damaged and the substrate is already under the risk. Such smart self-sensing composite structures capable to provide the information about the structural integrity.

Making predictions of the mechanical behaviour and response of these self-sensing structures with microencapsulated active materials embedded into polymer matrices by numerical simulations is a good possibility to understand a real phenomenon that occurs at the micro level of the composites and cannot be implemented in the existing analytical models. This also allows to speed up the trial and error experimental testing.

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One of the foremost progresses in contemporary structural components is the enhancement done on the materials to obtain the optimum behaviour relevant to its application. This is done through the exploitation of the materials' microstructure.

The authors of this study recently investigated the possibilities of using of smart polymer composite with microcapsules for damage sensing applications [4, 5] and prediction of mechanical properties of composite materials by numerical simulations [6-8]. The aim of this investigation is to determine the material properties of self-sensing composite structures using numerical finite element modelling of the composite microstructure.

2. Experimental

2.1. Materials

Papierfabrik August Koehler SE microcapsules were used. The shell of microcapsules was made from melamine-formaldehyde resin. The core contained the solution of colourless leuco dyes (colourformer). The oil is a mixture of diisopropylnaphthaline and dearomatized hydrocarbons. The colour former is cristalviolet lactone (CVL). SEM micrographs of microcapsules are presented in Figure 1. It was measured that the diameter of the microcapsule varied from 0.7 to 12 μm, the thickness of microcapsule shell wall was 0.1 μm. A polymer composite material was made by putting of 10, 20, 30, 50 weight % of microcapsules into polyvinyl acetate (PVA) matrix.

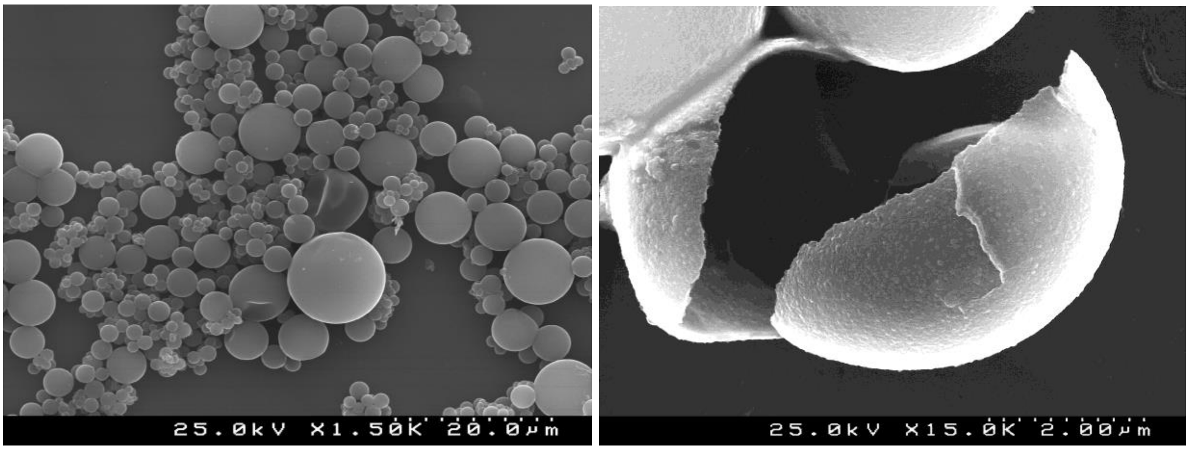

Figure 1. SEM micrographs of microcapsules.

2.2. Testing

Three types of specimens were prepared for testing. The specimens for compression test from the neat material of microcapsules shell melamine-formaldehyde (MF) resin were made. Specimens were as plates of irregular shape with average thickness of 1.7 mm. Area of the plates was measured by photos using ImageJ software for each sample, average area was ca. 30 mm^2. Compression tests were performed at room temperature and a rate of loading 0.5 mm/min using the universal testing machine ZWICK 2.5. Stress – strain curves were determined during this test (Figure 2., a). The next tension test was performed for specimens of PVA matrix composite. The stress – strain dependences of this test are presented in Figure 2., b. According to the results of these tests the mechanical properties of neat material of microcapsules and matrix material were obtained; they presented in Table 1.

