The OH stretch infrared band of water ice and its temperature and radiation dependence. U. Raut, M. J. Loeffler, R. A. Vidal, and R. A. Baragiola,.University of Virginia, Laboratory for Atomic and Surface Physics, Thornton Hall, Charlottesville, VA 22904, USA.

Introduction: Knowledge of the infrared spectra of water ice and its dependence on conditions and history is important for obtaining information about icy objects from remote sensing. The infrared absorption band corresponding to the OH stretch vibration at near 3.1 µm is the most prominent water band. Thus, it can be used to most sensitively detect the presence of water and is the first one to saturate with increasing optical path length. The literature of infrared spectra of low temperature water ice has been reviewed recently [1-2]. Recently, we have measured infrared reflectance spectra of transparent thin films of water ice under different conditions relevant to environments in the outer solar system and interstellar grains. Some preliminary results are given here.

Experimental details: Thin water ice films were grown by depositing high purity water vapor onto a cold gold mirror [4]. The gold substrate is one of the electrodes of a quartz-crystal microbalance, which allows an accurate determination of the amount of water deposited per unit area.

The infrared spectra were obtained in specular conditions for an angle of incidence of 45 degrees, using a Thermo-Nicolet Nexus 670 FTIR spectrometer at a resolution of 2 cm^{-1} and external mirror optics. The spectra were ratioed to the spectrum obtained with the bare gold mirror, and then converted to optical depth. Sequences of spectra were analyzed using factor analysis [5] to identify the distinct spectral structures and their evolution with thermal or ion-beam processing.

Compaction of microporous ice:

Fig. 1 shows the evolution of the IR spectra for an amorphous ice film grown at 20K as it is heated at a rate of 1 K/minute. The changes are irreversible; below about 125 K, they depend only on the maximum temperature to which the ice is heated and not on the heating rate. The changes are attributed to compaction due to the collapse of micropores.

Separation of the effect of compaction from the temperature dependence of absorbance is obtained by compacting (not completely) amorphous ice at 120 K (below the crystallization temperature) and measuring the band changes while lowering the temperature. The results in Fig. 2 show that compaction dominates spectral changes during annealing.

Dangling bonds. In addition to the main 3.1 µm OH band, much weaker sharp bands, characteristic of vapor-deposited ice appear due to dangling bonds in the surface of the ice and in the internal surface of pores [6]. In our non-grazing geometry, the contribution from the proper surface of the ice is small. We note that the bands disappear as ice is annealed past 90 K, as has been noticed earlier, or if it is irradiated with high energy ions (Fig. 3) . We can interpret the ion-induced pore collapse as the effect of annealing in the transiently 'hot' region around the ionization track produced by each individual ion.

Phase transitions:

Crystallization. Amorphous ice crystallizes at a rate that depends on temperature [2,3]. The effect of crystallization is to sharpen and shift the OH-stretch band, as shown in Fig. 1.

Amorphization of crystalline ice by ion irradiation. We grew cubic crystalline ice at 150 K and irradiated at 70 K with 100 keV Ar^+. The OH band transforms quickly to that of amorphous ice during irradiation (Fig. 4). The amorphization rate is quite higher than that found by Strazzulla et al. [7] using ions of a few keV.

Discussion: The spectrum of ice is characteristic of the highest temperature reached during its thermal history, in the absence of irradiation. Ion irradiation amorphizes crystalline ice and compacts microporous amorphous ice. The spectra of ice affected by meteorite and micrometeorite bombardment will depend on location and particle size. Vapor and liquid ejecta will cool extremely fast (hyperquench) during recondensation, leading to the formation of amorphous ice. In the impact region, ice will melt and then freeze at a rate that depends on the size of the impact region. Small impact regions will cool very fast, leading to amorphous ice, while the slow cooling of large regions will lead to the formation of crystalline ice.

