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Effect of Confinement on the Relaxation Dynamics in an Antiplasticized Polymer Melt ROBERT RIGGLEMAN, JUAN DE PABLO, University of Wisconsin, Madison — We have developed a coarse grained model which exhibits antiplasticization in a polymer melt. Using molecular simulations, we have characterized our model and investigated the effect of antiplasticization on the relaxation dynamics of the polymer in both bulk and free-standing thin film geometries. In the bulk, we show that antiplasticization reduces the size of the cooperatively rearranging regions (CRRs) and leads to a weaker temperature dependence of the relaxation times of the system. We also show that it decreases the fragility of the material. Upon confinement, we find that the CRRs in the pure polymer film are strongly heterogeneous, and more cooperative near the free surfaces, leading to a large decrease in the glass-transition temperature (Tg). In contrast, the antiplasticized film shows a homogeneous distribution of the CRRs, which eliminates the effects of the free surface, and causes little change in the material properties upon confinement, including Tg, offering an explanation of recent experimental results.

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