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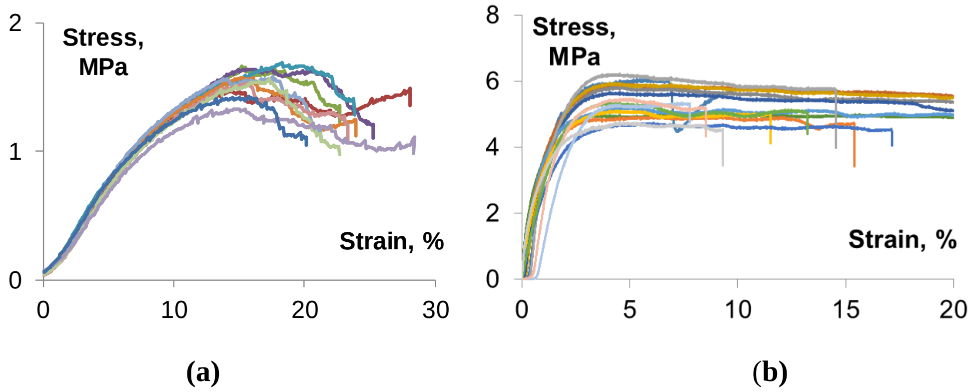

Figure 2. Stress – strain curves of: material of microcapsules shell (MF resin), compression (a); pure PVA matrix specimens, tension (b).

Table 1. Mechanical properties of materials.

Material	Young Modulus, *E* (MPa)	Poisson's Ratio, ν	Yield Strength, σ^* (MPa)
MF resin	17.0	0.3	1.5
PVA	310	0.4	5.5
Nitrocellulose [9]	2 200	0.3	60

PVA matrix composite specimens containing microcapsules were tested under tension as well. Yield strength dependences upon amount of microcapsules are presented in Figure 3.

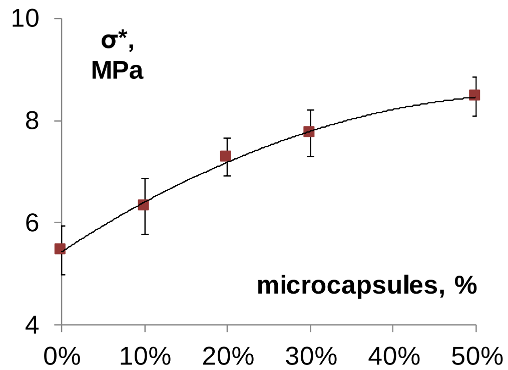

Figure 3. Yield strength of PVA matrix composite specimens for different amount of microcapsules by weight.

3. Modelling

The finite element (FE) analysis was used to study the mechanical behaviour of polymer composite with microcapsules. The analysis was performed by finite element code ANSYS R15.0. The well-known experiment on the compression of ping pong ball [9, 10] was used for the comparison with capsule compression behaviour and finding the suitable FE model (Figure 4., a). The behaviour under compression of nitrocellulose ping pong ball and MF resin ball (the same dimensions as nitrocellulose

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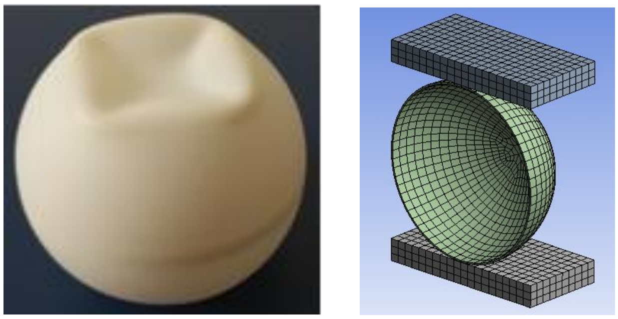
ball) was modelled. Mechanical properties of MF resin were experimentally tested and these of nitrocellulose were used according to other studies [9] (Table 1.). The balls' shells were created using SHELL181 elements. SOLID186 elements were used for supporting rigid plates. CONTA174 and TARGE170 elements were used for contact pair. For half symmetry model of the ball symmetry boundary conditions were used and FE mesh was generated (Figure 4., b). The bottom support plate was fixed and top one had displacement from 1 to 7.5 mm. The diameter of the ball was 40 mm. Bilinear Isotropic Hardening material model was used for nitrocellulose ball modelling and Multilinear Isotropic Hardening material model for MF resin. The dependences of compression force upon displacement obtained by FE modelling for nitrocellulose and MF resin were obtained.



(a) **(b)**

Figure 4. Testing and modelling: deformed shape of ping pong ball (a); FE model (b).

