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The influence of loading direction on micro-crack behaviour in polymer composite

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Abstract

In this paper polymeric particulate composites are studied. Especially on polypropylene (PP) matrix and mineral fillers was focused. Polymeric particulate composites are frequently used in many engineering applications. The composite was modeled as a three-phase continuum — matrix, interphase and particle. The properties of the particles and interphase (size, shape, material properties) have a significant effect on the global behaviour of the composite. On the basis of fracture mechanics methodology the interaction of micro-crack propagation in the matrix filled by rigid particles covered by the interphase was analyzed. Effect of the loading direction on mechanical properties of polymeric particulate composites is studied here.

Keywords: particulate composites, interphase, three-phase continuum

1. Introduction

Polymeric particulate composites with the polypropylene (PP) matrix and mineral fillers are of great practical importance due to the possibility of modifying mechanical properties and reducing the price/volume ratio of resulting material [1, 2]. Polymeric particulate composites are frequently used in many engineering applications. The properties of the particles themselves (size, shape, material properties) can have a significant effect on the global behaviour of the composite. Mainly, the addition of rigid particles to a polymer matrix will have an embrittling effect on the composite. The presence of the interphase between particle and matrix can change final mechanical properties of the composite.

The thickness of the interphase is usually determined indirectly from a composite property, but results depend very much on the method of determination. This fact is demonstrated in paper [1]. The presented interphase thickness of PP-$CaCO_3$ system using various methods based on global material properties of composite (modulus, yield stress, tensile strength) varies from $0.012\,\mu$m to $0.16\,\mu$m. In the paper [3] the interphase thickness is correlated with the work on adhesion and for the uncoated particles is estimated as $0.117\,\mu$m. The thickness of the interphases studied depends only on the matrix and particle chemical composition and seems to be independent of the size of the particle.

The main goal of the present paper is to estimate the influence of load direction on micro-crack propagation in the particulate composite. In the contribution the particle-filled polymer

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composite is modelled as three-phase continuum represented by infinite matrix with homogeneously dispersed identical coated stiff spherical particles. The studied composite corresponds to calcium carbonate ($CaCO_3$) filled polypropylene.

2. Determination of crack propagation direction

A propagation of a micro-crack in the matrix of particulate composite is controlled by its interaction with particles. To describe the interaction the further micro-crack propagation direction has to be known. Generally a crack propagates in direction leading to zero values of K_{II}. For determination of crack propagation direction numbers of criterions exist in the literature. In this paper maximum tangential stress (MTS) criterion [4] has been used. Determination of crack propagation direction Ω_s can then be expressed by the following equation:

$$\Omega_s = \arccos\left(\frac{3K_{II}^2 + K_I\sqrt{K_I^2 + 8K_{II}^2}}{K_I^2 + 9K_{II}^2}\right), \qquad (1)$$

where K_I and K_{II} are corresponding values of the stress intensity factors for normal and shear mode of loading.

3. Numerical model

Generally, it is presented configuration in fig. 1. It was found, that crack propagation is influenced significantly mainly by the nearest particles see [5, 6]. In this case, they are four particles around the crack. In the next, it is used configuration only with four particles ambient the crack.

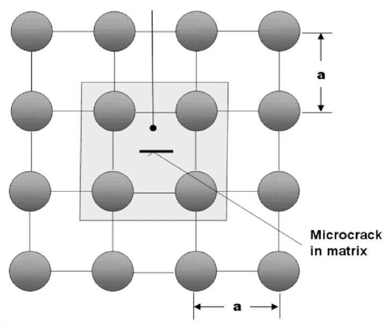

Fig. 1. Homogenous and regular distribution of the particles inside polymer matrix with micro-crack location

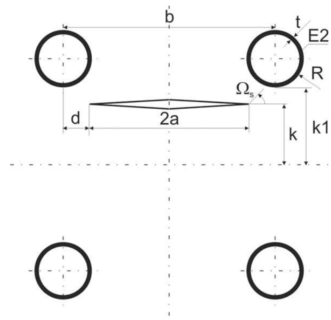

Fig. 2. The geometry of the 2D model used for estimation of micro crack behaviour in the studied particulate composite

To estimate the crack propagation direction the values of stress intensity factors for mode I and II have to be numerically calculated. To this aim the stress strain distribution of the three-phase composite with homogeneously distributed coated particles was numerically simulated on a microscopic scale using the finite element program ANSYS. A simplified 2D model has been used in the present contribution. The geometry of the model is shown in fig. 2.

