Raman microspectroscopy was used to determine the Fickian diffusivity of two families of low molecular weight molecules through amorphous polystyrene in the rubbery state. Different effects of the temperature on diffusivity for each of the families suggested that molecular mobility is controlled by both the volume and flexibility of the diffusing substance when the movement of polymer chains can generate stress induced deformation of molecules. The diffusing molecules were represented as Newtonian spring–bead systems, which allowed us to quantify their flexibility, in function of the vibration frequency of their bonds by reconstructing their theoretical spectra. Results showed that the use of molecular descriptors that take into account flexibility rather than the most stable conformation of the diffusing molecules may improve the description of the diffusion behavior caused by variations in shape and size of the free volumes of the polymeric matrix in the rubbery state.

Developing a Macroscopic Mechanistic Model for Low Molecular Weight Diffusion through Polymers in the Rubbery State

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