National Aeronautics and Space Administration

Amorphous and Crystalline Water-Ice in Space – Elastic and Inelastic Neutron Scattering

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Program: FY21 R&TD Innovative Spontaneous Concepts

Objectives

To determine the nanoscopic structural properties of amorphous ice, crystalline ice, and amorphized crystalline ice, which will provide better understanding of how non-ice molecules undergo chemistry, diffuse, aggregate, and are transported in icy materials in our solar system and interstellar medium.

Background

Water ice is present on the Moon, Mars, asteroids like Ceres, comets, the moons of Jupiter, Saturn, and beyond in our solar system as well as in the interstellar medium. Recent work shows that there is still disagreement between models based on lab data and ground-based observations on the crystallinity of Europa's surface ice [Berdis et al., Icarus, 341, 113999, 2020]. Water ice acts as a host matrix for several trapped species regulating conditions for complex chemistry. For this reason, it is important to understand water-ice solid structure at the nanoscopic level. In addition to relatively porous amorphous ice and more compact crystalline ice phases, amorphized crystalline ice can also be present under radiation and lower temperatures in our solar system.

Neutron scattering is ideally suited to investigate water ice, because of the high scattering cross-section of neutrons by protons (H). Elastic scattering provides structural information on the solid – both short-range and long-range. Inelastic scattering provides phonon (lattice) and molecular vibrational properties of the ice. While a couple of earlier works are published [Kolesnikov et al. Physical Review B. 59, 3569, 1999; Yamamuro et al. J Chem Phys, 115, 9808, 2001] on amorphous and crystalline ices with neutron elastic and inelastic scattering, to the best of our knowledge, no work is yet known on structural changes involving radiation-induced amorphization of crystalline ice, which is the focus of our study.

Approach and Results

Approach: Our approach was to obtain both the nanoscopic structural properties of the above three forms of ice as well as their infrared spectra that can be compared to in-situ or remote-sensing space observations. This involved amorphous ice deposited at 100 K and crystalline ice deposited at 150 K, both subsequently cooled down to 25 K and then warmed up to 150 K in steps of 25 K to provide unique data on how amorphous ice transforms into crystalline ice and how crystalline as well as amorphous ice structure changes with temperature. Subsequently, we planned to irradiate the crystalline ice at 125 K and below with 2 keV electrons to generate amorphized crystalline ice and study its structure and spectroscopy with elastic and inelastic neutron scattering. The JPL team worked with the ORNL team remotely to conduct experiments at ORNL and analyze the data.

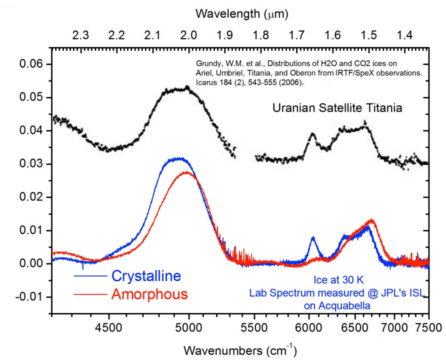

Figure 1. Top: Observed NIR reflectance spectrum of Titania inverted to compare with the laboratory data. Bottom: Absorbance spectra of vapor deposited amorphous ice and annealed and cooled crystalline ice at 30 K.

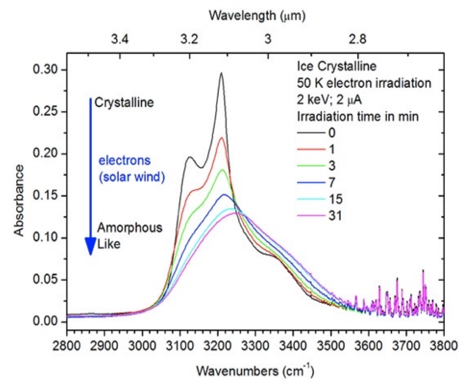

Figure 2. Change in the infrared spectral band shapes when crystalline ice at 50 K was bombarded with 2 keV electrons. The resulting spectrum after 30 min of irradiation is structure-less and resembles low-temperature deposited amorphous water ice.

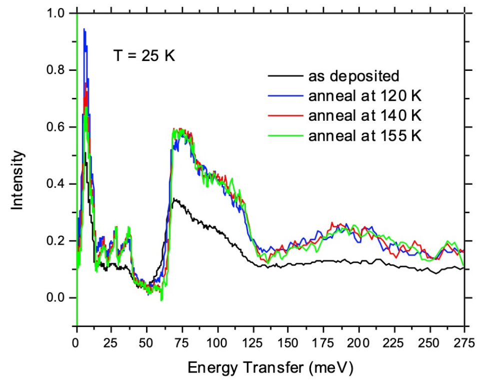

Figure 3. Inelastic neutron scattering spectra of amorphous (black line) and crystalline (rest of the colors) water ice. Energy transfer (meV) can be converted to cm^{-1} or mm to compare with infrared spectra.

Results: Due to the continued COVID19 pandemic in-person work that had been planned, had to be changed to remote collaboration and the same also resulted in significant slowdown in the project. However, we have made significant progress in obtaining for the first time both elastic and non-elastic neutron scattering data for vapor-deposited amorphous and crystalline water-ice at temperatures between 30 K and 150 K. We find that the vapor deposition rate of water has an effect on the purity of amorphous phase when deposited at 30 K. Slower deposition rate produced pure amorphous ice, whereas faster deposition resulted in small amount of crystallin ice formation. We are now in the process of data analysis and preparation of publication. Second part of the work with electron irradiation of crystalline and amorphous ices couldn't be achieved as planned due to the COVID19 related issues. We plan to conduct these studies in FY22.

Significance/Benefits to JPL and NASA

Understanding how water-ice structures transform between amorphous and crystalline phases on many solar system and interstellar ices would provide critically needed insight into how we can connect remote-sensing spectroscopic data to surface physics and chemistry. Particularly, Europa's surface ice spectra do not fit into either amorphous or crystalline phases, but looks like a combination of both, but it is not clear why. Similarly, interstellar ices are mostly amorphous whereas surfaces of KBO icy bodies are predominantly crystalline. Only neutron scattering will provide both structural and vibrational information simultaneously, unlike any other method - enabling us to link observational infrared data to microstructure environments.

Publication: One manuscript under preparation

Acknowledgments: A portion of this research used resources at the Spallation Neutron Source, a DOE Office of Science User Facility operated by the Oak Ridge National Laboratory. We also thank Jamie Molaison and Eric Novak of the Neutron Scattering Division, Oak Ridge National Laboratory, for helping with conducting the experiments and analysis of the data.

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Clearance Number:
RPC/JPL Task Number: R21246