

FINITE ELEMENT SIMULATION FOR YIELD STRESS OF HARD POLY(VINYL CHLORIDE)/ACRYLONITRILE-BUTADIENE-STYRENE BLENDS AT DIFFERENT CROSSHEAD SPEEDS*

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Abstract Hard poly(vinyl chloride) (PVC)/acrylonitrile-butadiene-styrene (ABS) blends were prepared using injection-molding and influence of crosshead speed on mechanical properties was examined. Based on morphology parameters obtained from transmission electron microscopy photography and the material parameters from true stress-strain curves of neat PVC and ABS, yield stresses of the blends at different crosshead speeds were simulated employing a two-dimensional nine-particle model based on the finite element analysis (FEA). The FEA results were compared with the experimental yielding stress and the good agreement validated the simulation approach. The FEA approach allowed establishing a yielding criterion related to local yielding of the interstitial matrix between ABS particles.

Keywords: Poly(vinyl chloride) (PVC); Acrylonitrile-butadiene-styrene (ABS) resin; Deformation and fracture; Simulation and modeling.

INTRODUCTION

Finite element analysis (FEA) is a powerful computational technique for approximate solutions to a variety of real engineering problems. A variety of finite element micromechanical models have been developed to model elasticity^[1–5], toughness^[6, 7] or fracture behaviors of polymer composites or blends^[8–12]. However, very limited modeling studies have been performed on rubber-toughened polymers to predict the yield strength at different crosshead speeds.

In the present study, hard poly(vinyl chloride)/acrylonitrile-butadiene-styrene (ABS) (PVC/ABS) blends are prepared through injection-molding. The mechanical properties of the blends at different crosshead speeds are investigated. Based on structural parameters determined through morphological observation and material parameters determined from true stress-strain curves of pure PVC and ABS, finite element simulation employing a two-dimensional representative volume element model is carried out to predict yield stress of the blends stretched at different crosshead speeds.

* This work was financially supported by Key Projects in the National Science & Technology Pillar Program (No. 2007BAE10B04).

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Received January 7, 2011; Revised, March 8, 2011; Accepted March 28, 2011

doi: 10.1007/s10118-011-1090-2

EXPERIMENTAL

One hundred phr (per hundred resin) PVC (S-700, Qilu Petrochem. Co., Shandong, China) and 0–28 phr ABS core-shell particles (HR-181, Kumho Petrochem. Co. Ltd., Korea, 12% acrylonitrile, 60% butadiene and 28% styrene) were used to prepare hard PVC/ABS blends. The additives incorporated in the blend included 2 phr organic tin (HTM-2010, Haipudun Chem. Co. Ltd., Zhejiang, China), 1.4 phr lanthanum stearate (Jiangyin Huashi Plastic Aids Plant, Jiangsu, China), 0.5 phr calcium stearate (Wenzhou Chem. Reagent Plant, Zhejiang, China), 4 phr glyceryl monostearate, 3 phr acrylate processing aid (ACR 401, Hangzhou Chuanhua Co. Ltd., Zhejiang, China). All additives and ABS were first mixed into PVC powders using a high-speed mixer (10 L, Wuhan Yiyang Plastics Machinery Co. Ltd., Hubei, China). The mixture was melt blended in a conical twin-screw extruder (Wuhan Yiyang Plastics Machinery Co. Ltd., Hubei, China) and the extrudate was pelletized by hot cutting. The pellets were then injection molded into tensile specimens according to GB16421-1996 using an injection molding machine (Boy 55, Germany). Tensile tests were performed using a universal testing machine (CMT4202, Shenzhen SANS Test Machine Co. Ltd., China) according to GB16421-1996 with a tensile velocity of 1 mm min⁻¹ to 500 mm min⁻¹ at 20°C. At least eight specimens were tested for each set of samples.

