

# Development of Microscopic Damage Model for Impact Failure Simulation of Polymeric Components

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## ABSTRACT

For simulating the final failure of the component made by polymeric materials based on the microscopic material properties, the craze density-based softening law was proposed phenomenologically. The microscopic experiment was conducted while the craze nucleation, growth and fibril failure were simulated with the coarse grained molecular dynamics model. The impact failure test was also conducted on the actual automotive part. The deceleration time history and damage zone development were compared with those obtained by the finite element (FE) analysis. As a result, the usefulness of the constitutive equations with microscopic material properties was validated.

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## 1. Introduction

Continuing efforts by automotive manufacturers to increase environmental and safety performance have generated increasingly diverse and sophisticated performance requirements for automotive components. To satisfy performance requirements that are expected to diversify even more in the future, further increases in product performance, crash performance and cost performance are being sought. This makes the study of the chemical composition of materials a greater part of the development process for automotive components.

Important components in terms of crash with pedestrians and the collision of passengers with the interior of the cabin are the instrument panel, the door lining, and the bumper face. These components are manufactured from plastics such as polypropylene, the crash performance of which is known to be determined to a large degree by the chemical composition of the material<sup>(1)</sup>.

To analyze the large deformation impact characteristics of these plastic components, it is essential to determine material constitutive laws dealing with the microscopic damage (craze) resulting from micro-voids and fibril failure that can be observed in glassy plastics. A great deal of research has already been conducted on the craze using micro-scale simulations<sup>(2)-(6)</sup>. These studies have clarified the fact that the initiation of the

craze growth is affected by the length of high molecular chains<sup>(2)-(3)</sup>, and the fact that fracture energy on the macro-level in glassy plastics is determined by the elastic property and the fracture stress of the craze, which represent physical quantities on the micro-level<sup>(4)</sup>. The mechanism of the craze is also being clarified using micro-scale simulations, for example simulations that express the mechanism of nucleation of the craze by means of molecular chain entanglements<sup>(5)-(6)</sup>.

Considerable research has also been conducted using macro-scale simulations in attempt to predict the behavior of glassy plastics after yielding<sup>(7)-(9)</sup>. However, while the constitutive laws developed by this research enabled the prediction of the nucleation of the craze, they could not predict the growth of the craze and the formation of shear bands. Research in this area was conducted by Shizawa, et al., resulting in the proposal of material constitutive laws that enabled prediction of both phenomena<sup>(10)-(13)</sup>. These constitutive laws (the Shizawa, et al. model) comprise a law of strain rate hardening, a law of the craze nucleation, and a law of the craze growth. Their material constitutive model demonstrated excellent correlation with the results of static tensile tests on polypropylene and polycarbonate in micro-scale simulations, but the validation for predicting the deformation and failure at the medium and high strain rates, which are generated in automotive crash has not been conducted. In addition, to conduct analyses from the chemical composition level to

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the component level, it is necessary to formulate material constitutive models and analytical method that link the micro- and macro-scales.

The present paper therefore proposes a craze density-based softening law as a phenomenological model to enable simulations of large impact deformation processes at the component level that include consideration of micro-scale material parameters. To this end, the softening law is proposed phenomenologically based on the modeling of final failure due to the nucleation and growth of the craze and fibril breaks, using the results of tests at the micro-scales and coarse grained molecular dynamics. The above-mentioned Shizawa, et al. model is modified by means of the incorporation of this softening law, and material constitutive laws that can now be used in analyses at the component level are proposed. Finally, the results of tests and analyses at the component level are compared and then the analytical method is validated.

## 2. Test Method

### 2.1. Test Specimen and Test Material

The material used for this research was thermoplastic semicrystalline polypropylene often used for the interior and exterior parts of automobiles. When this material is to be used for parts which are to be loaded by impact, elastomer is added to toughen the thermoplastic. Therefore, the materials are ductile up to the high strain rate<sup>(14), (15)</sup>. Polypropylene blended with elastomer was chosen as the test specimen for this research to evaluate the failure behavior of impact parts. Figure 1 shows a schematic of the test specimen. This was a compact tension test specimen, using the specifications stipulated by ASTM D5045-93. The specimen was cut from a bumper face. A 0.2-mm pre-crack was made at the crack tip using a sharp cutter knife prior to the tests.

