LCP-A2MC
Laboratoire de Chimie et Physique
Approche Multi-échelles des Milieux Complexes

Séminaire du LCP-A2MC

UNIVERSITÉ DE LORRAINE

Shear-stress relaxation in free-standing polymer films

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Using molecular dynamics simulation of a polymer glass model we investigate free-standing polymer films focusing on the in-plane shear modulus μ and the shear-stress relaxation modulus G(t) as a function of temperature T, film thickness H and sampling time t. Various observables, such as the glass transition temperature Tg, are seen to vary inversely with H demonstrating thus the (to leading order) linear superposition of bulk and surface properties. Confirming the time-translational invariance of our systems, μ is shown to be numerically equivalent to a second integral over G(t). As shown from the respective standard deviations, this is especially important for large times and for temperatures around the glass transition. Both μ and G are found to decrease continuously with T and a jump-singularity is not observed. Using the successful time-temperature superposition scaling of μ and G the shear viscosity can be estimated for a broad range of temperatures.

Salle de réunion du département de Chimie – ICPM

Vendredi 8 novembre 11:00h