FINITE ELEMENT ANALYSIS

Two-dimensional computational models were established to explore stress field distributions using ABSQUS 6.9 FEA software (dassault systèmes, France). Two reasonable assumptions were made for creating the FEA model. The first was that ABS particles were evenly distributed in the PVC matrix according to transmission electron microscopy (JEM-1230, JEOL Ltd., Japan) observations and the second was that the interaction between PVC matrix and ABS particles was strong enough so that no debonding occurred at their boundaries during fracture process. The second one was proposed according to dynamic mechanical analyses of the blends at frequency 10 Hz. Good compatibility between PVC and styrene acrylonitrile polymer (SAN) was assigned according to a unique thermal transition of the PVC/SAN rigid phase surrounding the rubbery polybutadiene phase, which allowed building strong interfacial adhesion between the PVC matrix and the ABS particles.

Two-dimensional nine-particle FEA models with spherulite-shaped ABS particles were constructed, as schematically shown in Fig. 1, to investigate distribution of stress field and yield stress for the blends. As the stress field was not evenly distributed, the nine-particle models allowed describing interaction of adjacent particles in different directions accurately in comparison with the one-particle models^[10]. According to morphological observation, ABS particles with diameter (d) ranged from 0.17 μm to 0.20 μm were approximately homogeneously dispersed in the matrix. Matrix ligament thickness (T) decreasing from 0.238 μm to 0.048 μm with increasing ABS content from 4 phr to 28 phr was determined according to $T = d \{ [\pi / (6\phi)]^{1/3} - 1 \}$ ^[13, 14]. Here, ϕ is volume fraction of ABS. The kinetic factor of the material microstructure is important for FEA. Density and Poisson's ratio used as input parameters for the models were supplied by the manufacturers. The dynamic mechanical responses of the model were related to the kinetic parameters of PVC matrix and ABS particles. Young's moduli as well as stresses at different plastic strains were evaluated according to true stress-strain curves of injection-molded PVC and ABS bars stretched at different crosshead speeds, which were used as input parameters for the FEA models. The yield stress of PVC was 54.9, 68.0, 74.7 and 86.5 MPa at the crosshead speeds of 1, 10, 100 and 500 min min⁻¹, respectively. Stress was applied on the FEA models along the y -direction in the Cartesian coordinates. The PVC matrix and the ABS particles in the model were meshed using CPS4R and CPS3 element types. The number of elements depended on T . Tie constraints were created at the boundaries of the PVC matrix and the ABS particles.

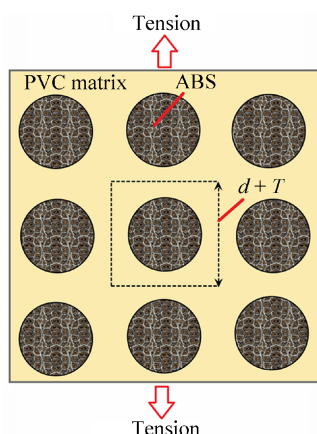


Fig. 1 Schematic of morphology-based nine-particle FEA model under tensile force

RESULTS AND DISCUSSION

Figure 2 shows true stress-strain curves for 4 phr ABS toughened PVC at different crosshead speeds. Figure 3 shows contour plots of von Mises equivalent stress for FEA model at applied stresses of 20.0, 50.0, 54.9 MPa, respectively, for the bar deformed at 10 mm min^{-1} . Increasing crosshead speed leads to increases in yield stress and elastic modulus with consumption of break strain. According to the evolution of stress distribution from FEA, the stress-strain curves can be divided into three regions: region I (elastic deformation region below 40.0 MPa), region II (subyielding region from 40.0 MPa to 54.9 MPa) and region III (postyielding region above 54.9 MPa). Regions II and III are divided by the yielding point at 54.9 MPa. In region I, the high stress region with local stress more than 10.0 MPa higher than the applied stress initiates around the equator side of ABS particles, while the low stress regions are located around the polar side of ABS particles. In region II, local stress in some sites in the high stress region reaches yield strength of PVC, which initiates local plastic deformation in the matrix. As the applied stress increases in region II, stress values of both the high and the low stress regions keep nearly constant while the yielded area expands rapidly along the equator side of the particles and tends to connect each other. The occurrence of yielding along the equator side is responsible for the decrease in slope of stress-strain curve in the subyielding region. In region III, the applied stress exceeds yield stress (54.9 MPa) of the blend, and the yielded areas extend along the equator direction of particles and interconnect throughout the interstitial matrix between the particles.

