

Abstract Submitted
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Studies of dynamical layering in adsorbed alkane films by molecular dynamics simulations and quasielastic neutron scattering.¹ F.Y. HANSEN, Tech.U. of Denmark, P. SOZA, P.U. Catòlica of Chile, A. DIAMA, H. TAUB, U. Mo.-Columbia, U.G. VOLKMANN, P.U. Catòlica of Chile — From experiments using a surface apparatus it is known that alkane fluids confined between two surfaces exhibit a layered structure at the molecular level. This static layering has motivated us to consider the possibility that the individual molecular layers in fluid alkane films adsorbed on a solid surface also exhibit different dynamical properties. Here we report molecular dynamics (MD) simulations of the diffusive motion in layers of tetracosane molecules ($C_{24}H_{50}$) (C24) adsorbed on graphite in time scales from 1 to 100 ps and from 1 to 4 ns and compare the results with high-energy-resolution quasielastic neutron scattering spectra that probe motions on these time scales. The MD simulations are set up to answer the questions: a) is interlayer diffusion of C24 molecules significant on these time scales? b) are the diffusive motions in the layers different? and c) what is the nature of the diffusive motions observed in the high-energy-resolution quasielastic neutron scattering experiments using the Disk Chopper Spectrometer (1-100 ps) and the High Flux Backscattering Spectrometer (1-4 ns) at NIST?

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