Simulated Ice Regelation by Nanowire

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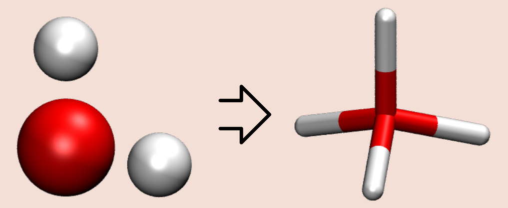
Regelation is the phenomenon where solid ice melts under high pressure and then resolidifies once the pressure is removed. We study regelation and friction in bulk ice on the nanoscale by simulating the passage of a nanowire, driven by an external force, through a lattice of solid ice.

Water Model

Water is described using the modified 3D Mercedez-Benz (MB) model which is a geometric coarse grained description on the molecular level. The method ignores the atomic structure of the water molecules, but includes dangling bonds in tetrahedral coordination. This results in a model that reproduces the correct local structure without computationally heavy long ranged forces.



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

$$U_{ij}^{\mathrm{HB}} = \varepsilon_{\mathrm{HB}} \sum_{\substack{k=1\\l=1}}^{4} b_i G_{ij}^{kl} \Phi_{ij}^{kl}$$

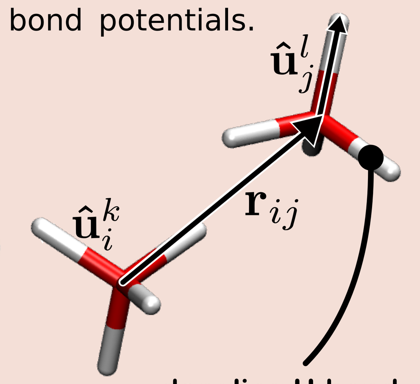
dangling bond potential

$$G_{ij}^{kl} = g\left(\frac{r_{ij} - R_{\mathrm{HB}}}{\sigma_{\mathrm{HB}}}\right) g\left(\frac{\hat{\mathbf{u}}_i^k \cdot \hat{\mathbf{r}}_{ij} - 1}{\sigma_\theta}\right) g\left(\frac{\hat{\mathbf{u}}_j^l \cdot \hat{\mathbf{r}}_{ji} - 1}{\sigma_\theta}\right)$$

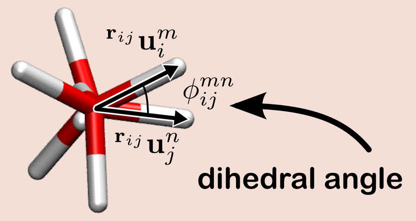
$$g(x) = \exp\left(-\frac{1}{2}x^2\right)$$

dihedral angle potential

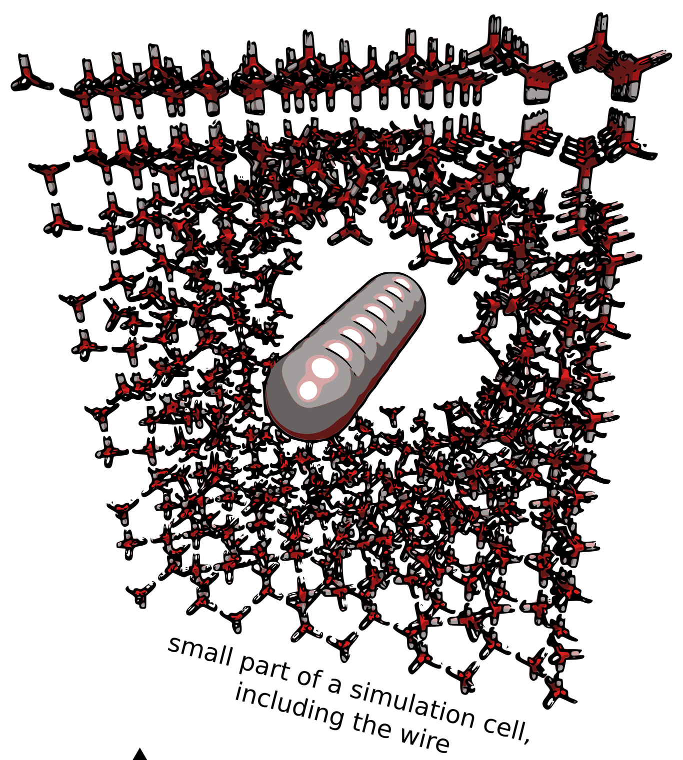
$$\Phi_{ij}^{kl} = 1 + \frac{\varepsilon_\phi}{2} \sum_{\substack{m\neq k\\n\neq l}} (1 + \cos 3\phi_{ij}^{mn})$$