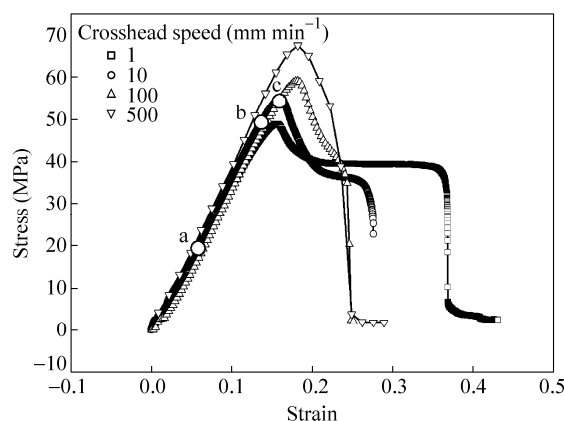


Fig. 2 True stress-strain curves for 4 phr ABS toughened PVC bars stretched at four different crosshead speeds
The stress data at points (a), (b) and (c) as marked on the curve at 10 mm min^{-1} were used for creating of FEA model.

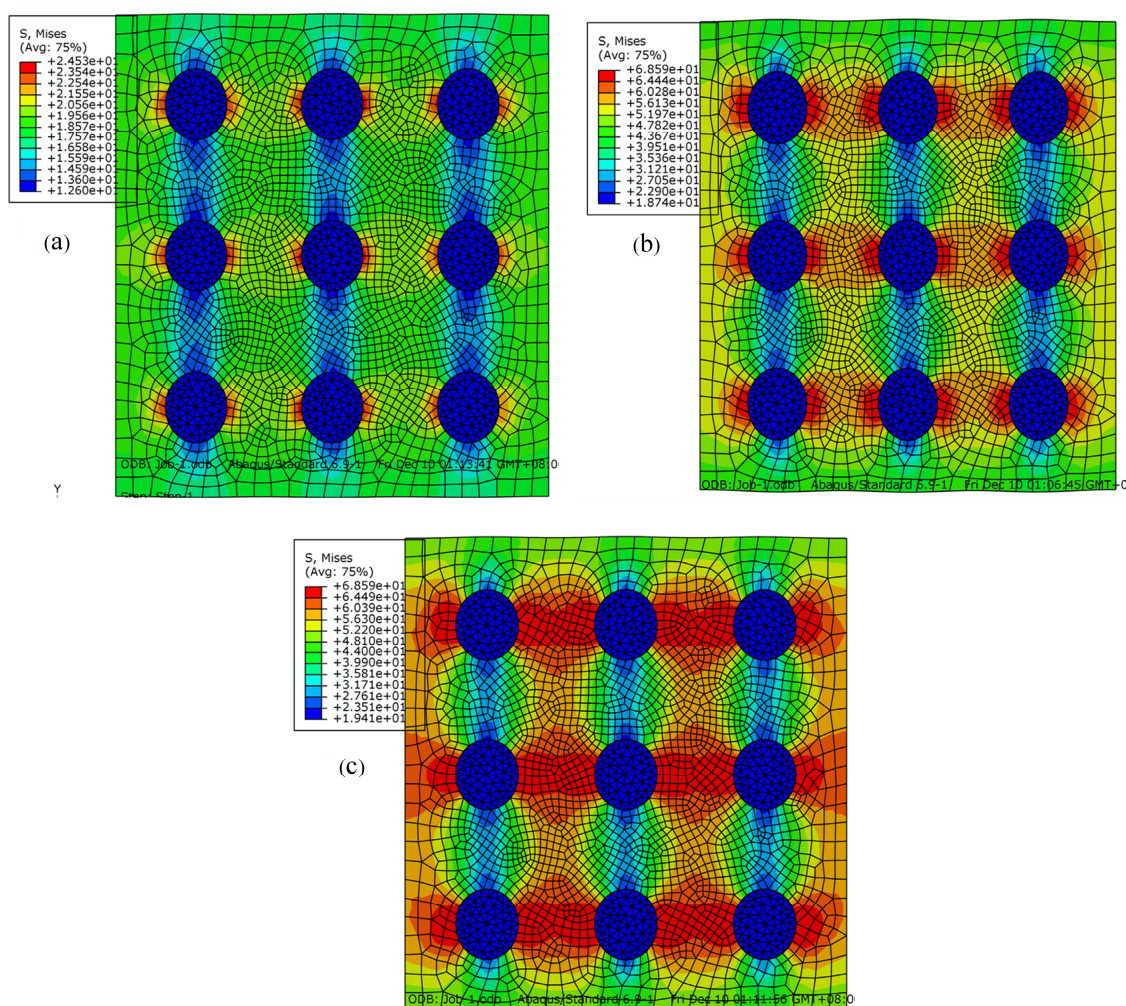


Fig. 3 Contour plots of von Mises stress for FEA model at applied stresses of 20.0 MPa (a), 50.0 MPa (b), and 54.9 MPa (c), respectively, for the bar deformed at 10 mm min^{-1}

The simulation reveals that the blend yields when local yielding areas in the matrix begin to interconnect throughout the interstitial matrix along the equator side of ABS particles. Yielding stresses of the blends at different crosshead speeds are predicted according to this yielding criterion. Figure 4 presents the predicted and the experimental yielding stress values of the blends. Yielding can be related to molecular relaxation that would be restricted at high strain rates, so the yielding stress of the blend increases with increasing strain rate^[15, 16]. The predicted yield stresses show good consistency with the experimental values, indicating that the morphology-based nine-particle FEM is efficient to estimate the yielding behavior of toughened PVC. The FEA results also indicate that T affects yielding stress of the blend by its influence on