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Computational estimation of micro-crack behaviour in polypropylene copolymer

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ABSTRACT

In many applications of polymeric materials mechanical properties are decisive or at least of non-negligible importance. Improvement of toughness is of particular interest, since the toughness of polymeric materials is an important selection criterion for many applications. Toughness is one of the most complex properties, so it is of fundamental importance to understand the relationship between the morphology, deformation and crack behaviour in modified polymer systems.

Presented work is focused mainly for the polypropylene based composite filled by mineral fillers like calcium carbonate $CaCO_3$. Generally, the addition of rigid particles to polymer matrix leads to embrittling effect on the composite. The presence of particles significantly influences the cure reaction, resulting in the formation of the third phase known as the interphase, which possesses property distinct from those of the matrix and the particle. This region controls the adhesion between particles and the matrix and plays an essential role in the composite resistance against crack propagation [1,2].

Computation of the internal stress and strain fields in the microstructural level of the studied composite and understanding of microcracks behaviour in the interaction with particles is the first step to understanding the global behaviour of the composite based on microstructural morphology. Therefore, particle reinforced composite has been modelled as a three-phase material with homogenously distributed coated particles and numerically studied on the microscopic scale using finite element modelling. The FEM modelling and unit cell models provide an effective tools for parametric study of the three-phase composite mechanical properties [3,4].

The material properties characterizing polypropylene based composite corresponding to calcium carbonate ($CaCO_3$) and polypropylene at room temperature are used. The properties of the interphase are varying in the interval given by literature data [2]. It is assumed that Young's modulus of the interphase is constant through the thickness and perfect adhesion between particles, matrix and interphase is considered. A micro- crack of length corresponding approximately to the distance between the particles was assumed in the matrix region and corresponding values of the stress intensity factors were calculated. A micro-crack path in the particle composite was predicted as a function of the interphase material properties and its relative thickness.

Generally, a crack propagating in the matrix has a tendency to deflect to the regions with stiffer materials. For perfect adhesion between particle and matrix (effect of the interphase is negligible) micro-crack is propagating in the matrix only, see fig.1-1. If the particle is coated, this effect is shielded by the existence of the softer interphase and under certain conditions (given by its thickness and material properties) the trend of crack propagation can be characterised by the attraction to the particle, see Fig.1-2.

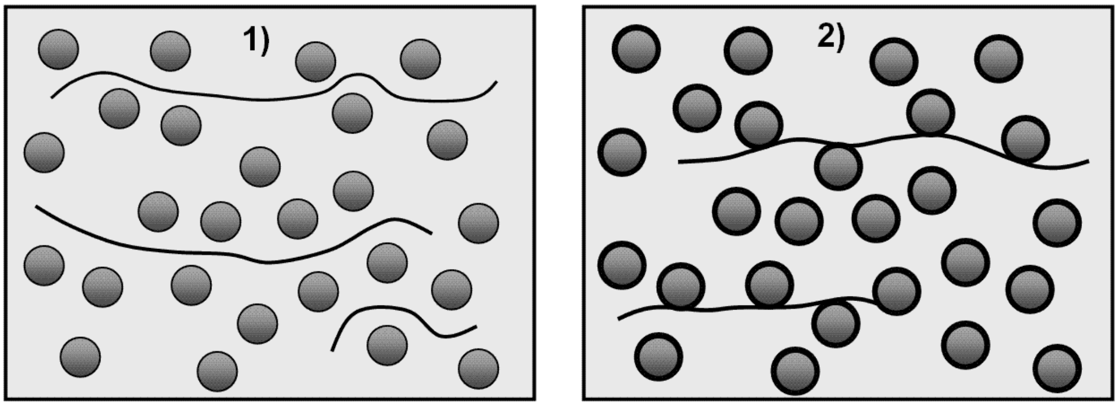

Fig.1. 1 - micro-crack propagation in the case of rigid particles without an interphase and 2- micro-crack propagation in the case of coated particles

It is suggested that the interaction between particles and micro-cracks plays a deciding role on fracture resistance of the composite. The basic mechanism consists in shielding the stiff particles by a softer interphase followed by the debonding. This is connected with a blunting of micro-cracks. The intensity of toughening depends on the size and quality of the interphase.

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