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Theoretical model of Case-II diffusion based on molecular-dynamics study of methanol in PMMA[1] JIAYUAN MIAO, Case Western Reserve University, MESFIN TSIGE, University of Akron, PHILIP TAYLOR, Case Western Reserve University — In Case-II diffusion, a sharp diffusion front moves at a nearly constant speed. An obstacle to the theoretical prediction of the form of this front lies in 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. We attempt to overcome this limitation by using the short-time results of atomistic molecular-dynamics simulations to construct a stochastic model valid over all time scales. The ability of this model to yield Case-II diffusion behavior was confirmed, and it was then developed into a continuum mathematical model in which the diffusivity D has a strong dependence on the concentration of the penetrant. We anticipate that solution of the appropriate non-linear diffusion equation will yield an accurate portrayal of the characteristics of the diffusion process.

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Jiayuan Miao
Case Western Reserve University

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