Development of Constitutive Equation for Polymer with microscopic damage


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1. Overview

Polymers which have effective properties such as lightweight, reasonable stiffness and molding characteristics, have been widely used at various industrial fields including automotive and home appliances. Additionally, the demand for resource saving and energy saving is promoting replacement of metallic structural material by polymers.

In order to design of products composed of polymers, the scientific method which can associate structural performances with the physical properties of polymers is required. To meet this requirement, we developed the computational technology which can predict the structural performances based on the mechanical properties of polymers.

2. Contents of technology

The biggest feature of our technology is that performance of polymeric products as well as parts products under large deformation and fracture with energy absorption can be predicted considering the accumulation of micro damage. The accumulation of micro damage is the characteristic peculiar to polymers, which cannot be considered by the previous constitutive equations. Furthermore, our technology is one of the multi-scale technologies which can handle different scales from the molecular level by coarse-grained molecular dynamics to the product level by FEM.

In this paper, we show examples of the application of our technology to the design of end products, where our technology was also applied to the design of polymer for achievement of the required performance of the end products.

The design scheme using our technology for industrial production is briefly shown in Fig.1. Our technology can be easily utilized as one of material models in commercial FEM applications because it is provided as the user-defined material model which is normally prepared in the commercial FEM applications. According to the flow chart as shown in Fig.2, we can predict the performance of polymeric products by using the relationship between the micro-scale calculation and the macro-scale calculation. The behavior of the micro damage calculated by coarse-grained molecular dynamics is integrated to the constitutive equation, which is the remarkable feature of our technology.

The verification results of our technology are shown in Fig. 3 and Fig. 4, which show the numerical and experimental results of the uni-axial tensile test and the impact test of the automotive bumper face, respectively. They reveal that the numerical results agree with the experimental results.

Furthermore, we show the flow chart of the material design of polymers for achievement of the required performance of final product performance in Fig.5.

3. Summary

As described above, our technology is a technology regardless of scale from material to final product. As a result, it is expected that it can be shared from material manufacturers to final product manufacturers, promote collaboration among different industries, and widely disseminate polymer materials as structural materials to the world.

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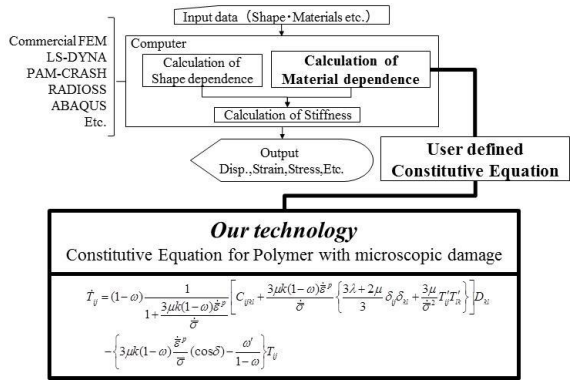

Fig. 1 The design with our technology for industrial production

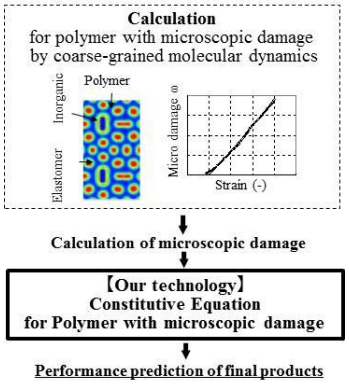

Fig. 2 The flow chart of performance prediction for products

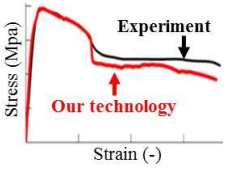

Fig. 3 Verification 1: Tensile test

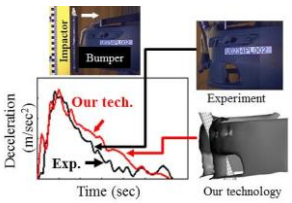

Fig.4 Verification 2: Bumper impact test

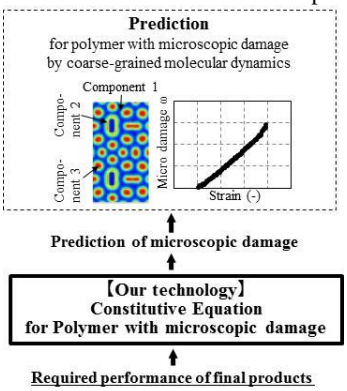

Fig. 5 The flow chart of prediction for material properties