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Predicting the Highly Nonlinear Mechanical Properties of Polymeric Materials[1]

DAVID PORTER, University of Oxford

Over the past few years, we have developed models that calculate the highly nonlinear mechanical properties of polymers as a function of temperature, strain and strain rate from their molecular and morphological structure. A review of these models is presented here, with emphasis on combining the fundamental aspects of molecular physics that dictate these properties and the pragmatic need to make realistic predictions for our customers; the designer of new materials and the engineers who use these materials. The models calculate the highly nonlinear mechanical properties of polymers as a function of temperature, strain and strain rate from their molecular structure. The model is based upon the premise that mechanical properties are a direct consequence of energy stored and energy dissipated during deformation of a material. This premise is transformed into a consistent set of structure-property relations for the equation of state, EoS, and the engineering constitutive relations in a polymer by quantifying energy storage and loss at the molecular level of interactions between characteristic groups of atoms in a polymer. These relations are derived from a simple volumetric mean field Lennard-Jones potential function for the potential energy of intermolecular interactions in a polymer. First, properties such as temperature-volume relations and glass transition temperature are calculated directly from the potential function. Then, the 'shock' EoS is derived simply by differentiating the potential function with respect to volume, assuming that the molecules cannot relax in the time scales of the deformation. The energy components are then used to predict the dynamic mechanical spectrum of a polymer in terms of temperature and rate. This can be transformed directly into the highly nonlinear stress-strain relations through yield. The constitutive relations are formulated as a set of analytical equations that predict properties directly in terms of a small set of structural parameters that can be calculated directly and independently from the chemical composition and morphology of a polymer. A number of examples are given to illustrate the model and also to show that the method can be applied, with appropriate modifications, to other materials.

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