Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

Diffusion of Small Penetrants in Polybutadienes AHMED E. ISMAIL, RWTH Aachen University, FLINT PIERCE, GARY S. GREST, Sandia National Laboratories — The diffusion coefficient D in the dilute limit for three different penetrants— oxygen, water, and methanol—in three different conformations of polybutadiene (all cis-1,4, all trans-1,4, and a random copolymer containing 50% trans-1,4, 40% cis- 1,4, and 10% vinyl-1,2 repeat units) has been computed using molecular dynamics simulations for temperatures in the range $T = 300$–$400\,\mathrm{K}$. Simulations runs of 25 and 50 ns made for each of the 45 combinations of penetrant, conformation, and temperature studied. Over this temperature range the density of the all-cis-1,4 conformation is higher than that of the all-trans-1,4 and random copolymer conformations, which are approximately equal. For all three conformations, D for oxygen and water are comparable and larger than that of methanol. However, for a given penetrant, strong differences were observed in the rate of increase of D for the three conformations. We find that the activation barriers for the three penetrants are generally between 20 and 30 kJ/mol, in agreement with experimental results. The magnitude of the activation energy is directly proportional to the size, rather than the mass, of the penetrant molecule. (Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy under contract DE-AC04-94AL85000.)

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Date submitted: 17 Nov 2010 Electronic form version 1.4