### 2.2. Test Equipment and Methods

#### 2.2.1. Tensile test inside environmental SEM

Tensile tests were conducted inside an environmental SEM to enable measurement of the large deformation and

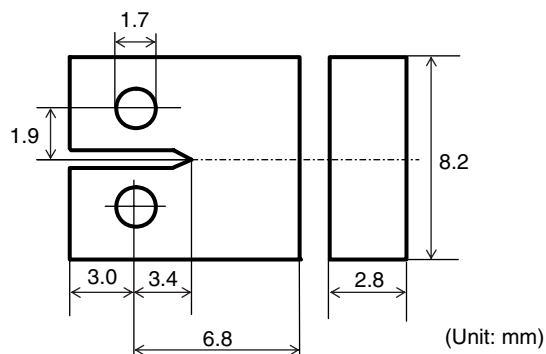


Fig. 1 Schematic illustration of compact tension test specimen

failure behavior of the craze at the micro level. A Deben M5000 micro tensile stage was placed in an environmental SEM (Quanta 600F manufactured by FEI Co.) and the compact tension test specimen was applied by tensile loading. Figure 2 shows a photograph of the specimen and the tensile stage in the ESEM. Tensile speeds were 0.5 and 4.0 mm/min, and the ambient temperature was 23 °C. As tensile force was applied, the deformed areas in which the craze occurred were recorded on video, at the same time as the load applied by the clamping devices was measured. After the tests, the fibril length was measured in the areas in which the craze had occurred using the video images until the macroscopic crack started to propagate. (Fig. 3).

#### 2.2.2. Bumper face impact tests

Bumper face impact tests were conducted using the pendulum test equipment as tests at the automobile component level. Figure 4 shows the test set-up. A

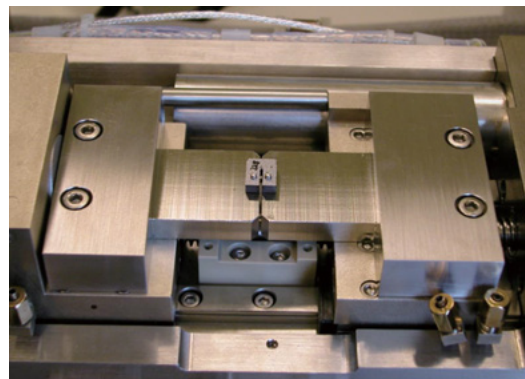


Fig. 2 Photograph of tensile stage and specimen in ESEM

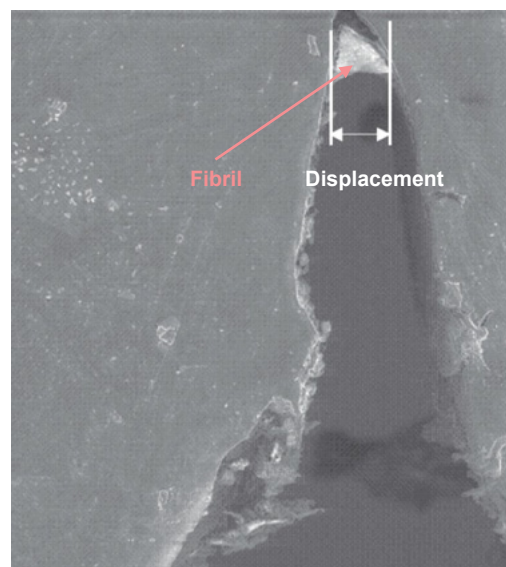


Fig. 3 Photograph of crack tip during tensile test

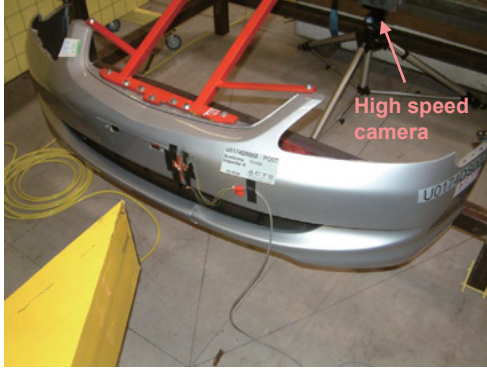


Fig. 4 Photograph of bumper face impact test

bumper face was fixed in an iron jig, and impacted by a wedge-shaped impactor at a velocity of 2.8 m/sec at an offset of approximately 40% from the center of the bumper face. The deceleration of the impactor was measured, and a high-speed camera positioned on the backside of the bumper face was used to record the progress of the craze damage development and fracture.

