Regelation and Surface Premelting of Ice

N. Samadashvili [1,2], A. S. Foster [1,2], Giulia Rossi [2],
T. Hynninen [1,2], V. Heinonen [2], C. L. Dias [3],
M. Karttunen [3], T. Ala-Nissilä [2]

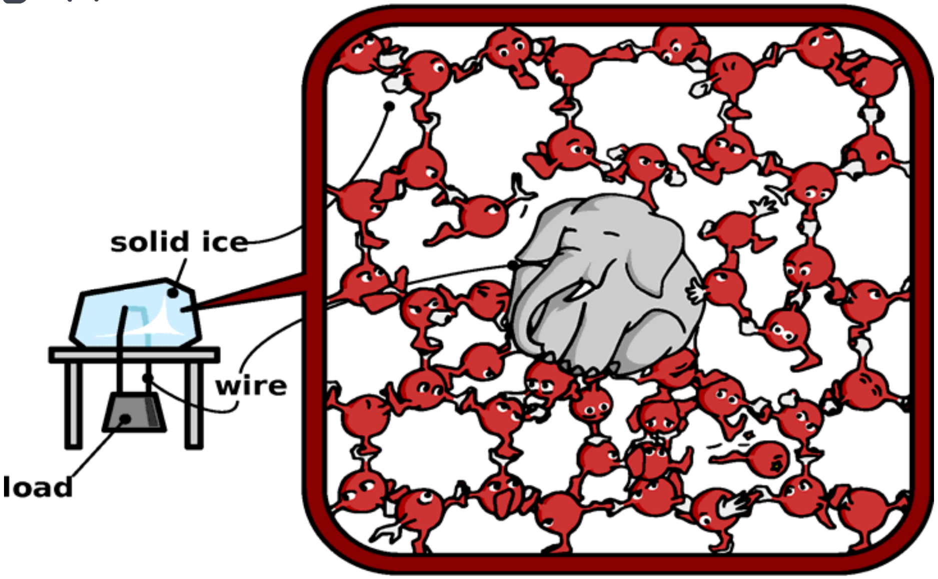
[1] Department of Physics, Tampere University of Technology, Finland
[2] Department of Applied Physics, Aalto University School of Science and Technology, Finland
[3] Department of Applied Mathematics, University of Western Ontario, Canada

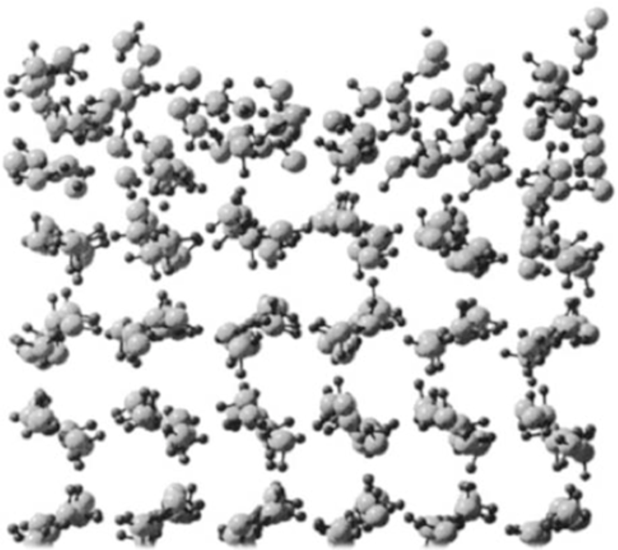
Tampere University of Technology

Surfaces and Interfaces at the Nanoscale

CONTENT

- ✓ Cutting Ice: Nanowire Regelation
- ✓ Theory Behind Surface Premelting



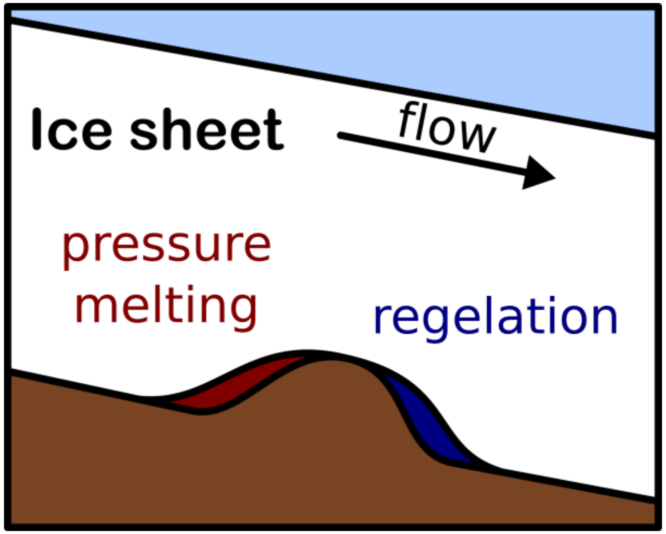


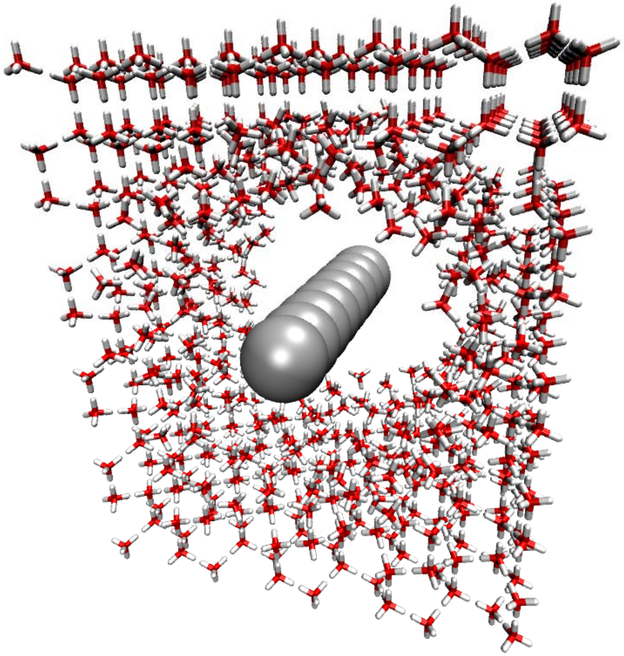
- ✓ Results of Simulation and Models Used
- ✓ Current Studies
- ✓ Conclusion

NANOWIRE REGELATION

Regelation is the phenomenon where solid ice melts under high pressure and then re-solidifies once the pressure is removed.

