NUMERICAL SIMULATION OF CRAZE INITIATION AND GROWTH IN GLASSY POLYMERS

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ABSTRACT

Crazing process in rubber particle modified glassy polymers is numerically simulated by using micromechanics and finite element methods. To simulate the initiation and growth of craze, craze elements are prearranged in the unit cell mode, in which Drucker-Prager's plastic constitutive relation is employed to describe the deformation behavior of craze elements. Modified Sternstein's criterion is used as the initiation criterion of craze in which effect of hydrostatic stress is considered. Effect of craze on the macroscopic deformation behavior of polymer is discussed. Moreover, effects of the volume fraction of rubber particle and craze on the macroscopic deformation of polymers are discussed in detail.

1 INTRODUCTION

Craze, a web of interpenetrating voids (~20*nm*) and fibrils (5~45*nm*) is a special phenomenon in glassy polymer. The fibrils are mainly oriented in the direction normal to the craze plane. The primary and secondary (or cross-tie) fibrils bridge the craze surfaces together. Such that load can be transmitted through the craze structure which results in the toughening of polymer. Usually, the crazing process in polymer includes three stages: initiation, growth and breakdown. Microstructure of craze consists of active zone, crack zone and matrix material. Bucknall and Smith[1] attributed the improvement of toughness of polymer to the formation of multiple crazes around the rubber particles, and gave a successful explanation to the toughening mechanism of rubber modified HIPS. Micromechanics method was used by Socrate et al. [2] to numerically simulate the crazing process in polymer. In the last decades, extensive works has been devoted to the crazing phenomenon and different models have been proposed [1-7]. However, it is still an open problem.

Here, crazing process in glassy polymer is investigated in the framework of micromechanics in which craze element is incorporated into representative volume element. Effects of the volume fraction of rubber particle and craze on the macroscopic deformation of polymers are discussed in detail.

2 CRAZE CRITERION AND CONSTITUTIVE LAW

We modify the craze initiation criterion proposed by Sternstein et al [3] as

$$f\left(\sigma_e,\sigma_m\right)=\sigma_e+k\sigma_m-\sigma_c=0$$

where σ_e is von Mises stress, σ_m is hydrostatic stress, σ_c is critical stress, and k is a constant. Here, we choose k=0.95 and σ_c =40MPa.

Once a mature craze structure formed, the growth of craze includes the propagation in its original direction and the increase in its thickness direction. Williams [4] neglected the microstructure of craze and treated the craze zone as a continuous zone, in which perfect-plasticity theory was employed to describe the mechanical behavior of craze zone. Here, we use the following well-known Druck-Prager plasticity theory instead of the perfect-plasticity theory employed by Williams [4] to consider the effect of hydrostatic stress,

$$f=\alpha I_1+\sqrt{J_2}-k=0 \quad \text{with} \quad \alpha=\frac{2\sin\phi}{\sqrt{3}\left(3-\sin\phi\right)} \quad \text{and} \quad k=\frac{6C\cos\phi}{\sqrt{3}\left(3-\sin\phi\right)}$$

where I_1 and J_2 are the first and second stress invariants, respectively, C is the cohesive value, and ϕ is the angle of inter friction. The dilatancy angle varies from 0^o to ϕ. Here, we choose ϕ=40^o and C=4.0MPa.

3 MICROMECHANICS MODEL AND CRAZE ELEMENT

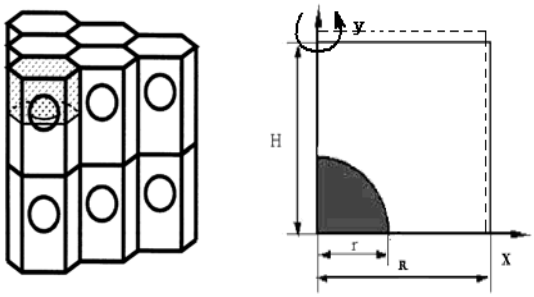
Socrate et al. [2] numerically simulated the crazing process in HIPS by using micromechanics and finite element methods. The axisymmetric unit cell mode, as shown in Figs 1(a) and 1(b) are used in computation where the following periodic boundary conditions are considered.