References:

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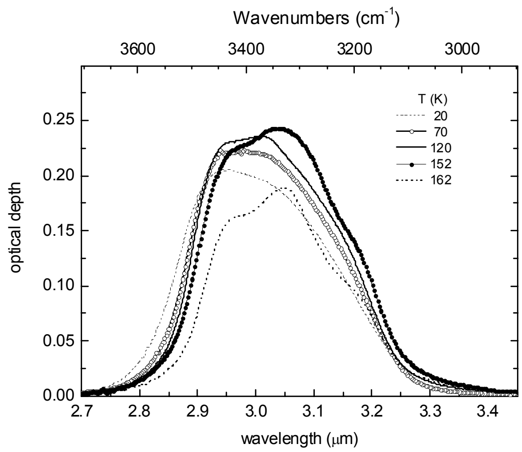

Figure 1 - Effect of temperature on the infrared spectrum of a 4.1×10^{17} H_2O/cm^2 amorphous ice film grown at 20 K and warmed up at 1 K/min. The notable decrease of band area at 162 K is due to mass loss by sublimation

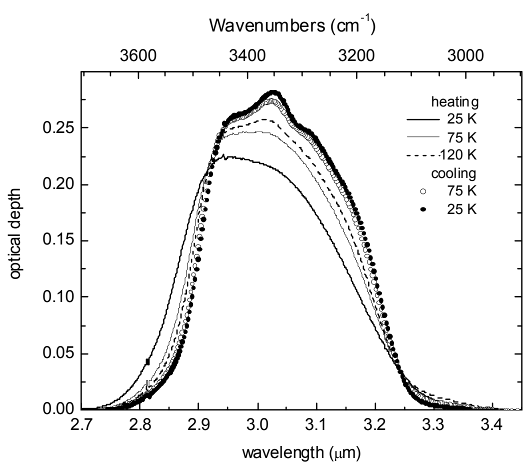

Figure 2 - Effect of temperature on the infrared spectrum of a 4.24×10^{17} H_2O/cm^2 amorphous ice film grown at 25 K warmed to 120 K at 1 K/min and then cooled back to 25 K.

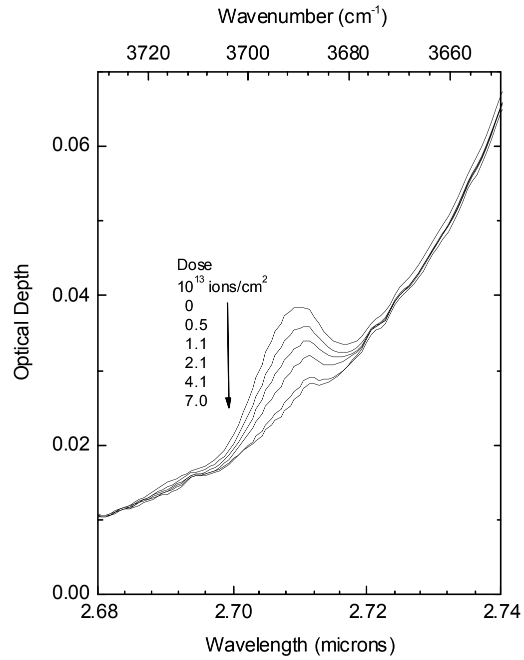

Figure 3 - Evolution of the 2.71 μm dangling bond band in a 6×10^{18} H_2O/cm^2 ice film grown and irradiated at 80K with 100 keV protons to the indicated doses.

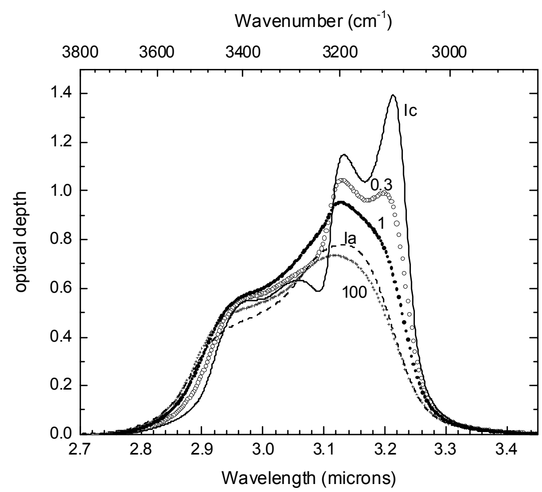

Figure 4 - OH band measured at 70K for a 1.02×10^{18} mol/cm^2 crystalline ice film grown at 150 K and irradiated at 70 K by 100 keV Ar^+ ions at normal incidence. Ic - unirradiated crystalline (cubic) ice. The sumbols denote spectra of Ic irradiated to different fluences indicated by the numbers adjacent to the curves, in units of 10^{13} ions/cm^2. The dashed curve labeled Ia is the spectrum of amorphous ice grown at 20 K and taken to 75K.