### 3. Coarse Grained Molecular Dynamics Model

This section will discuss the coarse molecular dynamics model used in the micro-scale modeling of the craze.

#### 3.1. Potential Function

A coarse grained molecular dynamics model was used for micro-scale modeling of the nucleation and growth of the craze. OCTA<sup>(17)</sup>, an integrated simulator available in the public domain, was used as the analytic solver. A bead/spring model was used in this analysis. The Lennard-Jones (LJ) potential expressed by Eq. (1) was used as the van der Waals force between the beads.

$$U_{nonbond}(r_{ij}) = 4\epsilon_{ij} \left[ \left( \frac{\sigma_0}{r_{ij}} \right)^{12} - \left( \frac{\sigma_0}{r_{ij}} \right)^6 \right] \quad (1)$$

Here,  $r_{ij}$  is the diameter of the LJ beads and  $\epsilon_{ij}$  is the strength of the mutually acting force. The simple harmonic potential function expressed in Eq. (2) is used as the bonding force between the beads.

$$U_{bond}(r) = \frac{1}{2} k (r - r_0)^2 \quad (2)$$

Here,  $k$  is the spring constant, and  $r_0$  is the equilibrium bond length of the spring in the initial balance state.

#### 3.2. Polypropylene Bulk Model

Figure 5 shows the coarse molecular dynamics simulation model. The model has the shape of an oblong box with dimensions of 14.1  $\mu\text{m}$  x 14.1  $\mu\text{m}$  x 50.0  $\mu\text{m}$ .

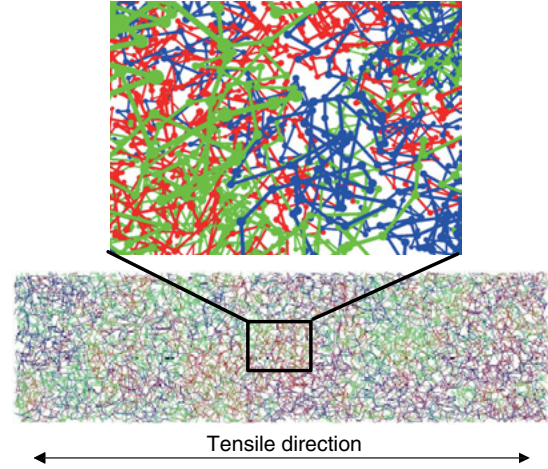


Fig. 5 Coarse molecular dynamics model

There are 10 000 beads in total and each bead contains a lamella structure of approximately 77 layers. Spring colors indicate different molecular chains respectively. After relaxation of the structure, the bond length is 1  $\mu\text{m}$ , and a linear chain structure is assumed as a molecular chain shape. In this model, one chain therefore corresponds to a bundle of fibrils. Staggered reflection was used as the boundary condition in the tensile direction, and cyclic reflection was used in other directions. Potential was automatically scaled<sup>(16)</sup> in the initial structural relaxation calculations; there were 50000 calculation steps. The mutually acting strength of the non-bond potential function,  $\epsilon_{ij}$ , and the bond potential spring constant,  $k$ , were established to ensure that the relationship between tensile load and displacement in the environmental SEM tests correlated well with the results of the simulation.

