Glass transition temperature of poly(vinyl chloride) from molecular dynamics simulation: explicit atom model versus rigid CH2 and CHCl groups model.

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Abstract

Mol. dynamics (MD) simulations were used to generate vol.-temp. (VT) data at const. pressure for poly(vinyl chloride) (PVC) over a temp. range that includes the exptl. glass transition temp. (Tg) to study the validity of MD simulation in predicting Tg of amorphous polar polymers. PVC contains a polar group (chloride) which induces a partial charge distribution on all at. sites of the polymer repeating unit. In an MD simulation, all at. sites were explicitly represented in the polymer chain model. In a second MD simulation, the CH2 and CHCl groups were modeled as rigid units to minimize the computational effort. The Tg obtained from the MD VT curves was slightly displaced upward relative to the exptl. Tg. The rigid unit model tends to under est. the liq. d. compared with the explicit atom model. MD simulation is a practical procedure for predicting the Tg of polar polymers. The rigid unit model provides substantial savings in computational effort without loss of accuracy.