Here b_i is a Tersoff-like factor which counts the first shell neighbors and penalizes overcoordination, i.e., configurations with more than 4 neighbors.

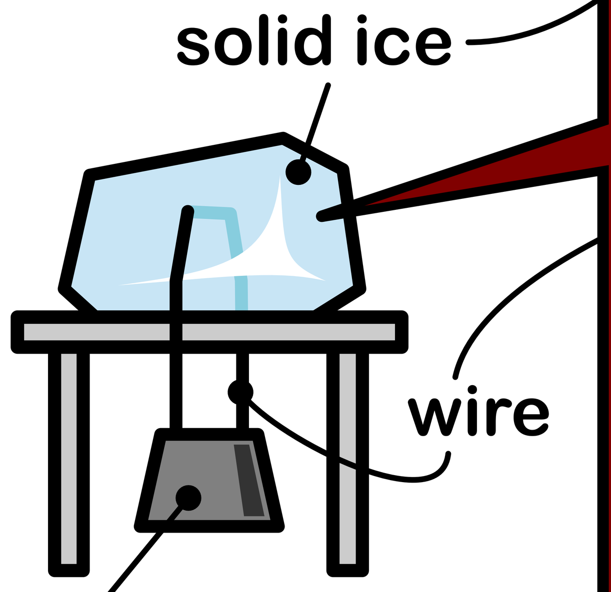


Nanoscale regelation and bulk friction are studied by molecular dynamics simulations of a nanowire, driven by external force, passing through an ice lattice. On this scale, different molecular mechanisms of movement are observed, depending on the size of the wire and the strength of the driving force.



