

Abstract Submitted  
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**Estimation of Linear Viscoelasticity of Polymer Melts in Molecular Dynamics Simulations Based on Relaxation Mode Analysis<sup>1</sup>**  
NOBUYUKI IWAOKA, Faculty of Science and Technology, Keio University, KATSUMI HAGITA, Department of Applied Physics, National Defense Academy, HIROSHI TAKANO, Faculty of Science and Technology, Keio University — On the basis of relaxation mode analysis (RMA), we present an efficient method to estimate the linear viscoelasticity of polymer melts in a molecular dynamics (MD) simulation. Slow relaxation phenomena appeared in polymer melts cause a problem that a calculation of the stress relaxation function in MD simulations, especially in the terminal time region, requires large computational efforts. Relaxation mode analysis is a method that systematically extracts slow relaxation modes and rates of the polymer chain from the time correlation of its conformations. We show the computational cost may be drastically reduced by combining a direct calculation of the stress relaxation function based on the Green-Kubo formula with the relaxation rates spectra estimated by RMA.

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