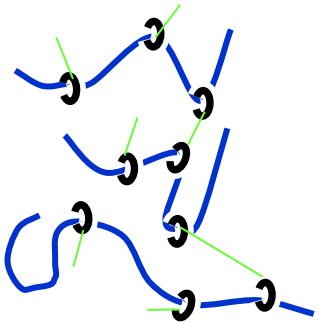
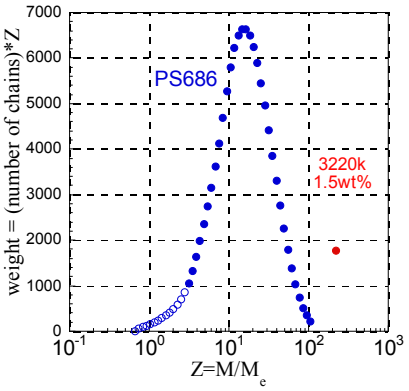
Prediction of Polymer Rheology by Simulation

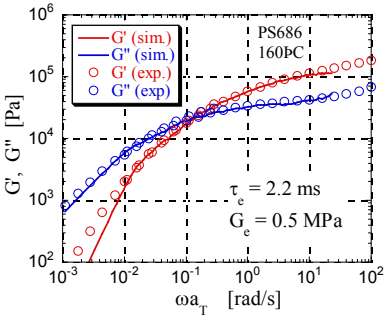
Professor Jun-ichi Takimoto



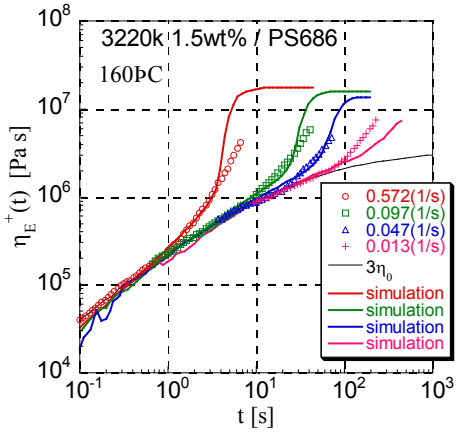
dual slip-link model for entangled polymer melts



Molecular weight distribution of a polystyrene sample



Prediction of the dynamic moduli



Effects of very high molecular weight components on elongational viscosity

Content:

Rheological properties of polymeric materials are the most important factors governing their processability. The rheology, on the other hand, is strongly affected by the molecular weight distribution and the architecture (branching structure) of the polymer. The objective of this study is to develop a simulation method for predicting rheological properties of polymeric materials from the knowledge of the molecular weight distribution and the architecture. This will enable us to design polymers with good processability from the molecular level.

The method we are using is based on a slip-link model, in which only the entanglements among polymer chains are explicitly taken account of. Currently we are able to predict various linear and non-linear rheological properties of linear and star-shaped polymers with molecular weight distributions. For example, we can correctly predict the strong enhancement of the strain-hardening of the elongational viscosity by the addition of a small amount of very high molecular weight chains. Extensions to more general architecture is now under way.

Yamagata University Graduate School of Science and Engineering
Research Interest : Polymer rheology

E-mail : takimoto@yz.yamagata-u.ac.jp
Tel : +81-238-26-3076

HP : http://ctwww.yz.yamagata-u.ac.jp/