

Abstract Submitted
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Dynamic Heterogeneity and Glassy Dynamics of Polymer Melts

ERICA SALTZMAN, KENNETH SCHWEIZER, University of Illinois at Urbana-Champaign — A statistical mechanical theory of collective dynamic barriers, slow segmental relaxation and the glass transition of polymer melts is developed by combining and extending methods of mode coupling, density functional and activated hopping transport theories. Analytic and numeric results are obtained for the crossover temperature, collective barrier, segmental relaxation time and glass transition temperature, and their relation to structural and thermodynamic properties of the polymer melt is established. A Gaussian “trap model” is constructed for the consequences of nanometer scale density fluctuations and barrier fluctuations. It predicts nonexponential relaxation with material and temperature dependent stretching exponents and decoupling of translational and relaxational processes. Correlations between the dynamic fragility, stretching exponent and degree of decoupling emerge which are consistent with experiments. Heterogeneity effects are much smaller for chain level properties thereby providing a basis for the failure of time-temperature superposition for polymer melts close to T_g .

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