Adapted Reissner equation [11] for elastic spherical shell loaded by force F was used also

$$F = \frac{4D\delta}{rc}, \tag{1}$$

where $D = Ehc^2$ is the bending stiffness of the wall; E is Young Modulus; h is wall thickness; $c = \beta h$ is the reduced thickness of the wall; $\beta = \sqrt{12(1-\nu^2)}$; ν is Poisson's Ratio; δ is the displacement; $r = d/2$ is spherical shell radius; d is spherical shell diameter. The dependences of compression force upon displacement for nitrocellulose and MF resin balls obtained experimentally, by finite element modelling and theoretical Reissner equation are presented in Figure 5. Von Misses stress of the balls under 7.5 mm displacement is presented in Figure 6.

For modelling of microcapsules in PVA matrix one eighth symmetry model RVE was created. Full RVE dimensions were 20×20×20 µm. The inner pressure in the capsule for the liquid effect assumed to be 10 kPa [12]. The diameter of microcapsule d varied from 1 to 12 µm. In this way the volume fraction of microcapsules was changed from about 0.01 to 11 %. Shell wall thickness h was 0.1 µm and in this stage of investigation was not changeable. FE mesh size did not exceed 2 µm (Figure 7.). Multilinear Isotropic Hardening material model was used both for MF resin and PVA. Nonlinear structural static analysis was performed to evaluate the influence of microcapsules diameter (volume fraction) to the stress-strain state of microcapsules and matrix. The constant displacement of 1 µm (applied strain 5 %) on the top surface of RVE was used for loading. Such deformation usually does not initiate the plastic strain in matrix, but the stress concentrations between the PVA and microcapsule surface can influence the stress-strain state changes in some areas.

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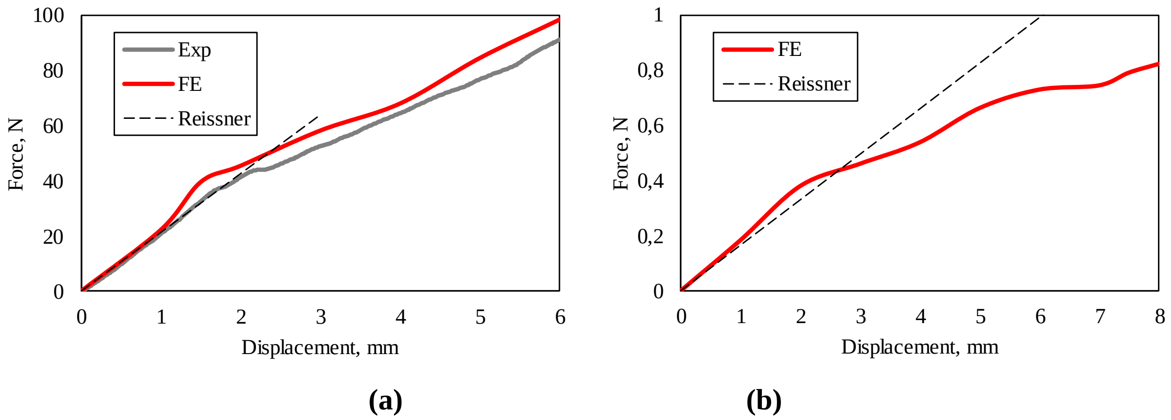

Figure 5. Dependences of compression force upon displacement obtained: experimentally, by finite element modelling and theoretical Reissner equation for nitrocellulose ping pong ball (a); by finite element modelling and theoretical Reissner equation for a ball from MF resin (b).

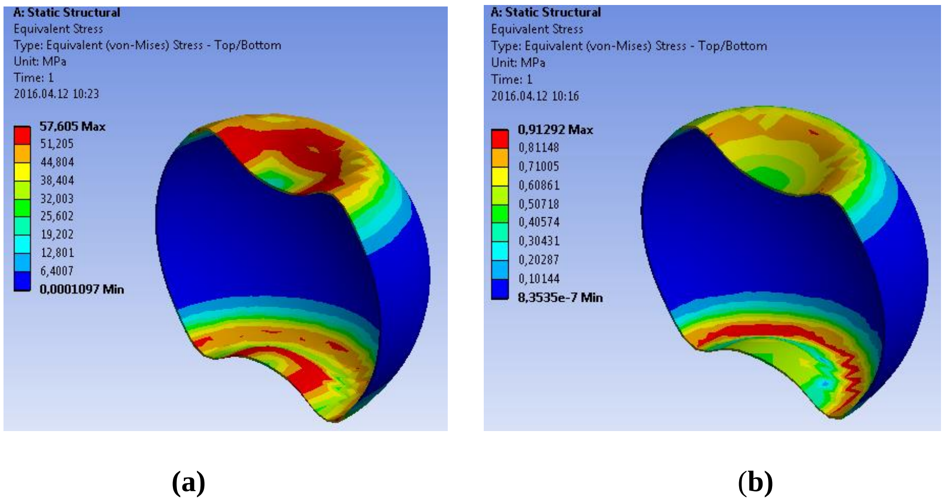

Figure 6. Von Misses stress in nitrocellulose (a) and MF resin (b) balls under displacement 7.5 mm.