Glacier may build up high pressure wherever the base of the ice sheet meets an obstacle. Pressure melting allows the glacier to pass. Water behind an obstacle re-freezes.





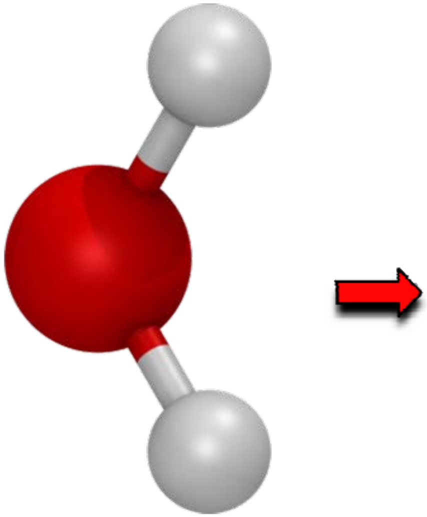
Simulation of a nanowire passage through a lattice of solid ice.

MERCEDES - BENZ MODEL OF WATER

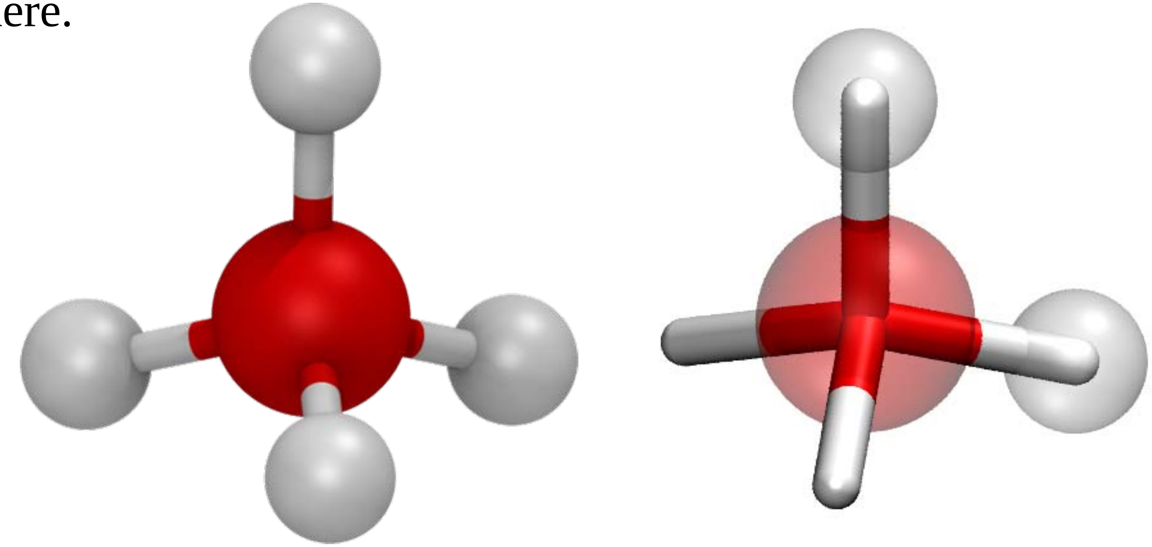
✓ Model ignores the atomic structure of water molecules (CG), but includes dangling bonds in tetrahedral coordination.

✓ Reproduces well some important properties of water.

✓ MB molecule is a LJ sphere.



