Thermodynamic Model of the Glass Transition Behavior of Polymer Nanocomposites

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We have developed a new molecular thermodynamic model to predict the glass transition temperature (T_g) of nanocomposites consisting of polymer (1) and nanoparticle (2) based on the configurational entropy model and the Flory-Huggins theory. Four configurational entropies have been taken into account in this study: the disorientation entropy of the polymer (S_{dis-1}), the confinement entropy of the nanoparticle (S_{con-2}), the mixing (S_{mix-12}) and the specific interaction entropies (S_{int-12}) of the polymer/nanoparticle. Quantitative descriptions according to the proposed model are consistent with experimental T_g data of polymer nanocomposites. Our results demonstrate that T_g values of polymer nanocomposites can be enhanced or depressed relative to neat polymer depending on the intensity of specific interaction between polymer and nanoparticles, which is quantitatively identified by physical parameter (γ_{int}) in this model.