$$x=0, U_x=0;\ y=0, U_y=0;\ y=H, U_y=U_0$$

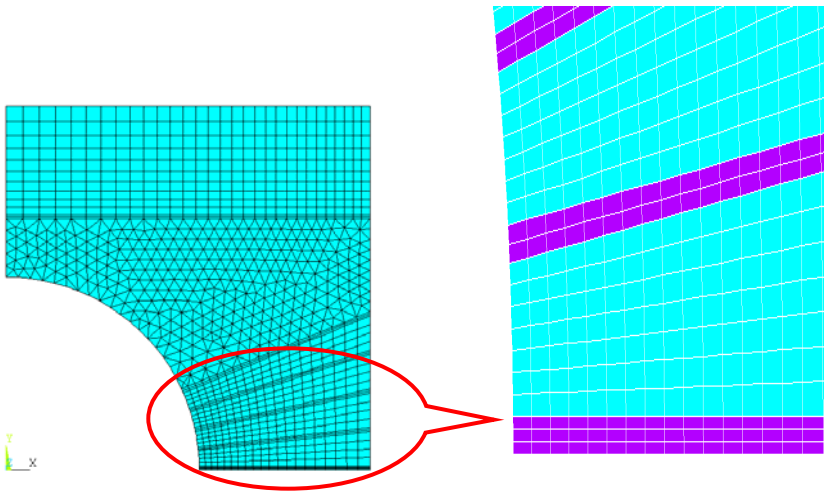
where U_x and U_y are the displacements in x and y directions, respectively, and U_0 is the applied displacement. The macroscopic stress is defined as $\Sigma=F/S$, where F is resultant force and S is true area. The macroscopic strain is defined as $E=\ln(H/H_0)$, where H and H_0 are true and initial length of the unit cell, respectively.

Huang and Kinloch [7] verified that the mechanical behavior of rubber particle modified polymer is almost the same as that of porous material. Such that one can use the unit cell mode with void instead of rubber particle in calculation. According to the experimental observation of crazing [6] and the results obtained by Socrate et al [2], craze elements are prearranged in the FEM meshes in six different places, as shown in Fig.1(c). Width of craze zone on the equator of particle is about 4% of rubber particle radius and otherwise it is about 2% of rubber particle radius. The

material parameters are the same as that used by Socrate et al [2]. In what follows, the well-known ANSYS 6.0 FEM code is employed to carry out the computation.



(a) SHA model (b) Axisymmetric unit cell mode



(c) FEM meshes with craze elements

Fig 1: Unit cell mode and FEM meshes with craze elements.

In numerical implementation, Young's and shear moduli of matrix material are 3.0GPa and 1.15GPa, respectively. Craze elements take different mechanical behavior in different stage of deformation, i.e. before craze initiation, the mechanical behavior of craze elements is the same as that of matrix, after craze initiation, the mechanical behavior of craze elements obey Drucker-Prager law. The stress-strain relation of matrix is shown in Fig.1. Using the unit cell mode shown in Fig.1, we obtained the stress and strain curves of rubber particle modified PS with and without craze. It is clear that the results obtained from the unit cell modes with void instead of rubber particle are almost the same which is in consistent with Huang and Kinloch [7]. On the other hand, we can see that the stress and strain curves of the material with craze is very different from that of

the material without craze. In other words, craze results in the toughening of polymer.

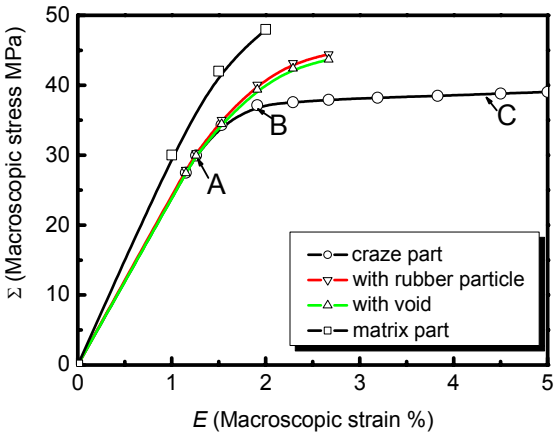
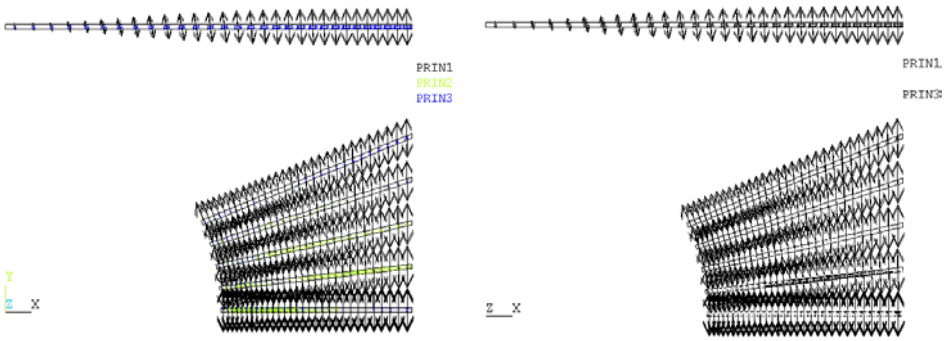


Fig. 2 Stress-strain curves of PS, rubber particle modified PS with and without craze.

The maximum principal stress vectors in craze elements during craze growth process obtained from our computation shown in Fig.3 indicate that the direction of maximum principal stresses are perpendicular to the direction of craze propagation, which is better than that obtained by Socrate et al [2]. In what follows, we will use the unit cell mode shown in Fig.1 to simulate the initiation and growth of craze in polymer.



