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Molecular-dynamics study of the Case-II diffusion of methanol in PMMA[1] JIAYUAN MIAO, Case Western Reserve University, MESFIN TSIGE, The University of Akron, PHILIP TAYLOR, Case Western Reserve University — In Case-II diffusion, a sharp diffusion front moves at a nearly constant speed. In the widely accepted Thomas-Windle model, swelling caused by the entry of solvents into the polymer matrix plays a central role in determining the speed of the diffusion front. The principal difficulty encountered in modeling this process is the large mismatch between the time scale of atomic motion, which is measured in femtoseconds, and the time scale of diffusion in a macroscopic sample, which is measured in millions of seconds. In the work reported here, we approach the problem as one in which the diffusivity D has a strong dependence on the concentration of the penetrant, and then assume that a numerical solution of the appropriate non-linear diffusion equation will yield an accurate portrayal of the characteristics of the diffusion process. In the calculation of D, we use a theoretical model to relate D to the mean squared deviations calculated in the atomistic molecular-dynamics simulations. The advantage of this technique is that the large mismatch in time scales can be bridged in a self-consistent approach to the Case-II diffusion problem that includes the effects of swelling.

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