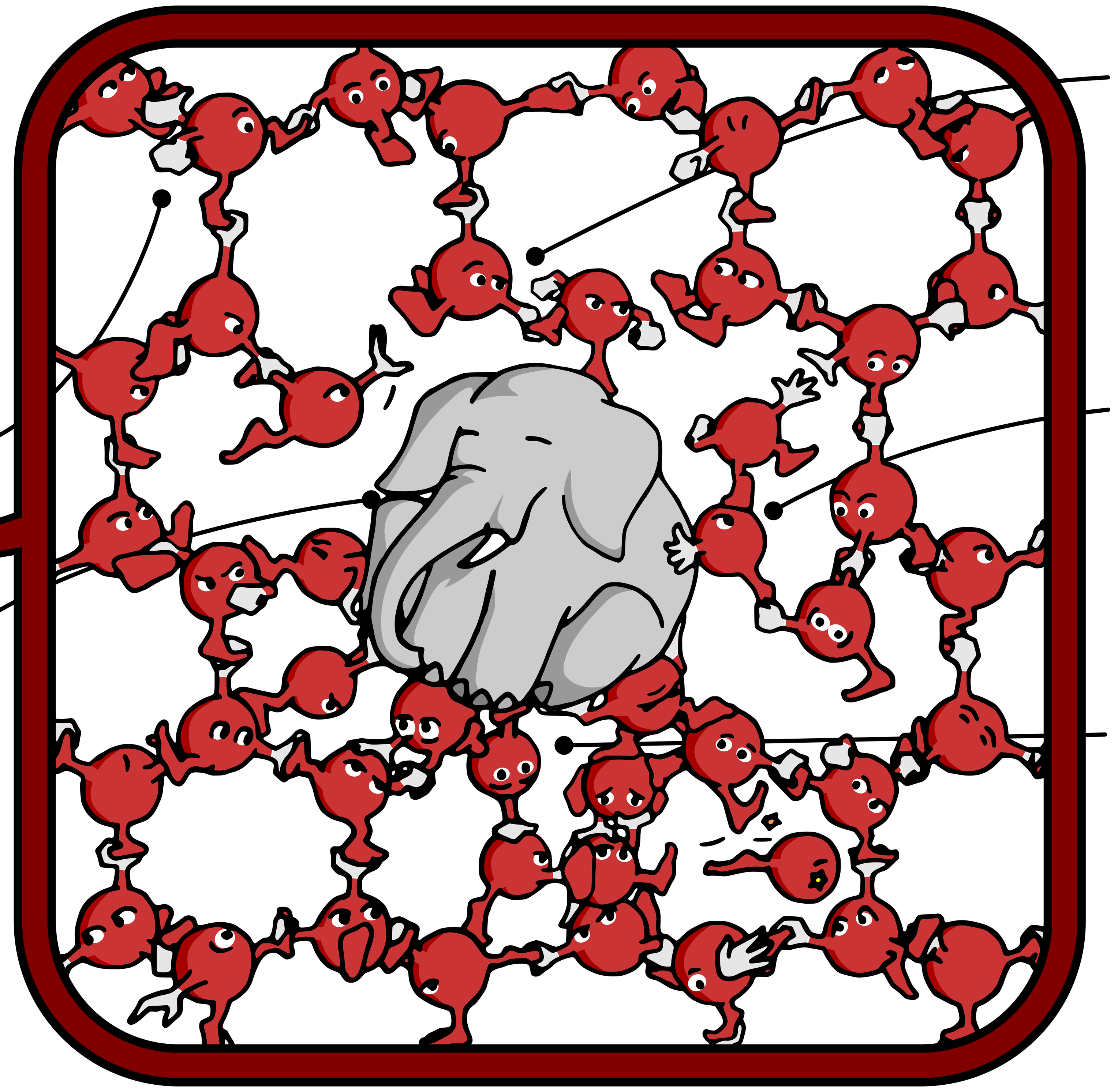
The Classic Experiment

Regelation is commonly demonstrated by setting a weighted wire on a block of ice, whereby the wire passes through the solid without actually cutting it.



load

Increases pressure excerted by the wire.



solidification

The pressure is relieved above the wire, allowing the water to freeze again, leaving behind an intact solid.

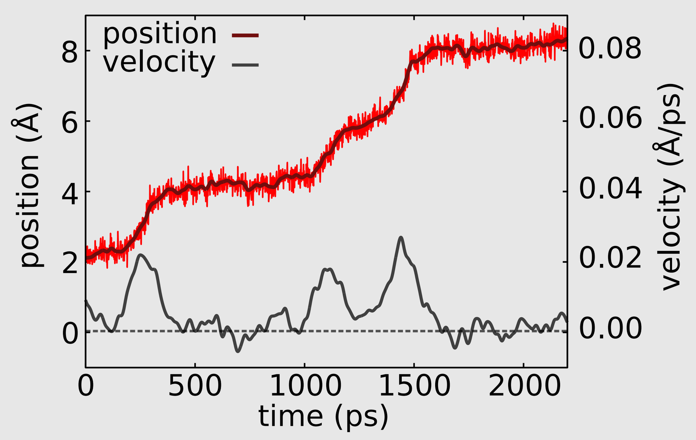
flow

A liquid layer forms around the wire. This liquid layer can flow around the wire and allows it to travel through the solid.