## 4. Results and Consideration

#### 4.1. Result of Tensile Test inside Environmental SEM

Figure 6 shows the relationship between load and fibril displacement as determined by the compact tension tests. This graph indicates that the maximum load

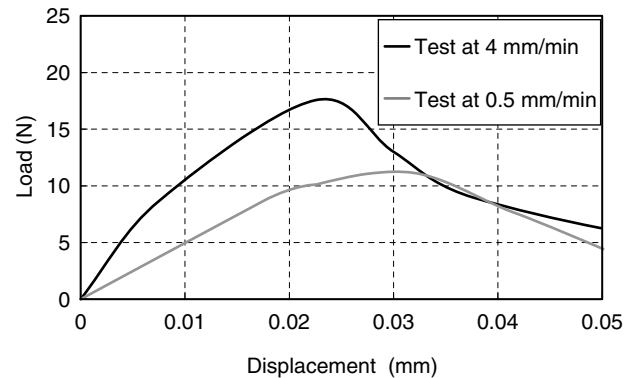


Fig. 6 Load displacement histories of crack tip

increases as the tensile speed increases. Figure 7 shows a photograph of nucleation of the craze at the crack tip during tensile loading. The fibril orients along the direction of tensile force, and then ruptures.

#### 4.2. Results of Coarse Molecular Dynamics Simulation

By analyzing parameters, it was previously demonstrated that the spring constant of the bond potential function shows a high sensitivity toward the gradient of the load-displacement relationship, and both the mutually acting force in the non-bond potential function and the bond potential function showed high sensitivity towards the maximum value of the load-displacement relationship<sup>(18)</sup>. These results were used to establish the parameters of the potential functions in the present simulation. The simulation results are shown in Fig. 8, and the simulated deformation at final failure is shown in Fig. 9. Both test results and simulation results demonstrated that after reaching the maximum load, the

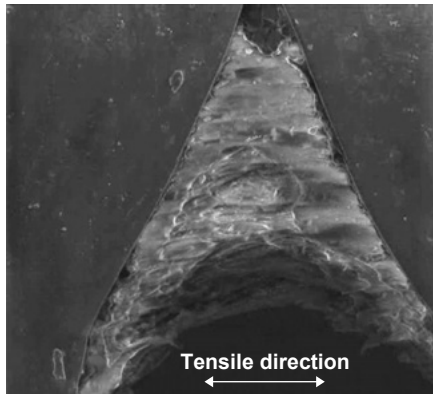


Fig. 7 Photograph of crack tip during tensile loading

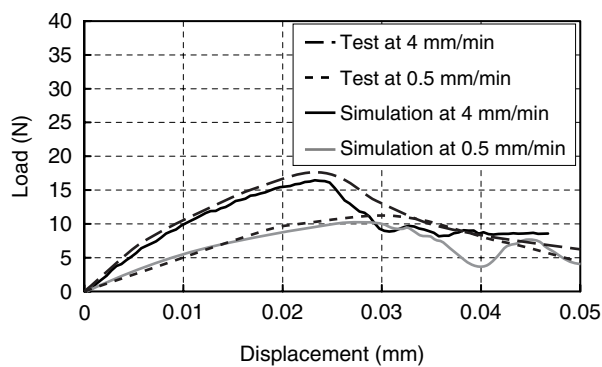


Fig. 8 Load displacement histories of bulk model



Fig. 9 Simulated deformation of crack tip in coarse molecular dynamics model

fibrils became oriented and the molecular chains loosened and fractured, making the load decrease. It is suggested that the incorporation of this softening behavior in FE models as a softening law would enable modeling the micro-parameters based modeling.

#### 4.3. Craze Density-based Softening Law and Constitutive Law of Elasto-viscoplastic Materials

The coarse molecular dynamics simulations and tensile test inside environmental SEM discussed above demonstrated that the fracture mechanism in the micro scale is determined by continuous failure of the fibrils in the craze. A softening law dependent on the craze density is next proposed to enable FE simulation of this phenomenon at the macro level. Figure 10 shows a schematic diagram of this softening law. The craze nucleation and growth are divided into Zone A and Zone B. Zone A is an area of microscopic damage, and Zone B is an area of macroscopic damage. In Zone A, the softening law is not operative, and the Shizawa, et al. model is used. When the craze grows and reaches Zone B, the softening law becomes operative, and simulations are conducted using a modified flow stress. The strong softening or weak softening can be simulated by changing the degree of softening effect.