Tensile load was applied via a prescribed stress in different angles. The finite element model boundary conditions are shown in fig. 3. For calculations plane stress conditions were assumed.

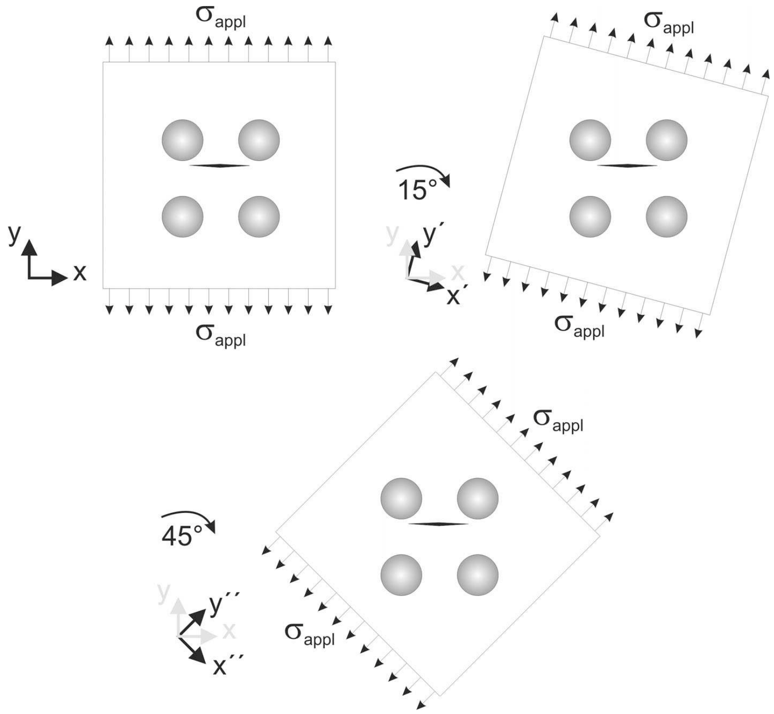

Fig. 3. Configurations expressed different loading directions

Two dimensional isoparametric elements (PLANE82) were non-homogenously distributed, because of the material inhomogenity and high stress concentration in the crack tip. The typical finite element model has about 40 000 elements, see fig. 3.

The material properties characterizing the composite corresponding to calcium carbonate ($CaCO_3$) — filled polypropylene (PP) at room temperature are used. The calculations have been performed for rigid particle dimension (given by radius of the $CaCO_3$ particles $R = 0.5\,\mu$m) and particulate filler volume fraction 25 %. The Young's modulus of the particles $E = 72$ GPa, and the value of Poisson's ratio $\nu = 0.29$. The corresponding parameters of the neat polymer matrix (PP material) are $E = 1.8$ GPa, $\nu = 0.29$. The thickness t of the interphase 117 nm is considered here. The perfect adhesion between particles, interphase and matrix was assumed. The stress and strain distributions in the matrix have been determined for these interphase properties. The value of Young's modulus of the interphase varies from 1.8 to 0.05 GPa. It is assumed that Young's modulus of the interphase is constant through its thickness. A micro-crack of length corresponding approximately to the distance between the particles was modelled and the corresponding values of the stress intensity factors K_I and K_{II} were calculated for different direct of load configurations (see fig. 3).

4. Numerical results

The corresponding values of stress intensity factors K_I and K_{II} were estimated using the standard KCALC procedure as implemented in ANSYS. The mesh around the crack tip has to be refined because of high stress concentration. Special "crack" finite elements with shifted midnodes and modelling the near tip stress singularity were applied. Obtained values K_I and K_{II} were used for estimation of further crack propagation direction Ω_s using eq. (1), see fig. 6.

The influence of the volume fraction of the composite on the crack located close to the particle, i.e. for $k/k1 = 0.9$ and $2a/b \to 1$ has been studied in [7]. Ratio $k/k1 = 0.9$ (it means that tip of crack is in proximity with particle with interphase) was chosen according to calculations in [5]. It was proved that in this configuration is interaction between particle, interphase and crack strongest, see fig. 5.