melting

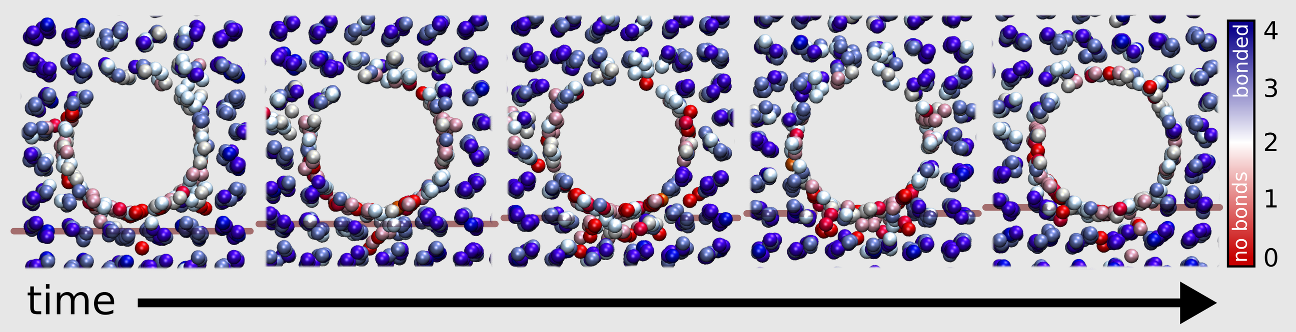
Pressure is greatly elevated under the wire. This lowers the melting point of water and melts the solid ice.

The Nanoscale Simulation



stick-slip motion

Stick-slip motion is seen once the force is strong enough to drive the movement. The wire pushes through molecular layers of the ice lattice in steps of one or one half layers (2-4 Å).



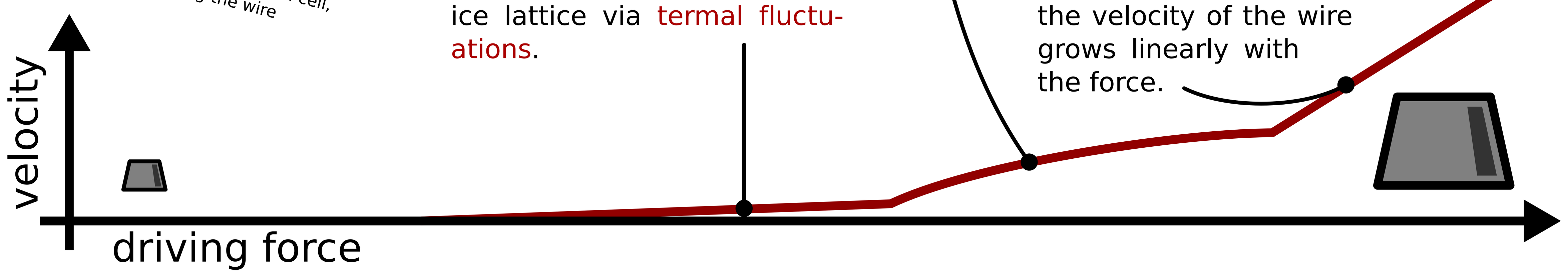
A molecular layer of ice remains intact close to the wire. Pressure rise directly below the wire disturbs the local order. The induced disorder spreads, melting the ice locally. The wire pushes in and through the liquid. The newly formed liquid joins the layer flowing around the wire.

creep

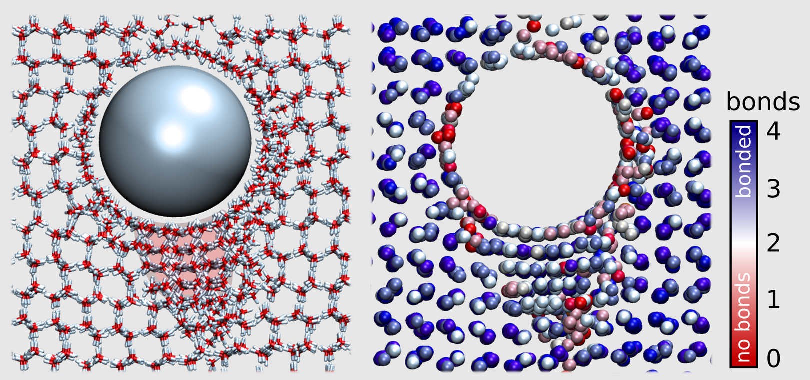
With very low forces, the pressure is not sufficient to melt the ice. Still, it is possible for a small wire to pass through layers of the ice lattice via termal fluctuations.

sliding

When the driving force becomes strong enough, the wire slides through the ice at a steady speed. In this region, normal sliding friction applies and the velocity of the wire grows linearly with the force.