To present the concept noted above, the following discussion offers the constitutive law proposed by Shizawa, et al. which considers the nucleation and growth of the craze, in addition to the modified flow stress equation and softening law developed in this research.

$$\overset{\nabla}{T} = C^v : \overset{\nabla}{D} - \dot{\epsilon}^p (\cos \delta) \mathbf{P}' - \dot{\omega} \mathbf{T} / (1 - \omega) \quad (3)$$

Here,  $\mathbf{T}$  is Cauchy stress,  $\overset{\nabla}{(\cdot)}$  is Jaumann velocity,  $\overset{\nabla}{D}$  is the deformation rate,  $\dot{\epsilon}^p$  is the corresponding plastic strain rate,  $\omega$  is the craze density, and  $\dot{\omega}$  is the craze growth rate.  $C^v$ ,  $\mathbf{P}'$  and  $\cos \delta$  are defined in the reference literature<sup>(10)-(13)</sup>, and therefore not noted here. The craze

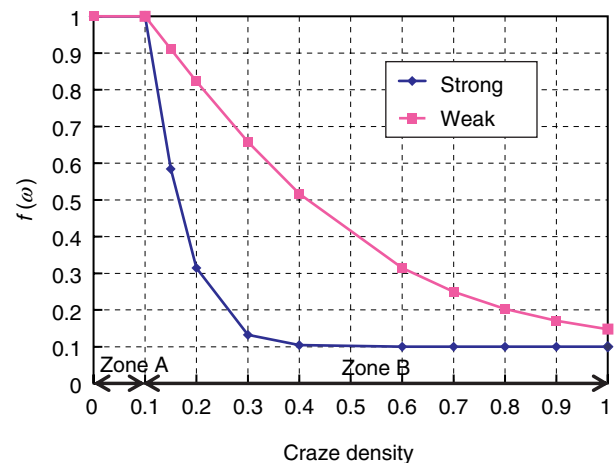


Fig. 10 Schematic explanation of softening factor and craze density

growth rate is expressed by the following equation:

$$\dot{\omega} = A(1-\omega)\langle \dot{\varepsilon}_m^p \rangle + B \cdot D_1 \cdot \dot{\varepsilon}_m^p \cdot 0.5[1 + \tanh\{-D_2(\bar{\varepsilon}^p - \varepsilon_c)\}] \cdot \dot{\varepsilon}^p \quad (4)$$

Here,  $A$ ,  $B$ ,  $D_1$ , and  $D_2$  are material parameters.  $\dot{\varepsilon}_m^p$  is the mean plastic perpendicular strain rate, and is expressed by the following equation:

$$\dot{\varepsilon}_m^p = d\{(q_1\omega)\cosh((q_2\omega+q_3)\sigma_m/\sigma_y)\}/dt \quad (5)$$

where  $\sigma_m$  is hydrostatic pressure,  $\sigma_y$  is yield stress, and  $q_1$ – $q_3$  are material parameters. The first term in Eq. (4) represents the creation of craze, and the second term represents nucleation and growth.  $\varepsilon_c$  is the strain at which the growth of the craze ceases. The craze is judged to have occurred on the basis of the following equation, which uses hydrostatic pressure criteria:

$$\sigma_b \geq A_1 + (B_1/3\sigma_m) \quad \sigma_b = \sigma_1 - \nu\sigma_2 - \nu\sigma_3 \quad (6)$$

Here,  $\sigma_b$  is the stress necessary to orient the fibrils,  $A_1$  and  $B_1$  are material parameters, and  $\sigma_i$  is the principal stresses. As shown in Eqs. (7) and (8), a strain hardening law is the general power law with the strain rate dependence coefficient  $m$ , and the flow stress,  $g$ , can express the increase of stress following secondary yielding, as observed in tensile load tests.

$$\dot{\varepsilon}^p = \dot{\varepsilon}_r \left| \frac{\bar{\sigma}}{g(\bar{\varepsilon}^p)} \right|^{1/m} \quad (7)$$

$$g(\bar{\varepsilon}^p) = \sigma_r \{ \tanh(k_1 \bar{\varepsilon}^p) + k_2 + H_e(\bar{\varepsilon}^p - \varepsilon_r)k_3(\exp \bar{\varepsilon}^p - \exp \varepsilon_r) \} \quad (8)$$

where  $\dot{\varepsilon}_r$  is the reference strain rate,  $\sigma_r$  is the reference stress, and  $\varepsilon_r$  is the reference strain.  $k_1$ – $k_3$  are material parameters.  $H_e(x)$  is the step function expressed by Eq. (9):

$$H_e(x) = \begin{cases} 1 & (x \geq 0) \\ 0 & (x < 0) \end{cases} \quad (9)$$

Equations (10) and (11) were used as flow stress equations in this research. Fracture caused by the craze occurs due to continuous fracture of several hundred to several thousand molecular chains. Use of the craze density-based softening law and flow stress to model this process phenomenologically enables simulation using micro-parameters of final failure originating in the growth of the craze.