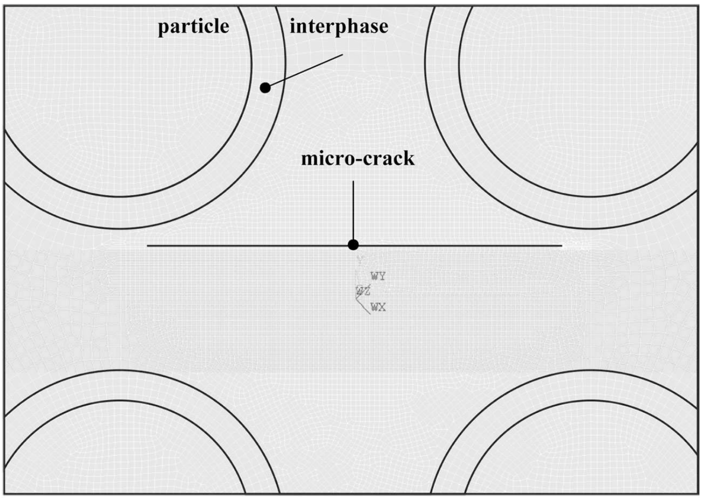

Fig. 4. Example of schematic FEM model

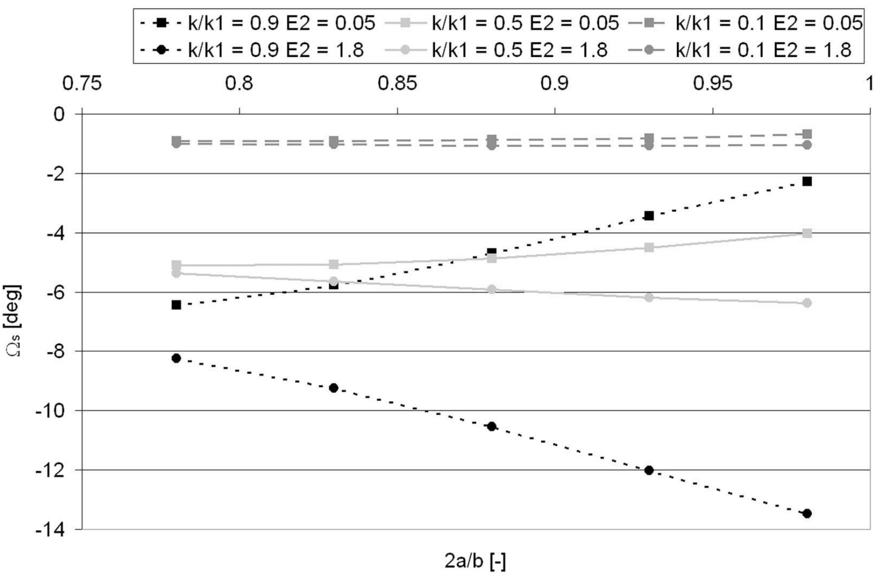

Fig. 5. Dependence of crack propagation direction Ω_s on ratio $2a/b$ for filler volume fraction 25 % for variety of ratio $k/k1$ and elastic moduli $E2$ of interphase

Six configurations were modeled: for three values of k/k1 ratio and for two limiting values of interphase moduli. The curves accordance with value of Young's modulus 0.05 GPa are marked by quads and curves accordance with value of Young's modulus 1.8 GPa are marked by circles. It has to be mentioned, that Young's modulus of the interphase 1.8 GPa corresponds to Young's modulus of the matrix and behavior of this configuration corresponds to the two-phase composite without interphase. Strong decrease of the angle of crack propagation Ω_s corresponds to Young's modulus 1.8 GPa. In this case the micro-crack propagates purely in the matrix and has a tendency to deflect to rigid particles. For this material configurations the direct interaction between particle and crack is rare and has no influence on fracture toughness of the composite.

Contrary to it for interphase with Young's modulus 0.05 GPa the influence of rigid particles is shielded by a soft interface and even for a small volume fraction of the interphase, the behaviour of the micro-crack can be changed. The crack deflection is much smaller and in some cases crack cannot avoid the particle and is attracted to it.

