Abstract Submitted
for the MAR07 Meeting of
The American Physical Society

**Local structure and the intermediate-energy fine structure in x-ray Raman scattering from ice Ih** G.T. SEIDLER, T.T. FISTER, C. HAMNER, F.D. VILA, University of Washington, J.O. CROSS, Advanced Photon Source, Argonne National Laboratory — The structure of the various different equilibrium and nonequilibrium phases of water ice is a topic of considerable interest, with strong relevance for geophysics, atmospheric sciences, and space sciences. Recent advances in non-resonant x-ray Raman scattering (XRS) provide a new method for studying local structure of water ices in extreme environments including especially in high-pressure cells. Here, we investigate two pragmatic issues: the optimum choice of momentum transfer $q$ for these measurements and the usefulness of the intermediate-energy fine structure as a strong fingerprint of local atomic structure out to several coordination shells. To this end, we present new XRS measurements of ice Ih with greatly improved statistics over earlier work, and also present extensive full-multiple calculations of the dependence of the intermediate-energy fine structure on local structure. We find that XRS measurements at high $q$, where the XRS cross-section is largest but where multipole transitions can be important, show little difference from dipole-limited soft x-ray absorption studies. In addition, our calculations predict significant sensitivity of the XRS intermediate-energy fine structure to different ice structures.

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Date submitted: 20 Nov 2006 Electronic form version 1.4