$$g(\bar{\varepsilon}^p) = \sigma_r \{ \tanh(k_1 \bar{\varepsilon}^p) + k_2 + H_e(\bar{\varepsilon}^p - \varepsilon_r)k_3(\exp \bar{\varepsilon}^p - \exp \varepsilon_r) \} \times f(\omega) \quad (10)$$

$$f(\omega) = 1 - \tanh((\omega - w_2)w_3) \quad (11)$$

Here,  $w_2$  is the craze density at which the softening equation is first applied, and  $w_3$  is a parameter that expresses the magnitude of softening. This softening law

Table 1 Material parameters

|                       |                             |            |              |
|-----------------------|-----------------------------|------------|--------------|
| $A$                   | 0.383                       | $\sigma_r$ | 100.55 (MPa) |
| $B$                   | 1.226                       | $\sigma_y$ | 17.432 (MPa) |
| $A_1$                 | 19.82 (MPa)                 | $k_1$      | 44.795       |
| $B_1$                 | 41766.5 (MPa <sup>2</sup> ) | $k_2$      | 0.863        |
| $D_1$                 | 0.999                       | $k_3$      | 1.243        |
| $D_2$                 | 100.541                     | $q_1$      | 0.0001177    |
| $\varepsilon_c$       | 1.087                       | $q_2$      | 12.44        |
| $m$                   | 0.069                       | $q_3$      | 2.908        |
| $\dot{\varepsilon}_r$ | 1                           | $w_2$      | 0.22425      |
| $\varepsilon_r$       | 0.0001                      | $w_3$      | 4.0968       |

multiplied by the right side of Eq. (11) gives the flow stress,  $g(\bar{\varepsilon}^p)$ . FE analysis was conducted by incorporating the material laws as a user subroutine of RADIOSS Ver. 4.4, a general explicit solver. The FE model of the bumper face for impact tests is shown in Fig. 11. The bumper face was modeled using shell elements.

#### 4.4. Results of Bumper Face Impact Tests and Simulation

A simple identification procedure of material parameters for the constitutive laws was already proposed, and the material parameters were identified for this concept<sup>(19)</sup>. Table 1 shows the materials parameters used in this FE analysis.

Figure 12 shows the results for deceleration obtained from the simulation and from actual bumper face impact

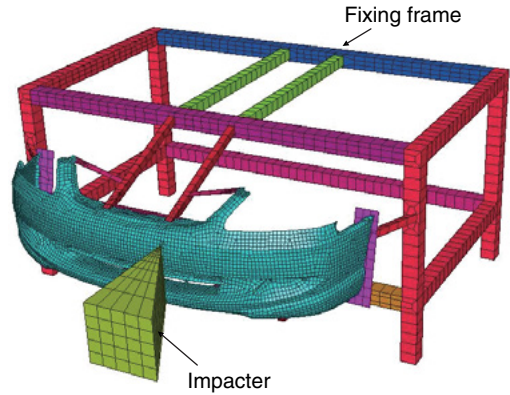


Fig. 11 Finite element model of bumper face

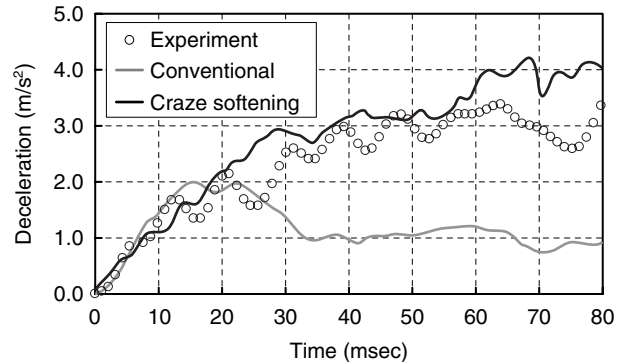


Fig. 12 Deceleration time histories of bumper face test

tests. The high-speed camera indicated that the craze occurred at 20 msec, and that cracks appeared at 40 msec. The results of the conventional simulation method that predicts fracture based on the strain showed fracture occurring earlier and at a lower level of deceleration than the test results. By contrast, the method using the constitutive material laws developed in this research showed good correlation with test results for the occurrence of the craze and the development of cracks.

