

## Development of an internal state variable model to describe the mechanical behavior of amorphous polymer and its application to impact testing

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### ABSTRACT

The use of lighter and impact resistant materials, such as polymers, in vehicular systems is an important motivation for the automotive industry as these materials would make vehicles more fuel-efficient without compromising safety standards. In general, polymers exhibit a rich variety of material behavior originating from their particular microstructural (long molecular chains) behavior that is strongly temperature, pressure, and time dependent. To capture such intricate behavior, a number of polymer constitutive models have been proposed and implemented into finite element codes in an effort to solve complex engineering problems (see [1] for a review of these models). However, developing improved constitutive models for polymers that are physically-based is always a challenging area that has important implications for the design of polymeric structural components.

The work describes the development of a material model for amorphous polymers based on a thermodynamic approach with internal state variables. The modeling approach follows current methodologies used for metals [2], and departs from spring-dashpot based models generally used to predict the mechanical behavior of polymers. To select the internal state variables, we used a hierarchical multiscale approach for bridging mechanisms from the molecular scale to the continuum scale. At this point of the work, we emphasize that molecular dynamics simulations results are mainly used as qualitative information for the continuum model. The continuum constitutive model applied a formalism using a three-dimensional large deformation kinematics and thermodynamics framework. The model predictions are then compared to compression, tensile and impact test data for a thermoplastic polycarbonate deformed at RT and at different strain rates.

Figure 1 presents the comparison between the model prediction and the experimental data for uniaxial compression at RT and different strain rates. All the curves show the expected features of the mechanical response for PC at temperatures below the glass transition: an initial linear elastic response followed by a non-linear transition curve to global yield, then strain softening and subsequent strain hardening. The model predicts well the mechanical behavior for both loading and unloading.

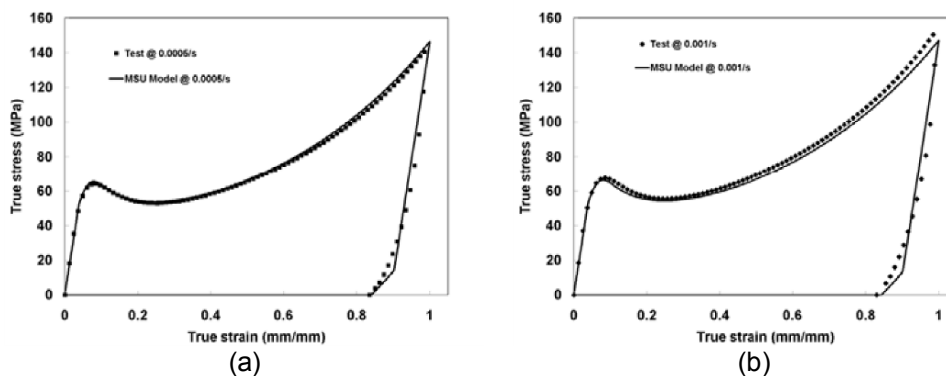


Figure 1: Comparison between model prediction and experimental data of PC in uniaxial compression at RT for

different strain rates: (a) 0.0005/s, and (b) 0.01/s.

Figure 2 displays the model predictions on tensile tests at 0.0005/s and 0.01/s. We can notice that the numerical simulations predict qualitatively the test results for the different regimes. However, the model seems to underestimate the yield peak and the softening/hardening response.

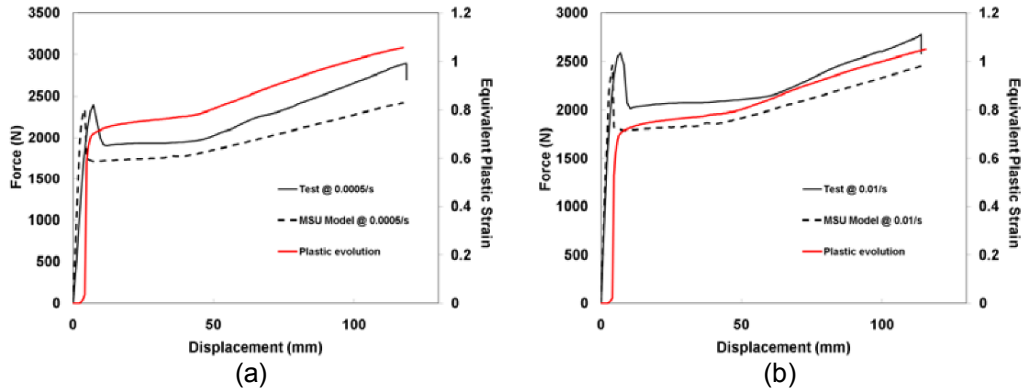


Figure 2: Comparison between model prediction and experimental data of PC in uniaxial tension at RT for different strain rates: (a) 0.0005/s, and (b) 0.01/s.

Figure 3(a) displays a comparison of the force-displacement curve between the model prediction and the impact test for a velocity of 3 mm/s. Figure 3(b) displays the stress contour at the maximum of deflection. As depicted in the figure, the numerical simulation result is in good agreement with the test data.

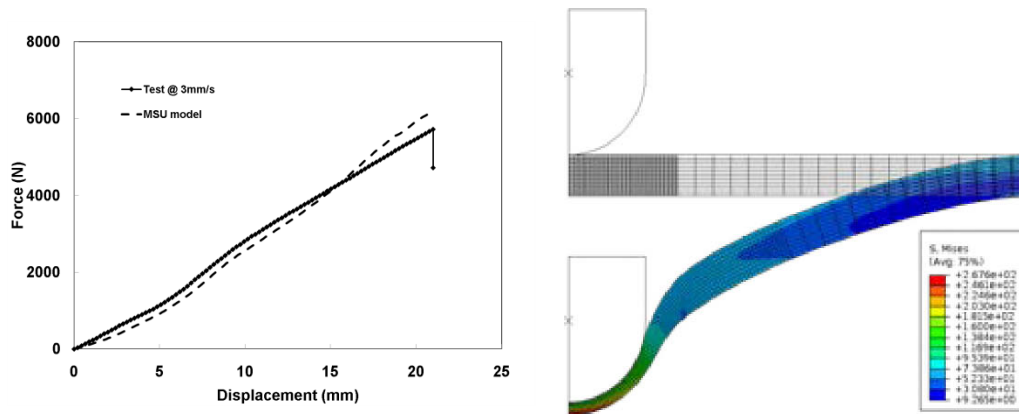


Figure 3: (a) Comparison between model prediction and experimental data for impact at 3 mm /s; (b) Stress contour at the maximum of deflection

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### References

- [1] Bouvard, J.L., Ward, D.K., Hossain, D., Nouranian, S., Marin, E.B., and Horstemeyer, M.F., 2009, Review of hierarchical multiscale modeling to describe the mechanical behavior of amorphous polymers, JEMT, DOI: 10.1115/1.3183779.
- [2] Bamman, D.J., Chiesa, M.L., and Johnson, G.C., 1996, Modeling Large Deformation and Failure in Manufacturing Processes, In: Tatsumi, T., Wanatabe, E., and Kambe, T. (Eds), Theoretical and Applied Mechanics, Elsevier Science, 359-376.