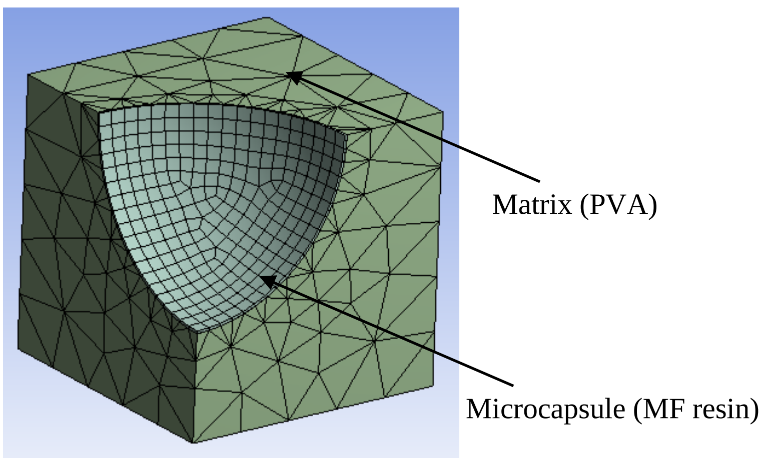

Figure 7. FE mesh of one eighth of RVE

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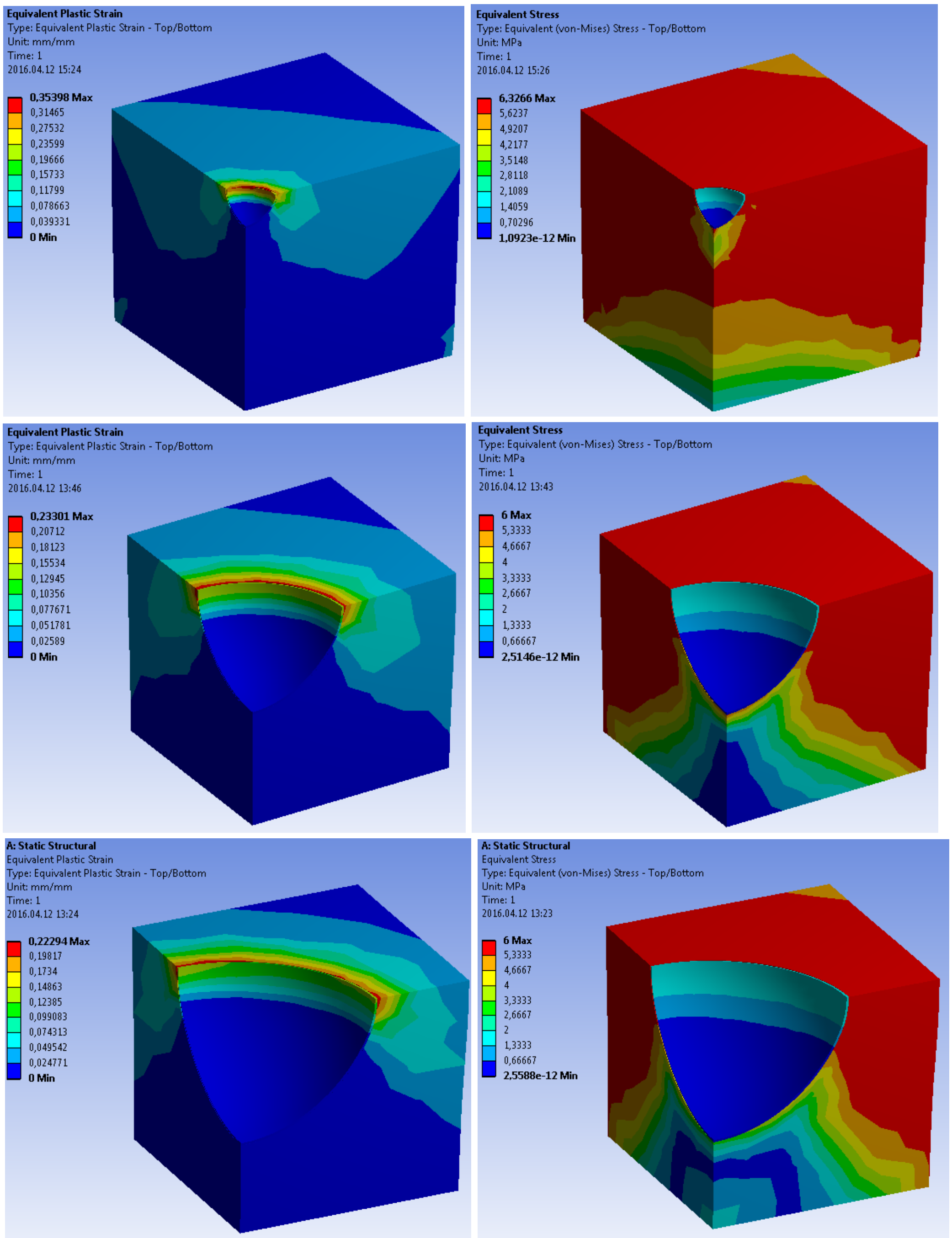
4. Results

