Abstract template:

Title

The Single Crystal, Basal Face of Ice I_h Investigated with Sum Frequency Generation

Reference

J. Chem. Phys. **2007**, *127*, 214502 pgs1-8.

Authors

Groenzin, Henning; Li, Irene; Buch, Victoria; Shultz, Mary Jane

Abstract

Sum frequency generation spectroscopy has been used to investigate the hydrogen-bonded region of single-crystal, hexagonal ice in the temperature range of 113–178 K. The temperature and polarization dependences of the signal are used in conjunction with a recent theoretical model to suggest an interpretation of the bluest and reddest of the hydrogen-bonded peaks. The reddest feature is associated with strong hydrogen bonding; the dynamic polarizability of this feature is primarily parallel to the surface. It is assigned to a cooperative motion among the companion to the free-OH and four-coordinate oscillators hydrogen bonded to dangling lone-pair molecules on the surface. The bluest hydrogen-bonded feature is similarly assigned to a cooperative motion of the OH stretch of dangling lone-pair molecules and of four-coordinate molecules in the lower half bilayer that are hydrogen bonded to free-OH molecules. Reconstruction induced strain is present at as low as 113 K. These results provide a richer picture of the ice surface than has heretofore been possible.