Water Molecule



MB Model of Water Molecule

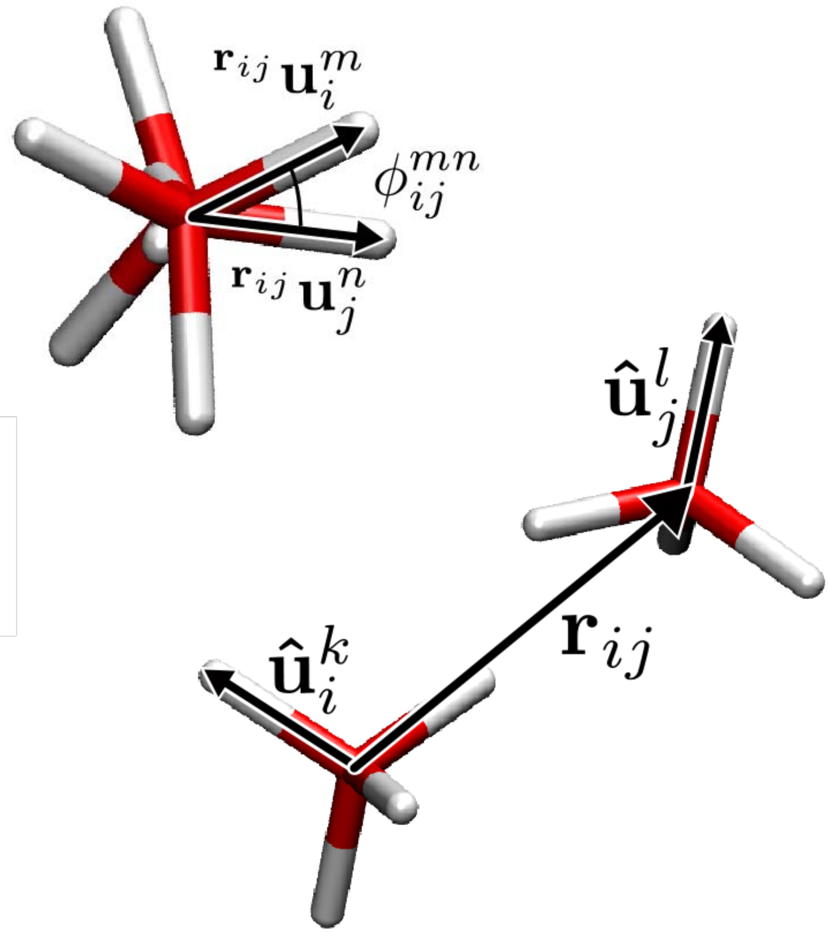
MB POTENTIAL

The MB potential is a combination of Lennard-Jones and bond potentials.

$$U = \frac{1}{2} \sum_{i,i \neq j} U_{ij}^{LJ} + U_{ij}^{HB}$$

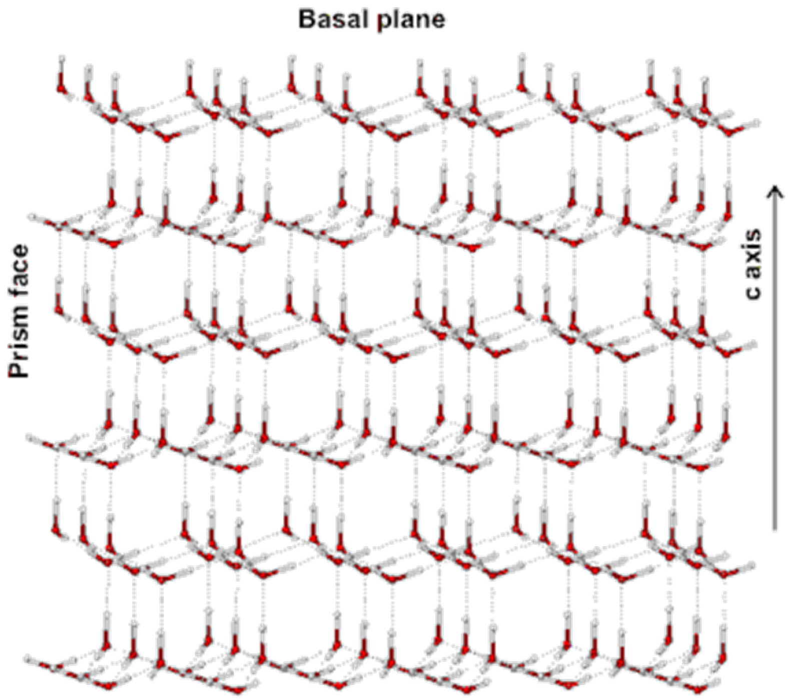
$$U_{ij}^{LJ} = 4\varepsilon_{LJ} \left[\left(\frac{\sigma_{LJ}}{r_{ij}} \right)^{12} - \left(\frac{\sigma_{LJ}}{r_{ij}} \right)^{6} \right]$$

$$U_{ij}^{HB} = \varepsilon_{HB} \sum_{k,l=1}^{4} b_i G_{ij}^{kl} \phi_{ij}^{kl}$$