Equivalent plastic strain and equivalent von-Misses stress in one eighth of RVE as the applied strain 0.05 are presented in Figure 8. The dependences of strain upon diameter of capsule are presented in Figure 9. The results show that that very small microcapsules or in other words small amount of microcapsules (~1 %) can cause the increase of plastic strains both in the matrix and in the microcapsules shells. In this case microcapsules act only as the stress and strain concentrators and can drastic decrease the mechanical properties of composite.



d = 3 µm

d = 9 µm

d = 12 µm

Figure 8. Equivalent plastic strain and equivalent stress of RVE as the applied strain 0.05.

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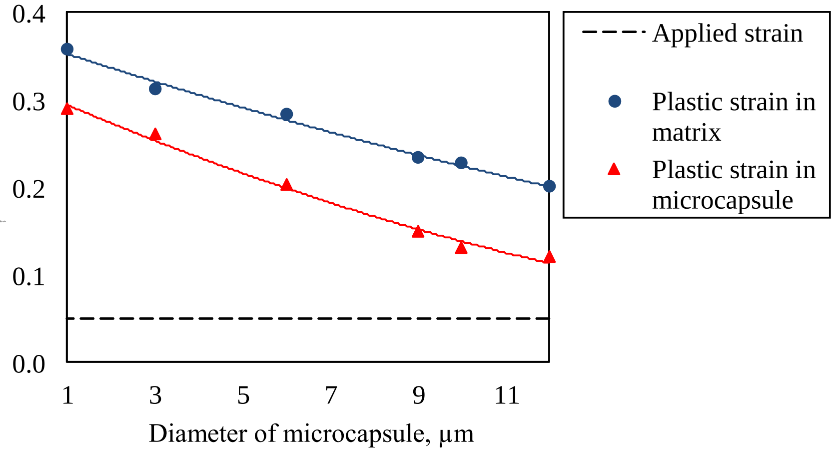

Figure 9. Dependences of strain upon diameter of capsule.

Unfortunately, such cases of very small volume fractions were not investigated experimentally and unambiguous prediction that very small amount of microcapsules works only negative cannot be made, because it was not taken into account that the shell thickness of smaller microcapsules like enough could be smaller as well and this could have the influence into this result. As the diameter of microcapsule increases the plastic strains in the matrix and microcapsule decrease. The experimental testing also shows strength properties increasing as the volume fraction of microcapsules increases.

5. Conclusions

The predictions of the mechanical behaviour and response of these self-sensing structures with microencapsulated active materials embedded into polymer matrices by numerical simulations was made to understand a real phenomenon that occurs at the micro level of the composites. This also allows to speed up the trial and error experimental testing.

Experimentally it was found that microcapsules embedded into PVA matrix increase the mechanical properties of composite. As volume fraction of microcapsules is 50 %, the strength of composite increase in 50 %.

The finite element modelling showed the analogical tendency of mechanical properties increasing. As the volume fraction of microcapsule increases the plastic strains in the matrix and microcapsule decrease.

This introduction research provides possibilities for further deeper micro- and macro-analysis of mechanical behaviour of such type of materials.

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