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Diffusion of small molecules in polymer nanocomposites: relationship between local free volume dynamics and penetrant diffusivity VICTOR PRYAMITSYN, VENKAT GANESAN, University of Texas at Austin — Polymer membranes are widely used as barrier or gas/vapors separation materials. Recent experiments have demonstrated that the barrier properties of the polymer nanocomposites (PNC) dramatically different from pure polymer. Usually such properties are quantified by the permeability P of the material to a penetrant which consists of two contributions: the penetrant solubility S and diffusivity D: $P = S\ D$ In present work we only discuss term D. We use the Bond Fluctuation Model, which allows us to model the diffusivity of the penetrant, the dynamics of the polymer and the dynamics of the polymer free volume in a single framework. We modeled PNC's at different particle load and the penetrant size and found that addition of nanoparticles increseses the penetrant diffusivity and selectivity to the penetrant size. This increase is attributed to the free volume increase and the acceleration of the free volume relaxation in PNC relatively to the pure polymer. We have compared the penetrant diffusivity in a rubbery and glassy PNC's and found than the effect of the PNC load on diffusivity and selectivity is much stronger for the glassy system which is due to rubbery system D is controlled by the rate of matrix free volume relaxation and in glassy regime it is controlled by the static free volume percolation, which is more sensitive to the PNC load.

Victor Pryamitsyn
University of Texas at Austin

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