Generalization of the results for various loading conditions is well documented in fig. 6, where four different configurations were modeled. The direction of the loading is changed from pure mode I loading (loading angle $0°$) to $45°$ of the loading direction, see fig. 3. The angles of the further crack propagation direction for the model with a particles covered by the soft interphase in the comparison with homogenous case is visible on fig. 6. The results are in fact superposition of the homogenous case and the effect of the particles with interphase. It means that decrease of the angle of further crack propagation Ω_s corresponds to Young's modulus 0.05 GPa for all mentioned cases is general. Therefore, even for loading direction different from pure mode I, the crack is more attracted by the particles. So, final configuration corresponds then to a micro crack with its tip on the interface between matrix and interphase. Due to existing high stress concentration matrix and particle are debonded and as a consequence, the crack is blunted. This is connected with strong decrease of the stress near the crack tip and the singular stress field is changed to regular one. The crack is transformed to a notch and arrested near the particle.

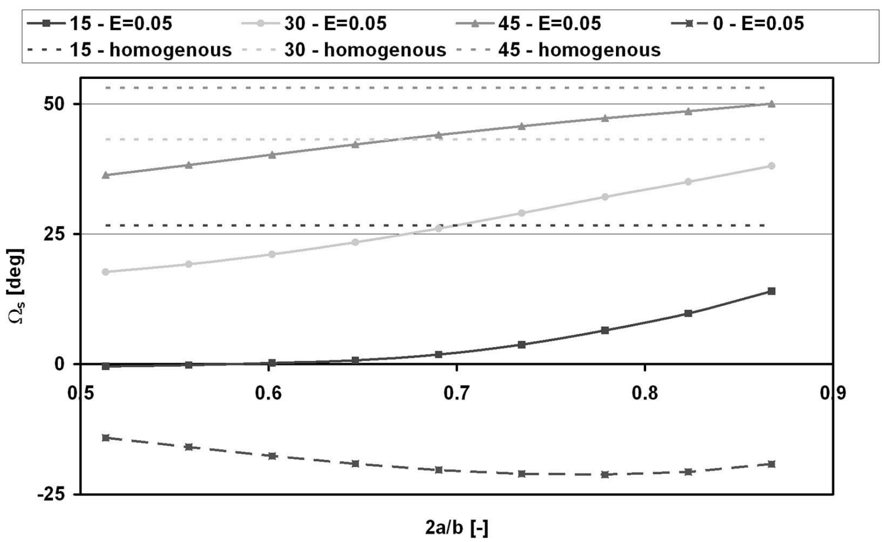

Fig. 6. Dependence of crack propagation direction Ω_s on ratio $2a/b$ for filler volume fraction 25 % for variety of loading directions

5. Conclusion

In the contribution finite element simulations based on the microstructure of polymer composite filled by coated particles are conducted in order to transfer the information from micro- to macro-scale. The simplified 2D model of a micro-crack interacting with the nearest particle was used. All results are generalized for different loading conditions. It was found, that results are in fact superposition of the homogenous case and the effect of the particles with interphase. It means that decrease of the angle of further crack propagation Ω_s corresponds to Young's modulus 0.05 GPa for all mentioned cases is general. Therefore, even for loading direction different from pure mode I, the crack is more attracted by the particles.

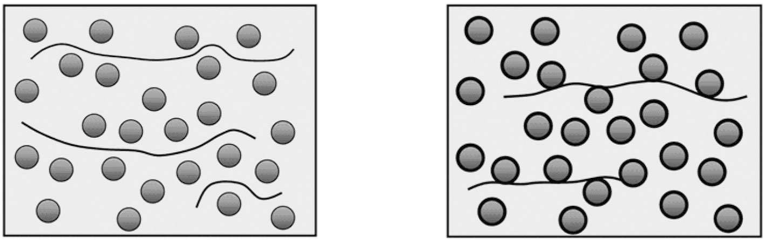

Fig. 7. Example of crack propagation in composite without interphase (on picture top) and in composite with interphase (on picture bottom)

The influence of the interphase between rigid particle and matrix on toughening mechanism was investigated as general. The basic mechanism of the composite toughening due to micro-crack propagation consists in shielding of rigid particles by soft interphase followed by debonding of the particle and the matrix. As a consequence, the crack is blunted and can be arrested on the particle. The intensity of this effect depends mainly on the size and quality of the interphase.

Acknowledgements

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