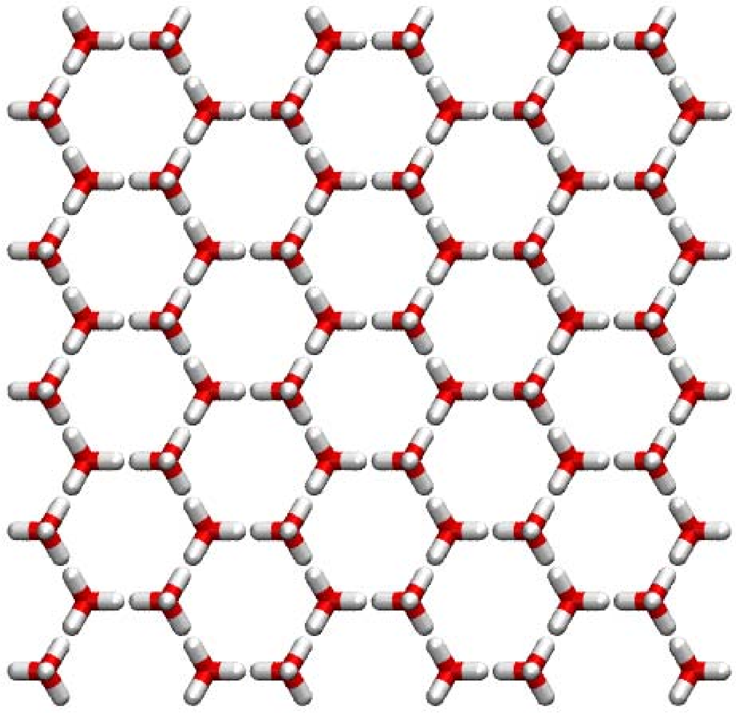


C. L. Dias, et al., J. Chem. Phys. 131(2009) 054504

LATTICE STRUCTURE OF ICE



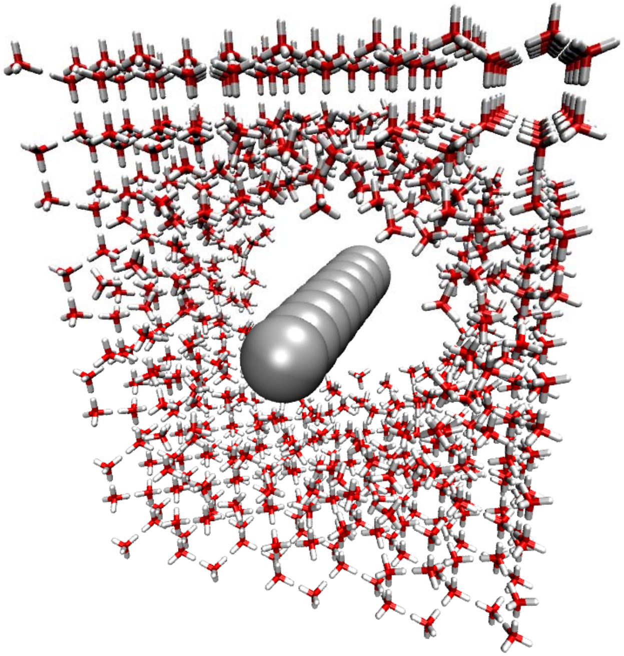
Hexagonal Ice, Ice Ih



MB Ice

SIMULATION DETAILS

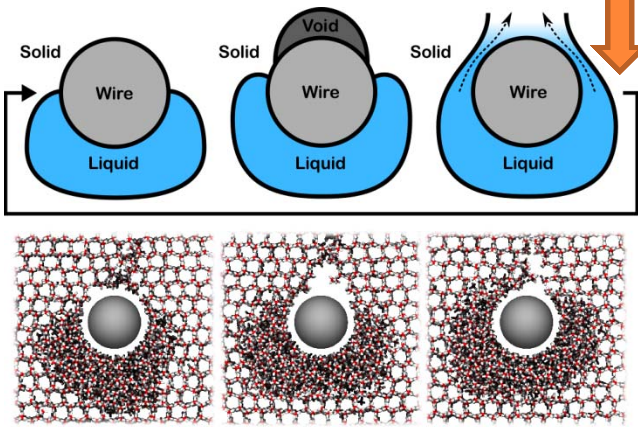
- ✓ The simulations were carried out using velocity Verlet algorithm.
- ✓ Melting point of the system was 270 K. Results were obtained at 260 K.
- ✓ The wire was described as a rigid string of beads.
- ✓ The simulations contained between 1000 to 10 000 water molecules.

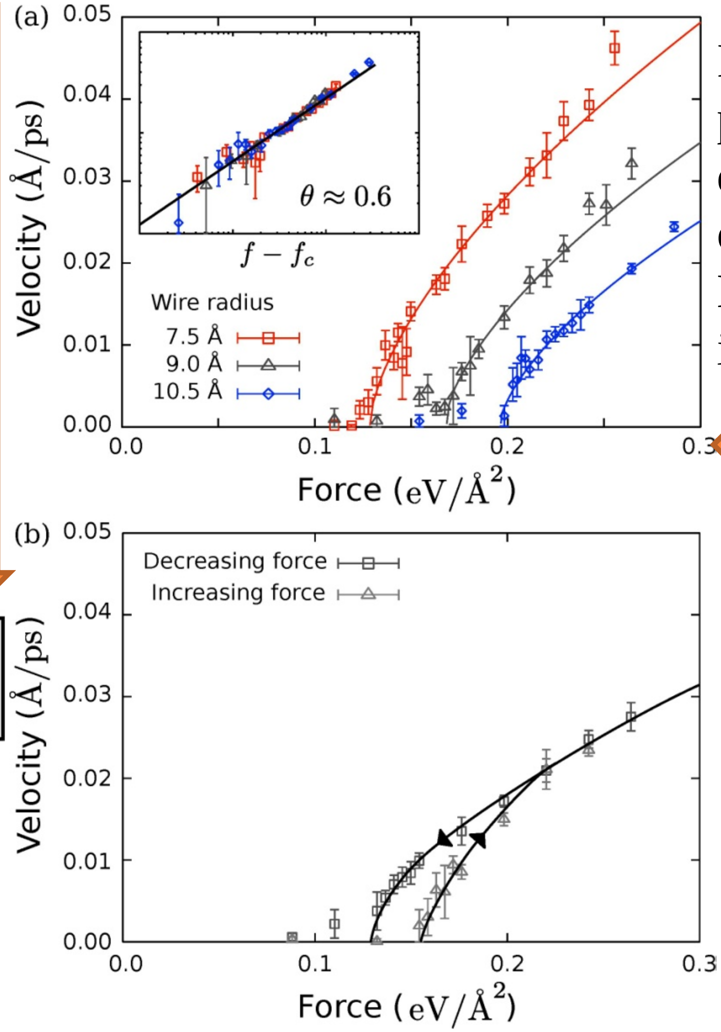


TWO DIFFERENT MODES OF NANOWIRE REGELATION

Hydrophobic wire

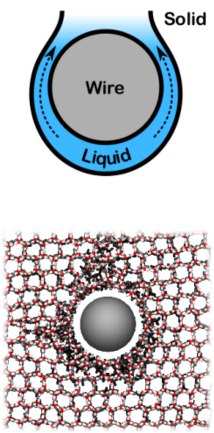
In case of hydrophobic wire, clear hysteresis was observed in depinning transition. When the force is gradually increased, the depinning is seen at a higher critical force than if the force is decreased.