Figure 13 shows the photographs of deformed bumper face at 40, 60, and 80 msec. Those photographs were taken by the high speed video camera located backside of the bumper face as shown in Fig. 4. The crack started propagating at 40 msec and continued propagating as the impactor penetrated to the bumper face. It was observed that the whitening at the crack tip was generated by the craze. It was found that the failure model observed in this test was formed due to the predominance of craze. Figure 14 shows the deformation with the simulated craze density distribution of bumper face at 40, 60, and 80 msec. In the simulated phenomena at 40 msec, the crack initiated and propagated show the same trend as the experiment. And the trends of the test and simulation results were the same in the craze density distributions at the crack tip and

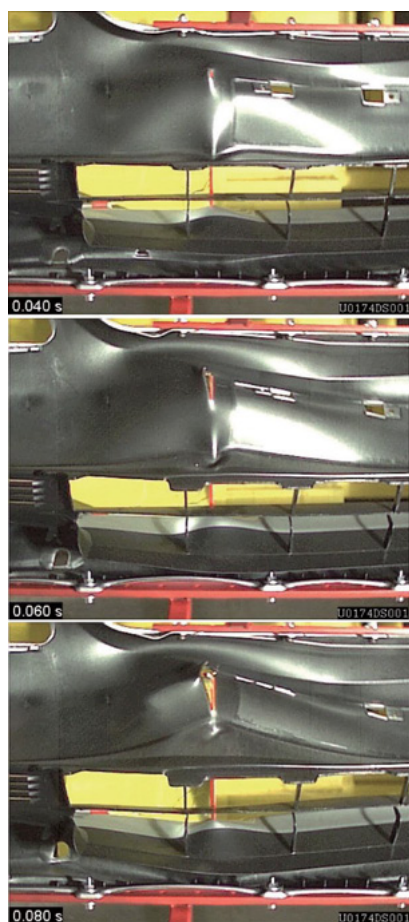


Fig. 13 Deformation of bumper face

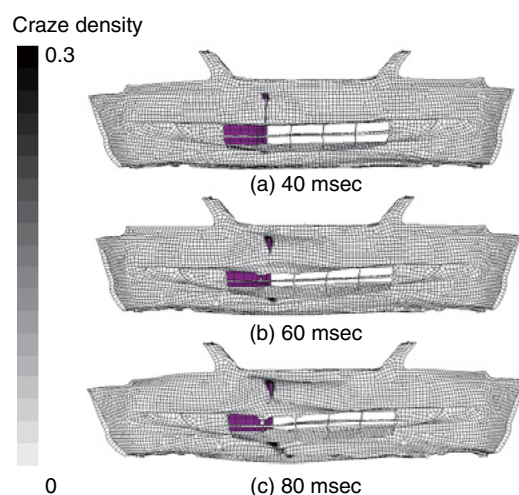


Fig. 14 Simulated deformation and craze density distribution of bumper face

around the impactor impact area. These results confirm the validity of the new method from the perspective of both deceleration and deformation. This confirms that the method proposed by this study can analyze macro-scale large deformation and impact behavior of polymeric materials using micro- material parameters.

## 5. Conclusion

The craze nucleation and growth and fibril fracture were modeled using the results of micro-scale tests and coarse grained molecular dynamics, and a phenomenological softening law that considered final failure process was proposed to analyze impact large deformation at the component level with micro-scale material parameters. This softening law was used to modify the model proposed by Shizawa, et al., and the modified model was used in the analysis of impact large deformation at the component level. Results obtained using the new method showed good correlation with the test results at the component level, confirming the validity of the method.

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