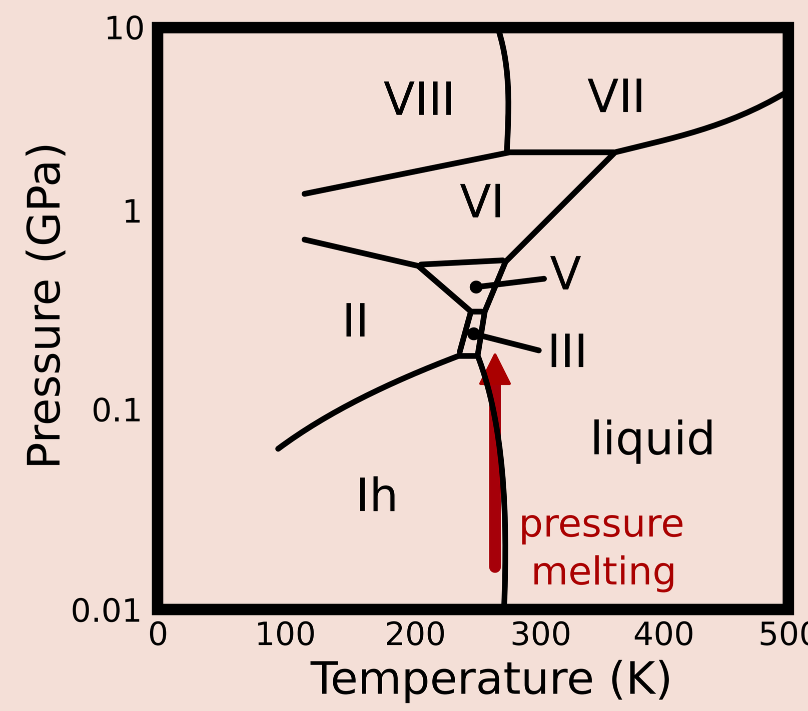


secondary phase



For a large enough wire (1 nm radius), ice-VII is seen to appear briefly. This introduces another stick-slip mechanism: Formation of the solid stops the wire, its breaking results in rapid movement.

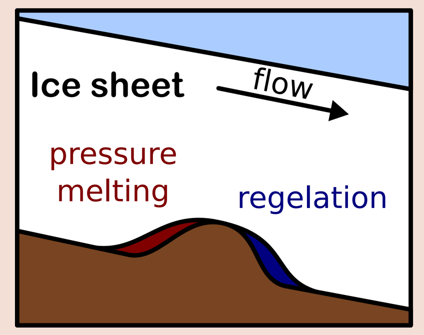
Phases of Water



Normal ice has the property that it melts under high pressure, as shown by the arrow in the phase diagram. This is unusual, since usually liquids solidify under increased pressure. It also makes the regelation phenomenon possible for water. Besides normal ice, ice-Ih, water has many other exotic solid phases as well, some of which are marked on the diagram. These phases appear only in very cold conditions or under extremely high pressure and thus are not normally seen in nature.

Regelation in Nature

Natural regelation occurs, for instance, in glaciers. As a glacier flows over rough terrain, it may build very high pressure wherever the base of the ice sheet meets an obstacle. This pressure may lower the melting point of the ice enough to form a liquid layer and allow the glacier to pass. Once behind the obstacle, the pressure becomes lower again and water freezes to reform the bottom of the glacier, essentially allowing the ice to flow around obstacles.



Premelting

Even tens of Kelvins below the melting point, ice surfaces and interfaces are covered by an extremely thin amorphous or quasiliquid layer. This is called premelting. The layer forms because the water molecules on the surface are not fully coordinated and are thus only weakly tied to their lattice positions. Regelation processes are also affected by premelting, which provides a pressure-independent mechanism for liquid layer formation at interfaces. Combined with premelting, regelation may occur at lower pressures than if pressure melting was the only mechanism driving the liquid formation.