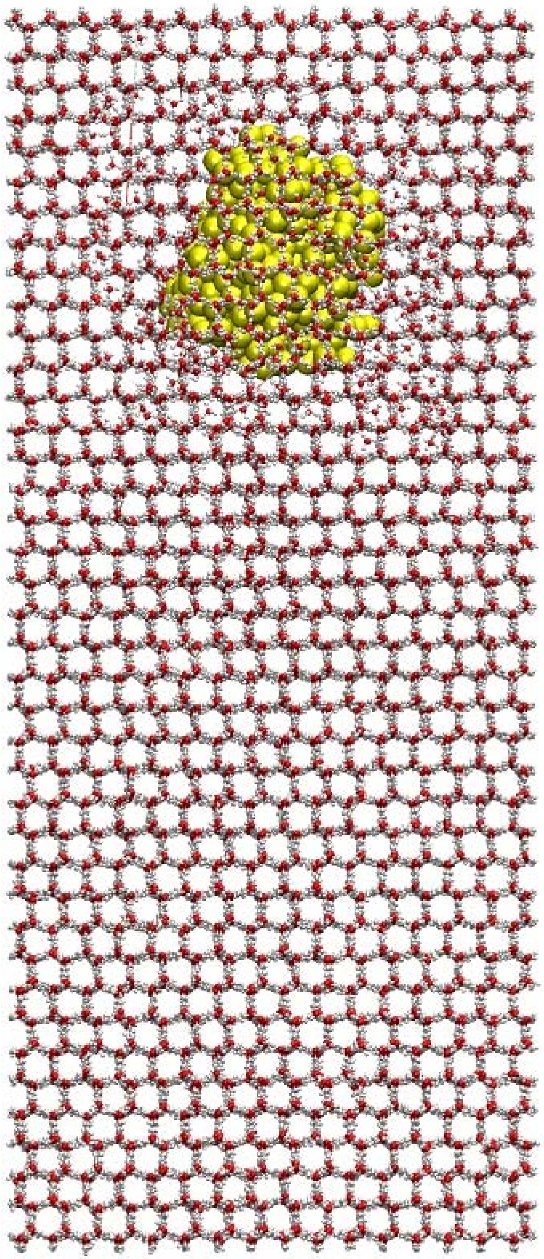
Hydrophilic wire

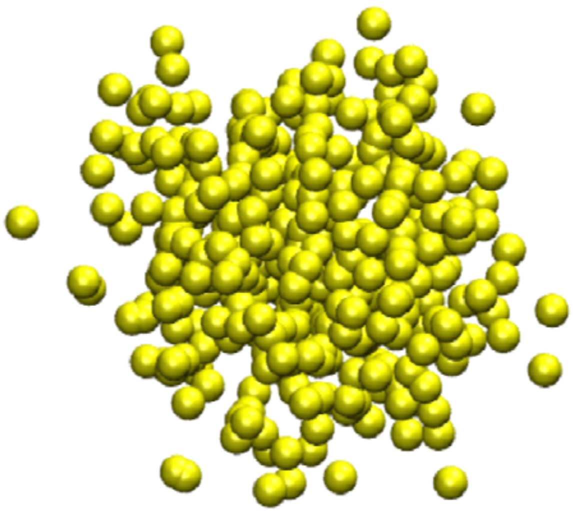
If a hydrophilic wire is placed in bulk ice, the depinning transition occurs continuously. No hysteresis was seen in the simulations.



T. Hynninen et al., PRL 105, 086102 (2010)

POLYSTYRENE REGELATION





PS

- ✓ Nanowire is replaced by Polystyrene (PS).
- ✓ PS is described as a chain of 400 beads, interacting through spring potential with each other.
- ✓ Driving force is applied to MB molecules.
- ✓ Force is applied to Polystyrene beads .

FRICTION OF ICE AT THE ATOMIC SCALE

- ✓ Very little work has been done to study the friction, or slipperiness, of ice, at the atomic scale.

- ✓ Nanoscale understanding of the friction of ice may provide new routes to control friction on this ubiquitous surface.

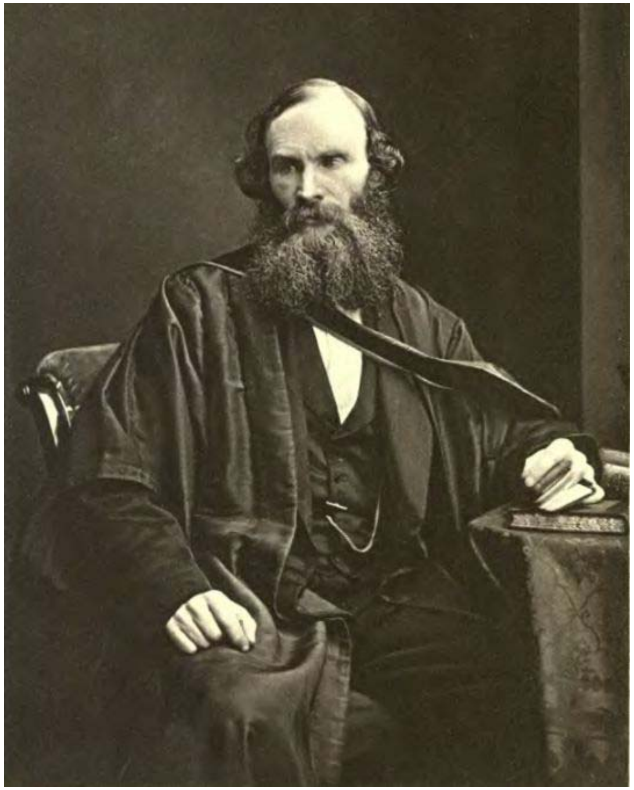
- ✓ The overall goal of this project is to use simulations to provide directions for understand--ing and control of friction of ice at the atomic scale.

- ✓ Premelting is not unique for ice, it characterizes other solids surfaces as well.

SURFACE PREMELTING OF ICE

Existence of thin liquid-like layer on ice surface at temperatures well below the bulk transition is called premelting. Combined with pressure melting, regelation may occur at lower pressures than is pressure melting was the only mechanism driving the liquid formation.

