Prediction of the Glass Transition Temperature of Polymer Systems

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Abstract

An explicit expression based on the configurational entropy model, the Flory–Huggins theory and Guggenheim's form of Debye-Hückel theory has been derived for predicting the glass transition temperature (Tg) of binary semicrystalline polymer/salt complexes The proposed configurational entropy of polymer/salt systems consists of the disorientation entropy of polymer 1, the dissociation entropy of salt, the mixing entropy and the specific interaction entropy. In particular, the effect of crystalline segments was accounted for by the current model. The prediction of the proposed Tg model is in good agreement with experimental data. Our results demonstrate that the small change of the Tg in semicrystalline polymer/salt complexes compared to amorphous systems is mostly attributable to the reduced configurational entropy due to the presence of crystalline segments. Also, a new mathematical model was derived based on configurational entropy and Flory-Huggins theory to predict the T_g of miscible polymer blends. The new model adequately predicts the T_g dependence on blend composition for the cases of (1) maximum behavior with positive deviation and (2) simple linear additivity obeying the Fox equation.

Keywords: configurational entropy model; Flory–Huggins theory; glass transition temperature.