行政院國家科學委員會專題研究計畫 期中進度報告

高分子運動及黏彈性：電腦模擬,理論及實驗之互補互成
(第 1 年)
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Progress Report (2007 – 2008)
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Polymer Dynamics and Viscoelasticity: Interplay of Computer Simulations, Theories and Experiments

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Fundamental issues in polymer dynamics and viscoelasticity have been investigated emphasizing the interplay of theory, computer simulation and experiment. The studies have led to important groundbreaking results, including (1) revealing the universality in the glass transition-related thermorheological complexity in polystyrene melts, entangled or not; (2) showing that the two seemingly unrelated phenomena: thermorheological complexity and breakdown of Stokes – Einstein relation share the same cause or mechanism; (3) developing the dynamic structure factor for single chains well entangled in polymer melts based on the Rouse – Mooney picture, accurately predicting the distribution of the q-split plateaus in the long-time region as observed by spin-echo neutron scattering; and (4) demonstrating by the Monte Carlo simulations the contribution of the inter-segmental interactions to the thermorheological complexity as a generic phenomena in polymer melts in the temperature region close to the glass transition point.

The above listed achievements are related, in majority closely related, to each other as presented in the following four papers:

(1) Y.-H. Lin, *Glass Transition-Related Thermorheological Complexity in Polystyrene Melts*; J. Phys.: Condens. Matter **19**, 466101 (2007).
(2) Y.-H. Lin and C.-F. Huang, *The Rouse – Mooney Model for Coherent Quasi-Elastic Neutron Scatterings of Single Chains Well Entangled in Polymer Melts*; J. Chem. Phys. (2008), in press.
(3) Y.-H. Lin, *Thermorheological Complexity in Polystyrene Melts and Breakdown of the Stokes–Einstein Relation in o-Terphenyl*; to be resubmitted.
(4) Y.-H. Lin and A. K. Das, *Thermorheological Complexity as a Generic Phenomenon in Polymer Melts: Effects of Inter-Segmental Interactions Studied by Monte Carlo*

Simulations on Viscoelasticity of Entanglement-Free Fraenkel Chains; to be resubmitted.

The contents in the above listed papers are of pioneering nature and some are simultaneously extensive and intensive; thus, they are not always easy for the referees to digest. Papers (3) and (4) will be rewritten and resubmitted.