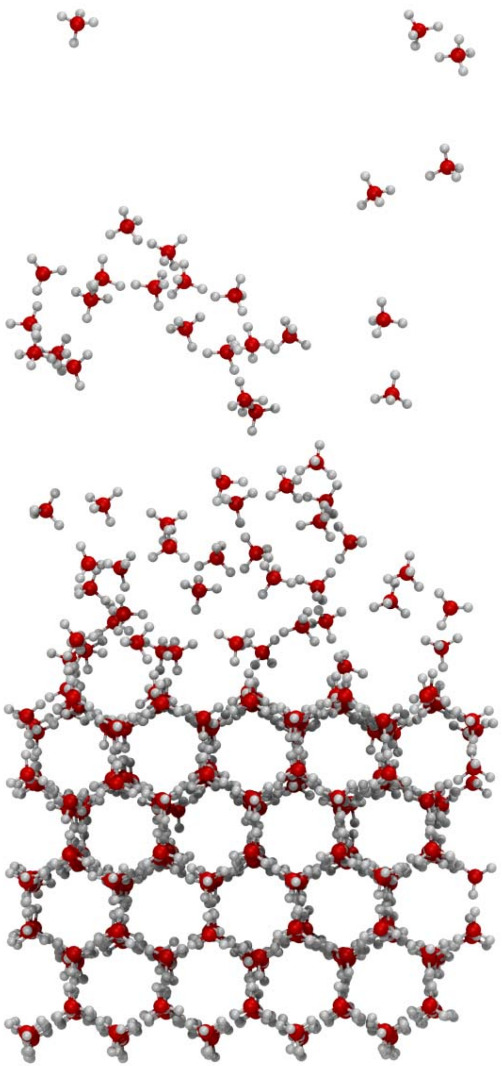
VS

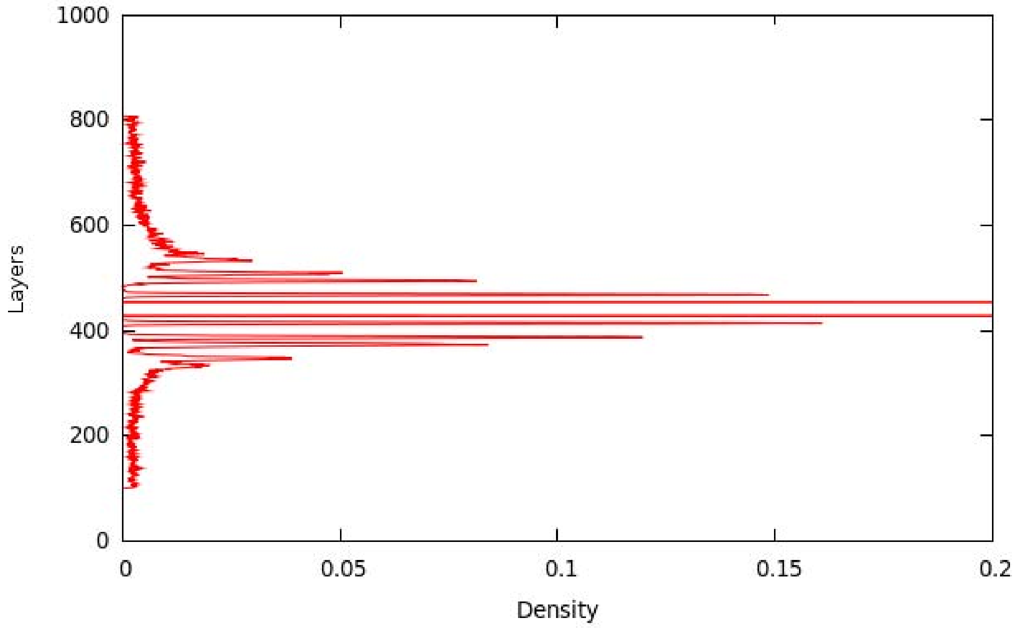


Michael Faraday (1791-1867)

James Thomson (1822-1892)

ICE SURFACE SIMULATION WITH MB WATER MODEL

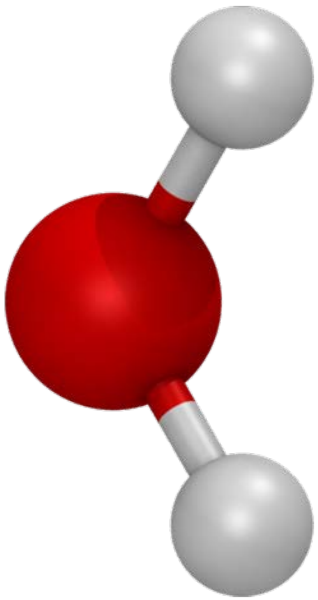




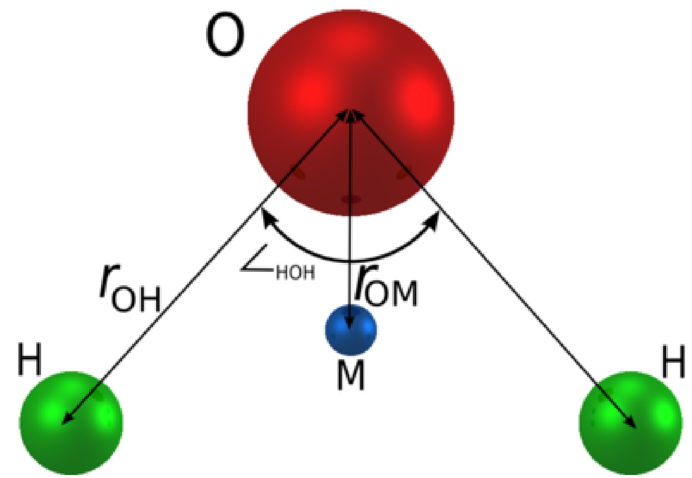
Simulation showed ice surface evaporation. No surface premelting was observed.

