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NUMERICAL ESTIMATION OF MICRO-CRACK PATHS IN POLYMER PARTICULATE COMPOSITE

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Abstract: *Determination of composite mechanical behavior is one of important part during the composite tailoring. The aim of the present work was to estimate a micro-crack behavior in a polymer particulate composite. The composite was investigated by means of the finite element method - using ANSYS software. A two-dimensional three-phase finite element model was developed to analyze the crack growth behavior. The assumptions of the linear elastic fracture mechanics were considered and the Maximum Tangential Stress (MTS) criterion was used to predict the direction of the crack propagation. The effect of the elastic modulus of the interphase on the micro-crack propagation was investigated. The properties of matrix and particles were taken from experiment. It was shown that the interphase properties influence the stress intensity factor K_I as well as the micro-crack paths. The results of this paper can contribute to a better understanding of the micro-crack propagation in particulate composites with respect to the interphase.*

Keywords: Polymer Composite, Fracture Mechanics, Interphase, Finite Element Method.

1. Introduction

Generally, composites are vastly used in many engineering applications. The main advantage of composites is that mechanical properties can be adapted according to the needs of individual applications. There are many different types of composite materials. One of them is particulate composites, especially the composite with rigid particles and soft matrix, where the particles are used to reinforce the material properties of the matrix. The mechanical behavior of the composite depends on many factors which are associated with particles size, matrix properties, volume filler fraction, etc. (Demjen et al., 1998; Park et al., 2004; Majer et al., 2013). The polymer particulate composites are studied by many authors experimentally (Muratoglu et al., 1995), analytically (Pal, 2005) as well as numerically (Majer et al., 2012). The analytical description of these structures is relatively complicated and the experiments are expensive and time consuming. On the other hand, the numerical approach is easily accessible and could solve many issues in a very short time. Of course, the numerical results should be compared with experimental data (observation) to confirmation.

During the production of the polymer composites the rigid mineral particles are added to the soft polymer matrix. In addition, the mineral particles are usually chemically treated on surface by stearic acid to better dispersion in matrix. This process causes creation of the third phase of the matrix-particle interface, generally called “interphase” (Fu et al., 2008; Kozak et al., 2004). The interphase is a region of a few up to a few hundred nanometers in size. In fact, the interphase controls the adhesion between the matrix and the fillers. The interphase can affect the behavior of the polymer particulate composites. An estimation of interphase properties is not simple due to size of interphase. The properties can be estimated indirectly but the results are significantly dependent on the method of determination (Mesbah et al., 2009). In the paper (Moczo et al., 2002) the interphase thickness was correlated with the work of adhesion and for the polypropylene particulate composite the interphase thickness t of 100 nm was determined.

The aim of the present work was to estimate a crack behavior in a polymer particulate composite using the finite element method. The stress intensity factor K_I versus the crack length was shown.

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2. Computational Model

2.1. Numerical model

A two-dimensional three-phase numerical model was developed, see Fig. 1a. The particles were uniformly dispersed in the matrix with a distance between the particle centers d of 1.25 μm. The diameter D of the round particles was chosen as 1 μm and the thickness of interphase t of 100 nm was used. The initial crack was modeled at a distance c of 0.55 μm from the center line and with an initial length a_i of 0.5 μm.

