SUMMARY OF Ph.D. DISSERTATION

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Title

Molecular Chain Plasticity Model Like Crystal Plasticity Theory and FE Simulation on Large Deformation of Glassy Polymer

Abstract

Polymers have widely been used as structural materials under severe mechanical conditions and it is necessary to develop a material model that can precisely describe a mechanical response of polymers. On the other hand, studies bridging between solid mechanics and polymer science have recently been done. The molecular chain network theory is a typical example of such attempt. However it neither can directly express orientation of molecular chains nor can represent nonlinear viscoelastic response before the initial yielding. In this thesis, a molecular chain plasticity model based on crystal plasticity theory for metals is newly proposed and a probabilistic inelastic response law considering change of local free volume is adopted as a hardening law. An FE simulation on large deformation of glassy polymer is conducted using this model and a new scheme of multiscale analysis for polymer is developed.

Chapter 1 describes a background, problems of previous studies and aims of this study.

In chapter 2, a concept of molecular chain slip system is proposed. The orientation of molecular chains is expressed by use of a method like crystal plasticity by considering the kink rotation in molecular chain as an elementary process of plastic deformation of polymer.

Chapter 3 devotes kinematics. Inelastic deformation rate and inelastic spin are kinematically determined without their plastic constitutive equations. The evolution equations of molecular chain base vectors are modeled allowing independent rotation of each slip system differently than the crystal plasticity for metals so as to represent directly molecular chain orientations.

In chapter 4, some internal forces conjugate to internal variables, e.g., a deformation induced anisotropy parameter are thermodynamically defined. Mechanical balance equations, equation of energy and entropy inequality are formulated in the form of internal variable theory.

Chapter 5 explains about development of constitutive equations. Anisotropic elastic constitutive equation is derived from the Clausius-Duhem inequality. Elastoviscoplastic constitutive equation is obtained by unifying the elastic constitutive equation and the inelastic deformation rate obtained in chapter 3. Moreover, in order to express the amorphous state of glassy polymer, a poly-entangled point model is constructed applying the extended Taylor model of polycrystals to polymer. An intensity of orientation anisotropy is defined and the anisotropy parameter mentioned above is practically represented by use of this intensity.

In chapter 6, a probabilistic response law of inelasticity based on the change of local free volume is adopted as a hardening law. This law enables the present model to express the nonlinear viscoelastic response before the initial yielding and strain softening after the yielding.

In chapter 7, an FE simulation based on this model is carried out for a PMMA (Polymethyl Methacrylate) plate subjected to tensile load. Formation of micro shear band due to sub-structural heterogeneity and its propagation are reproduced, and the orientation of molecular chains is visualized. It is shown that the present model can predict the rehardening behavior arising with neck propagation without the backstress model used in the conventional molecular chain network theory. Also, anisotropic change of elastic modulus is calculated according to molecular chain orientation.

Chapter 8 summarizes the conclusions obtained in this study.