Geophysical Research Abstracts
Vol. 13, EGU2011-10404, 2011
EGU General Assembly 2011

Ice from Supercooled Water: Neither Hexagonal nor Cubic

Tamsin Malkin (1), Benjamin J. Murray (1), Andrey V. Brukhno (2), Jamshed Anwar (3), and Christoph G. Salzmann (4)

(1) Institute for Climate & Atmospheric Science, School of Earth and Environment, University of Leeds, Leeds, LS2 9JT, UK. (t.l.malkin@leeds.ac.uk), (2) Centre for Molecular Nanoscience (CMNS), University of Leeds, Leeds, LS2 9JT, UK., (3) Institute of Pharmaceutical Innovation, University of Bradford, Richmond Road, Bradford, BD7 1DP, UK., (4) Department of Chemistry, Durham University, South Road, Durham, DH1 3LE, UK.

Under atmospherically relevant conditions both the stable hexagonal phase (ice Ih) and a metastable phase of ice I that lacks hexagonal symmetry can form. The ice which initially crystallises from pure water or solution droplets that freeze homogeneously has been identified in the past as being cubic ice (ice Ic) and it was suggested that this ice contains hexagonal like stacking faults [Murray et al., 2005; Murray and Bertram, 2006]. Here we show through X-ray diffraction experiments and a computational study that ice that initially crystallises from water when it freezes homogeneously is neither cubic nor hexagonal. It is in fact in fact, a mixed form of ice I, which randomly switches between sequences of cubic and hexagonal layers alternating perpendicular to the basal face {0001}. Normally it is assumed that a distinct phase crystallises rather than ice which lacks either cubic or hexagonal symmetry.

Droplets of pure water suspended in an oil emulsion of median diameter 0.9 μm were cooled down within a powder X-ray diffractometer at 30 K min^{-1} and froze homogeneously at around 232 K. The diffraction pattern of these frozen droplets lacks some of the peaks associated with hexagonal symmetry and the patterns are similar to other ice Ic patterns in the literature. Modelling of these diffraction patterns reveals that the ice is ice I with randomly stacked cubic and hexagonal sequences. Hansen et al. [2008 a,b] concluded that ice I recrystallised from ice V and ice IX is also a mixed structure with 25 - 60% hexagonal sequences in ice Ic. Our result is important because it suggests that what has been called cubic ice is in fact ice I with random stacking sequences lacking the pure cubic and hexagonal symmetries.

We also conducted Monte Carlo simulations of homogeneous ice formation in bulk water in which ice I crystallisation is encouraged, but no preference is made between hexagonal and cubic structures [Brukhno et al, 2008]. The resulting ice is most often a mixed cubic-hexagonal structure.

The experimental and computational studies show that the growth of ice I from supercooled water yields neither cubic nor hexagonal forms, but rather a mixed ice structure with random alteration between cubic and hexagonal sequences. These results suggest that ice growth is primarily governed by the nearest neighbour environment, making stacking faults a general feature.

Murray, B. J. et al., Nature, 434, 202-204 (2005).
Murray, B. J. and A. K. Bertram, Phys. Chem. Chem. Phys,. 8, 186-192 (2006) .
Hansen, T. C. et al., J. Phys. Condens. Matter, 20, 285104 (2008a).
Hansen, T. C. et al., J. Phys. Condens. Matter, 20, 285105 (2008b).
Brukhno, A. et al. J. Phys. Condens. Matter, 20, 494243 (2008).