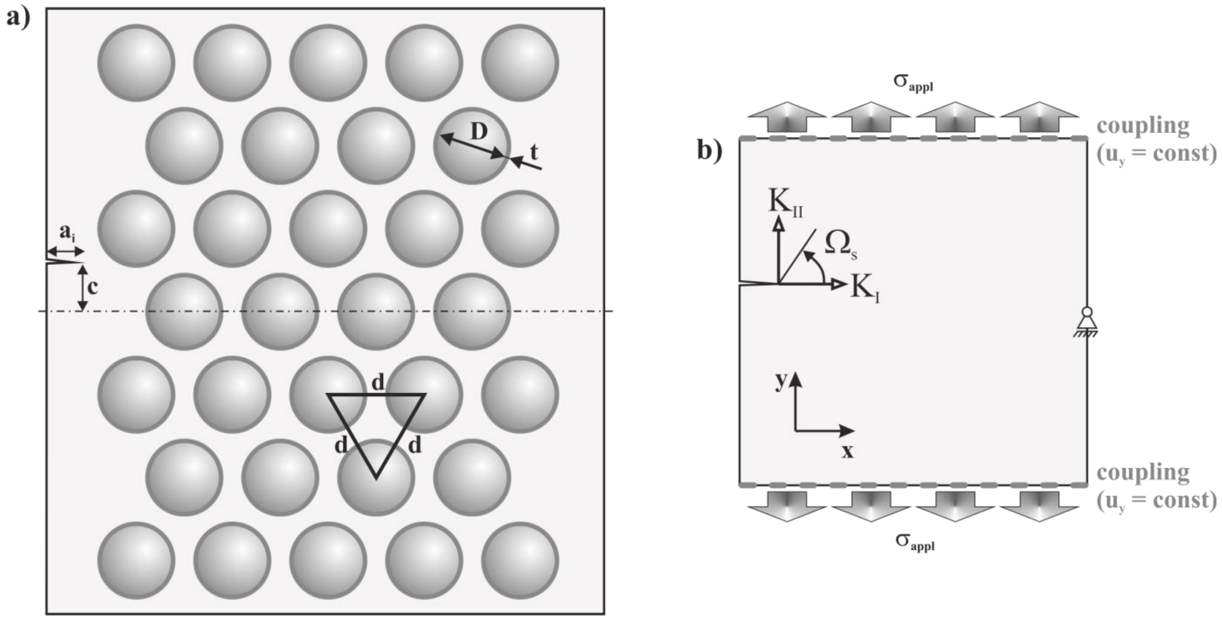

Fig. 1: a) Geometry of the finite element model; b) Used boundary conditions and scheme of the crack propagation direction Ω_s.

Ideal adhesions between matrix, particles and interphase were assumed in the model. The nodes on the top and at the bottom of the model were coupled in the y-direction, see Fig. 1b. A mean stress σ_{appl} of 100 MPa was applied in those regions and held constant throughout the calculation (Majer, 2013). A node on the right of the model was constrained in y direction, as shown in Fig. 1b. Only elastic behavior of the matrix and the particles was considered.

Plane strain condition and elements with quadratic displacement function (ANSYS type “PLANE183”) have been used. The high stress distribution is usually situated around the micro-crack tip and it is important significantly refine the mesh in this area. Moreover, special “crack” finite elements with shifted mid-nodes to capture the stress singularity at the crack tip were used. The values of the stress intensity factors K_I and K_{II} were calculated using the standard KCALC procedure implemented in ANSYS. Obtained values K_I and K_{II} were used for estimation of the direction of the crack propagation.

2.2. Maximum Tangential Stress (MTS) criterion

The propagation of a micro-crack in the matrix of the particulate composite is influenced by its interaction with particles. To describe of the interaction the micro-crack propagation direction has to be known. For the determination of crack propagation direction, numbers of criteria exist in the literature (Sih, 1991). In this paper the Maximum Tangential Stress criterion has been used (Erdogan and Sih, 1963). The criterion assumes that the crack propagates in the direction leading to zero K_{II} values. Determination of crack propagation direction Ω_s can then be expressed by the following equation:

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

where Ω_s is micro-crack propagation direction and K_I and K_{II} are stress intensity factors for mode I and II, respectively.

2.3. Material properties

The experiments were performed at the Institute of Material Science and Engineering, Faculty of Mechanical Engineering, Brno University of Technology in cooperation with the Polymer Institute Brno, spol. s.r.o. A co-polymer well known as PP SHAC KMT 6100 was used as the matrix (produced by Shell International Chemical Co. Ltd.) and its behavior under different load conditions was measured (Mollikova, 2003; Majer & Novotna, 2011).

The Young´s modulus of matrix E_m of 4 GPa was measured (at temperature -50°C) and corresponds value for particles E_p of 72 GPa. The interphase Young´s modulus was considered in range from 0.5 GPa to 4 GPa. The value of Poisson's ratio ν of 0.29 was considered for all phases.The particle size was determined from experiment as 1 μm.

3. Results and Conclusions

A simplified finite element model of micro-crack growth in polymer particulate composite has been developed and stress intensity factors K_I and K_{II} were calculated on the base of the linear elastic fracture mechanics. Only the selected results are shown.

Influence of stress intensity factor K_I (mode I) on the micro-crack length *a* was determined, see Fig. 2. The values K_I were calculated for four configurations; interphase Young´s modulus of 500, 1000, 2000 and 4000 MPa (in fact without interphase). With decreasing of interphase Young´s modulus the value of stress intensity factor increases. It means that the micro-crack could propagate faster in composite with any kind of softer interphase. This effect of interphase is negative.

