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Enhancing polymer T_g and tuning mechanical properties with stiff molecular additives JAYACHANDRA HARI MANGALARA, DAVID SIMMONS, University of Akron — Small-molecule additives are commonly employed to alter glass formation, mechanical, and transport properties of polymers. For example, plasticizers are used to suppress polymer T_g and soften the glassy state, while antiplasticizers, which stiffen the glassy state of a polymer while suppressing its T_g, are employed to enhance protein and tissue preservation. Recent advances in the understanding of additives' effects on glass formation suggest that additional combinations of temperature-dependent alterations to properties including T_g, viscosity, and glassy moduli can be obtained via rational selection of additive properties. Here we employ coarse-grained molecular dynamics simulations to study the effect of introducing a stiff molecular additive to an unentangled polymer melt. Results indicate that, in contrast to plasticizer and classical antiplasticizer additives, these stiff molecular additives enhance the T_g of the matrix polymer. We further examine the impact of these additives on glassy moduli and yield stress of the polymer. These results highlight the importance of additive stiffness as a design parameter enabling more rational control of glass formation behavior.

David Simmons
University of Akron

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