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Molecular Dynamics Simulation of friction in contact-mode Atomic Force Microscopy of alkane films and nanoparticles[1] F.Y. HANSEN, Tech. U. of Denmark, P. SOZA, P.U. Catolica Chile, H. TAUB, U. Mo-Columbia, U. VOLKMANN, P.U. Catolica Chile — In addition to sample topography, contact-mode Atomic Force Microscopy (AFM) can yield the lateral frictional force experienced by the AFM tip as it moves across a surface. This frictional force is measured by the torsional angle of the microscope's cantilever arm, which, in the case of a surface composed of highly anisotropic alkane molecules, can depend on the molecular orientation. We have conducted molecular dynamics simulations of an AFM tip moving over films and nanoparticles of $C_{24}H_{50}$ (C24) in the contact mode. For films in which the long axis of the C24 molecules is oriented parallel to the surface, we find a smaller frictional force in a scan direction perpendicular to the long axis than parallel to it. On surfaces where the alkane molecules are oriented perpendicular to the interface, we find that in all scan directions the frictional force is less than when the long molecular axis is parallel to the interface. All of these findings are consistent with experimental observations [2]

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[2]S. Trogisch *et al.*, J. Chem. Phys, **123**, 154703 (2005).

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