Nanoscale Friction of Ice

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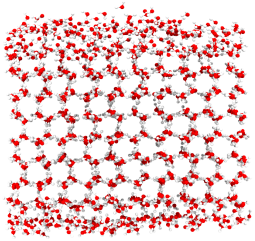
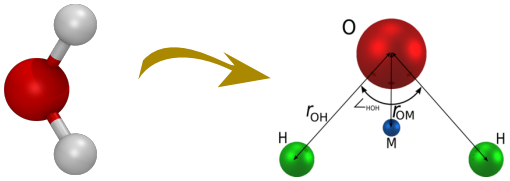
INTRODUCTION

Existence of thin liquid-like layer on ice surface well below the melting temperature is called premelting.

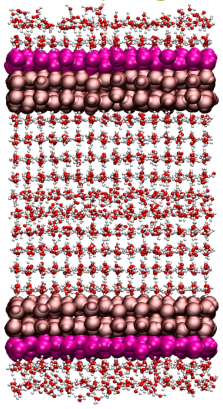


TIP4P/ICE POTENTIAL

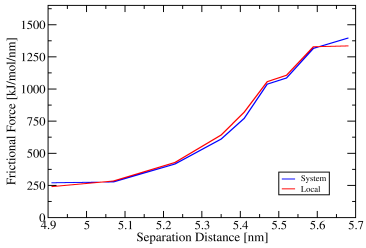


Oxygen site carries no charge. Negative charge is located at the dummy site which is placed at the bisector of HOH angle.
The pairwise potential function is composed of two terms: Lennard-Jones and Coulomb terms.

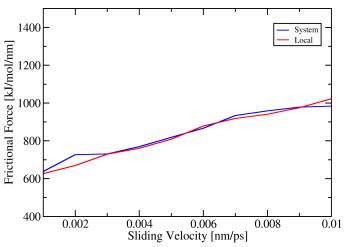
Local Coupling Scheme



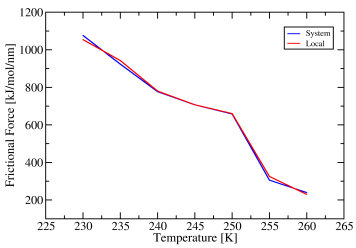
Load Dependence



Velocity Dependence



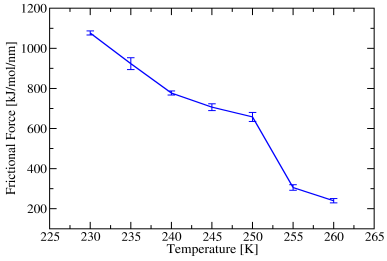
Temperature Dependence

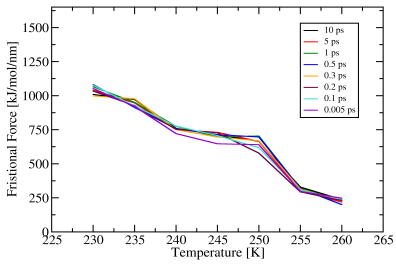


FRICTION

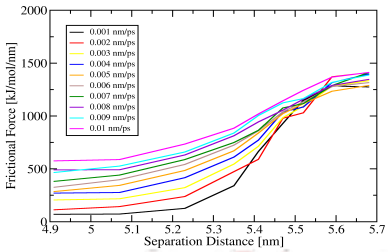
We calculate friction by bringing two surfaces together. The pull force is applied to both blocks of ice in opposite direction. Frictional force is obtained by calculating the pulling force and averaging over 5 ns simulation time. Eventually, the frictional properties as a function of temperature, sliding velocity and load are calculated.

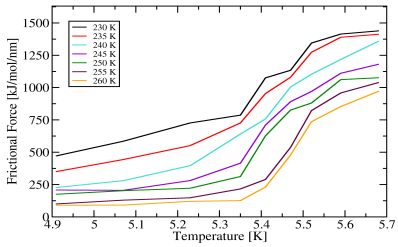
Frictional Force Dependence on Temperature for Different Coupling Constants of Nose-Hoover Thermostat





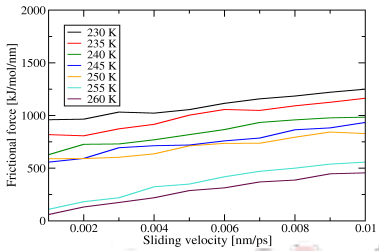
Frictional Force as a function of Applied Load



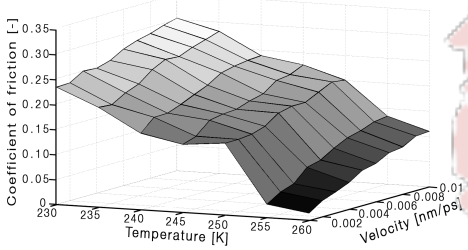


Dependences were obtained in two different cases: when the thermostat was applied to the entire system (right side) and locally (left side). Results presented here show no significant difference between the frictional forces in each case.

Friction Force as a Function of Sliding Velocity



Coefficient of Friction



As it is shown here, at all temperatures with increasing velocity the friction coefficient increases and at all velocities with increasing temperature the coefficient decreases.

Further Reading: A Potential Model for the Study of Ices and Amorphous Water, J. Chem. Phys. 122, 234511, 2005
Why is Ice Slippery, Robert Rosenberg, Physics Today, 2005
Ice Nanocolumns: A Molecular Dynamics Study, J. Chem. Phys. C, 113, 2009, 12699-12705