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Predicting glass transition temperatures from simulation studies[1]
SOLOMON DUKI, PHILIP TAYLOR, Case Western Reserve University — We have been seeking techniques by means of which the glass transition temperature T_g of a polymer can be predicted with minimal computational effort. With this goal in mind, the glass transition in syndiotactic poly(methyl methacrylate) was studied through atomistic molecular-dynamics simulations performed at temperatures in the range from 320 K to 700 K. The mean squared deviations of atoms, monomers, and molecules from their initial positions were analyzed by several different techniques. The most direct method looks at the long-time diffusive motion, and detects a characteristic change in the diffusion constant at T_g. This approach required lengthy computer runs to achieve meaningful results. Other techniques study the velocity correlation functions and the short-time vibrational motion. All three yield identical values for the glass transition temperature, but it is found that the method that is most economical of computing resources is the analysis of the short-time departure from ballistic behavior. The apparent softening of the "cage" in which a monomer or chain segment oscillates coincides with the onset of diffusive motion.

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