the interconnection of local yielding areas. On the other hand, crosshead speed affects the yielding stress of the blend mainly by its influence on yielding strength of the PVC matrix. The size of the dispersed ABS spherulites remains almost constant, which excludes the influence of ABS size on yielding stress of the blend. However, a variation in acrylonitrile content in the ABS core-shell particles would influence the compatibility between ABS and PVC, which undoubtedly impacts on the toughening behavior of PVC blends. The morphology-based nine-particle FEM method will be applied to study the influence of ABS size on the yielding and toughening behavior of PVC blends, which will be reported later.

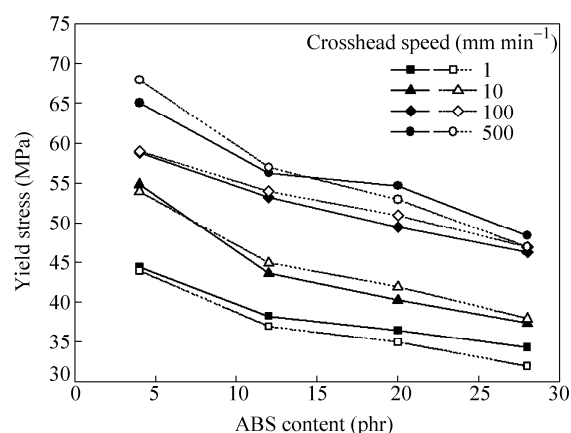


Fig. 4 Comparison between the measured (solid symbols) and the simulated (hollow symbols) yield stresses

CONCLUSIONS

The yielding behavior of PVC/ABS blends has been numerically estimated using two-dimensional nine-particle FEA models. FEA results show that the blend yields when local yielding areas in the matrix begin to interconnect throughout the interstitial matrix between the particles. The key factors dominating the yield stress of the blends are the stress value of the high stress area and the distance between adjacent high stress areas.

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