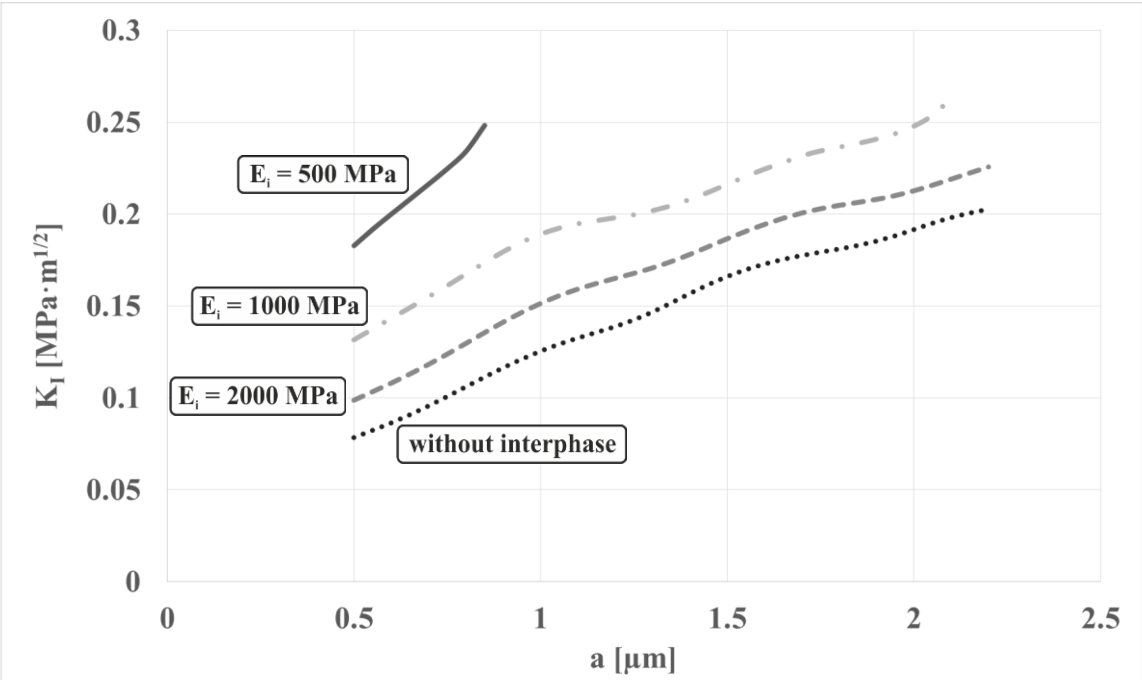

Fig. 2: Calculated values K_I for particulate composite. The initial crack at the distance c of 0.55 μm from the middle plane was considered. Four values of interphase Young's modulus were considered.

On other hand, micro-crack paths influenced by interphase are shown in Fig. 3. It is seen that for two softest interphases (500 and 1000 MPa) the micro-crack is practically attracted to the rigid particle. In fact, for interphase with Young´s modulus of 500 MPa the micro-crack touches immediately to the closest particles covered by interphase. For 1000 MPa the micro-crack is not so strongly attracted; nevertheless, micro-crack encounters to other particle. Consequently, the particle can be fully debonded because of high stresses in the interphase which is damaged. As a result, the micro-crack is blunted and stays arrested on the particle. For re-initiation it needs some time and much more energy. The blunting of micro-cracks in connection with debonding can contribute to an increase in the fracture toughness of the composite. The results of this paper can contribute to a better understanding of the micro-crack propagation in particulate composites with respect to the interphase.

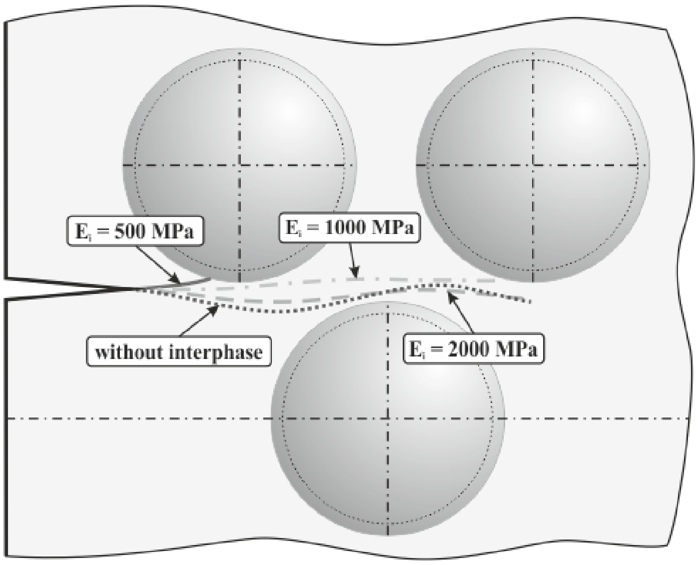

Fig. 3: The paths of the micro-cracks for the distance c of 0.55 μm are shown.

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