MB Model does NOT reproduce surface properties of ice with the set of parameters used!

TIP4P MODEL OF WATER



Water Molecule



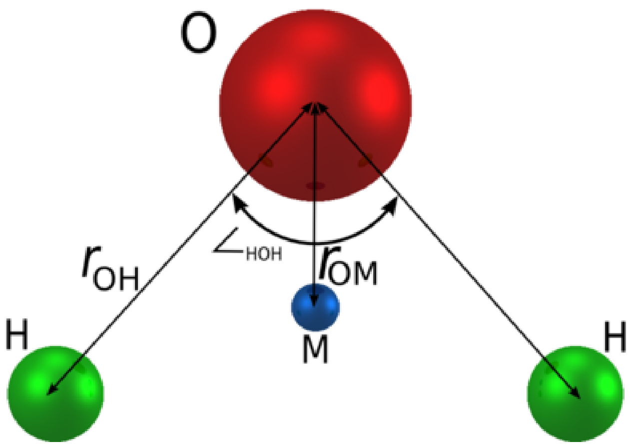
TIP4P Water Molecule

TIP4P POTENTIAL

✓ The total potential energy of the system is the sum of the pair interactions between molecules.

✓ The pairwise potential function is composed of two terms. Lennard-ones and Coulomb terms.

✓ Oxygen site carries no charge. Contributes to the LJ term.



$$U_{LJ} = 4\varepsilon\left[\left(\frac{\sigma}{r_{oo}}\right)^{12} - \left(\frac{\sigma}{r_{oo}}\right)^{6}\right]$$

$$U_{el} = \frac{e^2}{4\pi\epsilon_0}\sum_{a,b}\frac{q_a q_b}{r_{ab}}$$

SIMULATION DETAILS

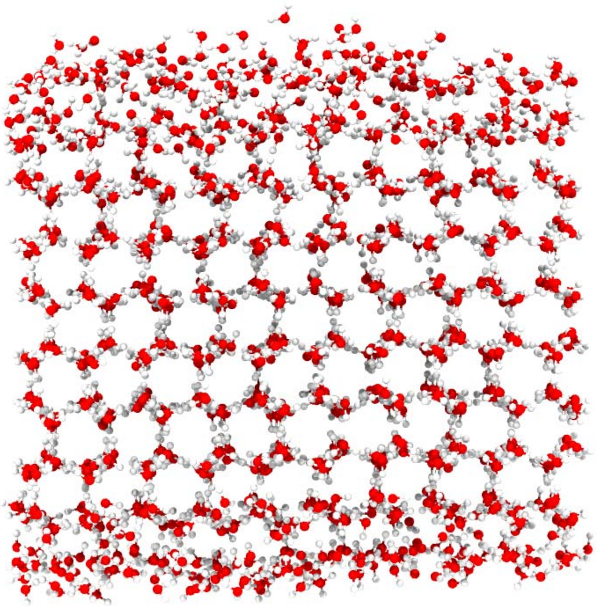
- ✓ We have performed molecular dynamics simulations of ice systems using the GROMACS simulation package.

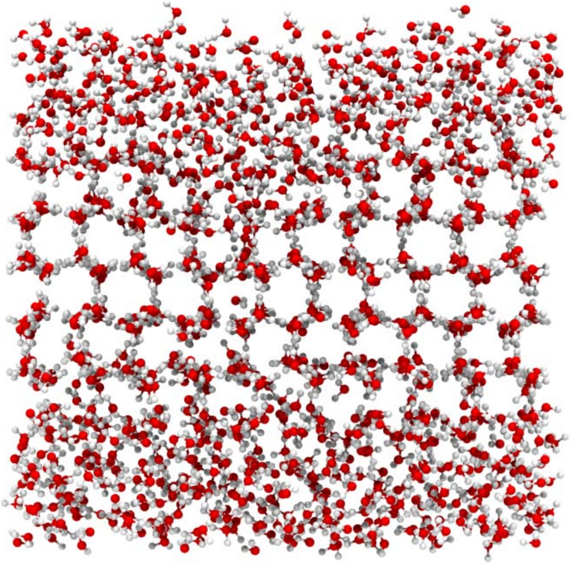
- ✓ There have been some parameterizations of the TIP4P model for specific uses. (TIP4P/Ice, TIP4P/2005 and TIP4P-Ew)

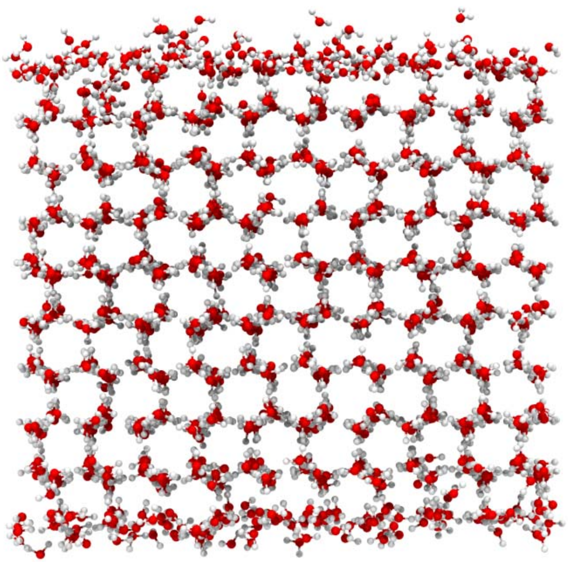
- ✓ Some of these parameterized models that have been used for our calculations are TIP4P/Ice and TIP4P/2005.

- ✓ We simulated the system of ice of 1600 water molecules over 2 ns. The temperature range of 100-275 K was probed.

