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A molecular dynamics simulation study of the segmental relaxations in model polymer blends DMITRY BEDROV, University of Utah — Molecular dynamics simulations of model miscible polymer blends consisting of chemically realistic 1,4-polybutadiene (CR-PBD) (slow component) and PBD chains with reduced dihedral barriers (LB-PBD) (fast component) have been performed in order to study the influence of blending on segmental relaxation processes. We find that blending with a slow (high glass transition temperature, or T_g) component significantly increases the separation between the α - and β -relaxations of the fast (low T_g) component, which may be unresolvable or nearly unresolvable in the pure melt. Detailed analysis of the dielectric response of the blend allows us to conclude that the high-frequency loss observed in numerous dielectric spectroscopy studies of miscible polymer blends that is apparently uninfluenced by blending can be due to the intrinsic β -relaxation of the fast component and not due to concentration fluctuations and/or structural heterogeneities within the blend. In other words, instead of assuming that some fraction of the fast component is not affected upon blending due to presence of the pure melt-like local environments. We further investigate the segmental relaxations by examining torsional autocorrelation functions, dipole moment autocorrelation function, and dielectric response for each component and for the blend as a function of temperature and concentration.

Prefer Oral Session
 Prefer Poster Session

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