(a) Onset of macroscopic yield (b) about 4% axial strain

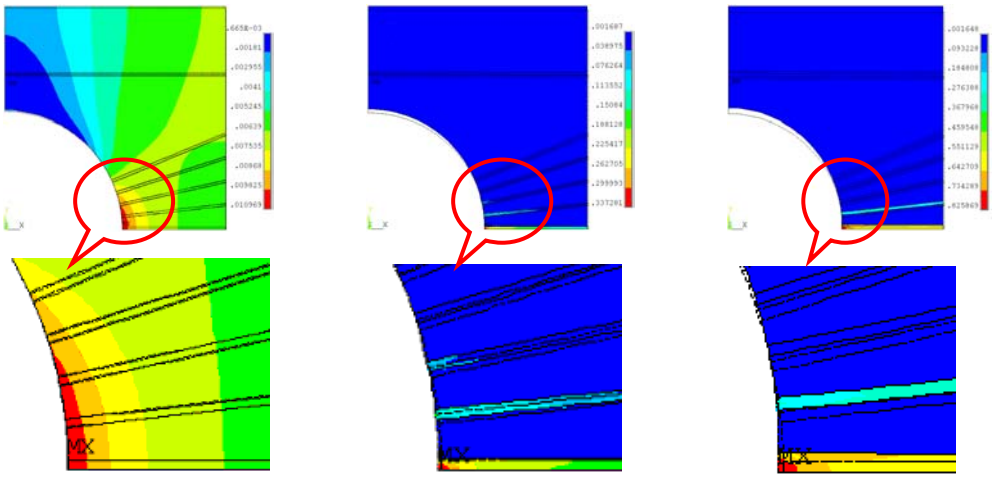
Fig. 3 Maximum principal stress vectors in craze elements at different deformation stage.

4 CRAZING PROCESS AND ITS EFFECT ON THE TOUGHENING OF POLYMER

4.1 Crazing process

Microscopic strain distribution at three different deformation stages corresponding to points A

(about 1.2% axial strain), B (about 1.8% axial strain) and C (about 4% axial strain) shown in Fig. 2 are shown in Fig. 4, respectively, from which one can see the crazing process in glassy polymer. At elastic deformation stage, deformation localized in the equator of particle, and matrix and the craze elements have the same deformation behavior, as shown in Fig. 4 (a). After yield onset, deformation manly localized in the craze elements, the craze propagates in its original direction and grows in the thickness direction, see Fig.4 (b) and (c) for more detail.



(a) axial strain 1.2%, (b) axial strain 1.8%, (c) axial strain 4%

Fig. 4 Microscopic strain distribution in the matrix and craze elements.

4.2 Effects of rubber particle volume fraction and craze on macroscopic deformation

Numerical calculations are carried out to investigate the effects of rubber particle volume faction and craze on the macroscopic deformation behavior of polymers. The volume fraction of rubber particle are 5%, 10% and 15%, respectively. For each case, the unit cell mode with and without craze elements are considered, respectively. The numerical results are shown in Fig.5, from which one can see the clear effects of particle volume fraction and craze on the macroscopic deformation behavior of polymer, particularly the toughening effect induced by crazing.

5 CONCLUSION

Crazing process and its effect on the toughening of glassy polymer are numerically investigated by using micromechanics and finite element methods. In analysis, craze elements are prearranged in the matrix. At elastic deformation stage, the material behavior of craze elements are the same as matrix. After onset of yield, the material behavior of craze elements are different from matrix and are assumed to obey the well-known Drucker-Prager law. Modified Sternstein's criterion is used as

the initiation criterion of craze in which effect of hydrostatic stress is considered. It is seen that crazing process can effectively be simulated through the above mentioned method and theory. One can see that crazing process has significant effect on the toughening of polymer.

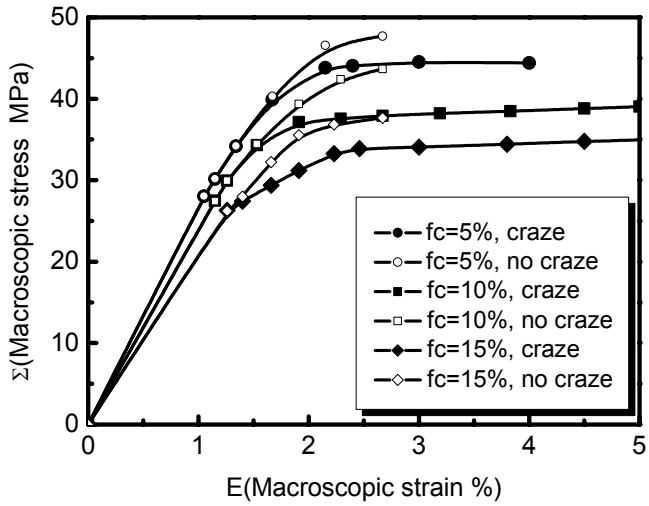


Fig. 5 Stress-strain curves for polymers with different particle volume fraction.

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