SIMULATION RESULTS







- ✓ TIP4P Potential

  TM – (230-235) K

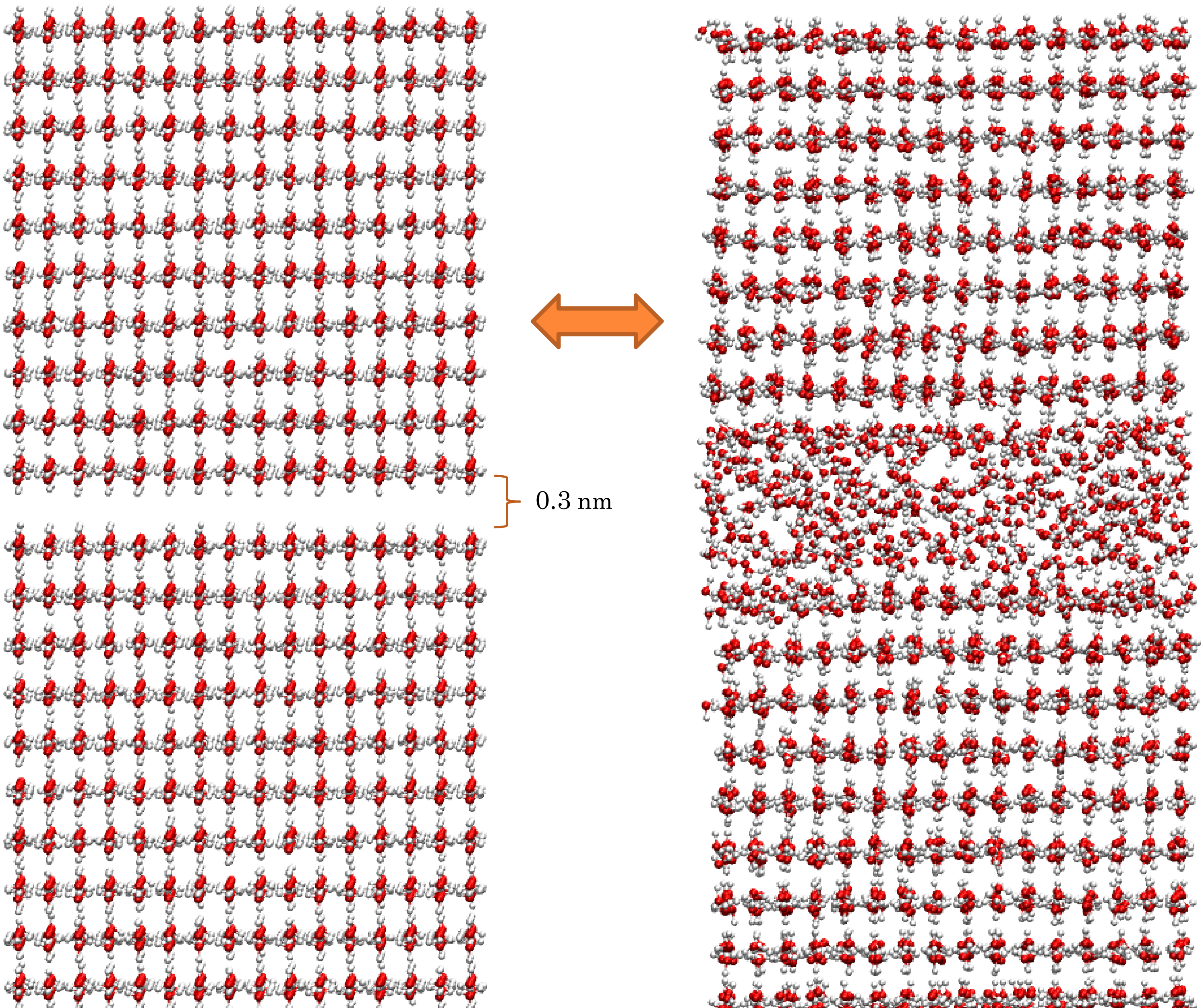
- ✓ TIP4P/2005 Potential

  TM – (255-260) K

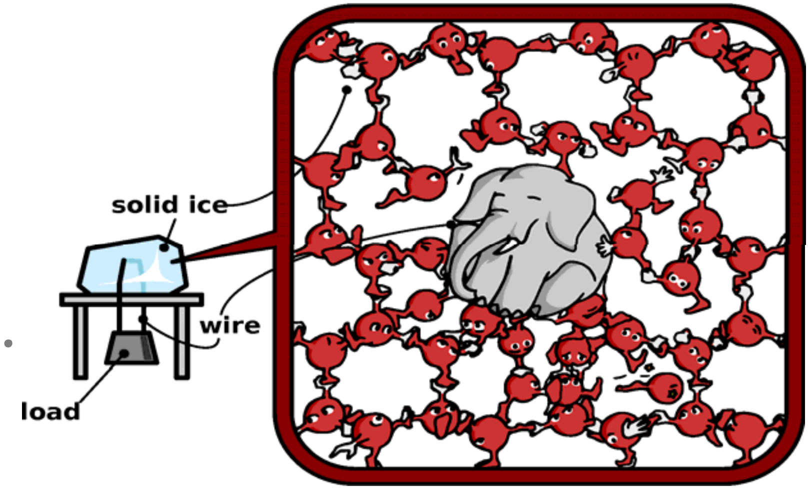
- ✓ TIP4P/Ice Potential

  TM – (273-275) K

FRICTION STUDIES



CONCLUSION



- Cutting ice: Nanowire regelation.
- For bulk ice simulations MB model was used.
- Transition in two different cases. Simulations were carried out using hydrophilic and hydrophobic wires.
- Polystyrene regelation.
- Slippery when wet: Surface Premelting of ice.
- Ice surface simulations with MB and TIP4P water models.

THANKS FOR LISTENING