Animated Movie of Ice

January 7 2008

An animated movie shows an ordered structure dissolving little by little into a disordered mess after a light pulse: Swedish researchers from the University of Uppsala have used a computer to simulate ice melting after it is heated with a short light pulse.

As they report in the journal Angewandte Chemie, the absorbed energy first causes the OH bonds to oscillate. After a few picoseconds (10^{-12} s) the energy is converted into rotational and translational energy, which causes the crystal to melt, though crystalline domains remain visible for quite a while.

The common form of ice crystals is known as hexagonal ice. In this form the oxygen atoms of the water molecules are arranged in a tetrahedral lattice. Each water molecule is bound to four neighboring molecules by means of bridging hydrogen bonds, leading to an average of two bridges per molecule. In water, there are, on average, only 1.75 bridging hydrogen bonds per molecule.

What happens in the process of melting? Carl Caleman and David van der Spoel have now successfully used a computer to simulate “snapshots” of melting ice crystals. These molecular dynamics simulations are ideal for gaining a better understanding of processes like melting or freezing because they make it possible to simultaneously describe both the structure and the dynamics of a system with atomic resolution and with a time resolution in the femtosecond (10^{-15} s) range.

The simulation demonstrated that the energy of the laser pulse initially causes the OH bonds in the water molecules to vibrate. Immediately after the pulse, the vibrational energy reaches a maximum. After about a picosecond, most of the vibrational energy has been transformed into rotational energy.

The molecules begin to spin out of their positions within the crystal, breaking the bridging hydrogen bonds. After about 3 to 6 picoseconds, the rotations diminish in favor of translational motion. The molecules are now able to move freely and the crystal structure collapses. This process starts out locally, at individual locations within the crystal.

Once the symmetry of the structure is broken, the likelihood of melting processes occurring in the area immediately surrounding the crystal defect rises significantly. The melting process thus spreads out from this point little by little. At other locations the ice can maintain its crystalline structure a little longer.

A movie is available online at
xray.bmc.uu.se/molbiophys/images/Movies/melt.mpg

Citation: David van der Spoel, Picosecond Melting of Ice by an Infrared Laser Pulse: A Simulation Study, *Angewandte Chemie International Edition*, doi: 10.1002/anie.200703987

Source: Angewandte Chemie

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