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Dependence of Tg on interfacial energy and "hardness" of confinement in multi-nanolayered polymers[1] DAVID SIMMONS, RYAN LANG, WESTON MERLING, University of Akron — Numerous studies have demonstrated that polymers and other glass-forming materials confined to dimensions under 100 nm can exhibit large deviations from bulk glass formation, mechanical, and transport behavior. The magnitude and direction of these alterations appears to depend on both the interfacial energy and the "softness" of confinement, among other variables, with implications both for the practical design of nanoscale materials and for the mechanistic understanding of nanoconfinement effects. Here we describe molecular dynamics simulations of multinanolayered polymers in which we systematically vary the interfacial energy and the relative glass transition temperatures of the domains. Results suggest a simple functional form that describes the combined dependence of nanoconfined T_g on interfacial energy and the relative Debye-Waller factors of the two domains. We suggest that this functional form may describe the T_g of nanoconfined materials more broadly, with implications for the design and understanding of nanostructured materials.

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