

Supporting information for the paper:

**Structural reorganization on amorphous ice films below 120 K revealed by
near-thermal (~1 eV) ion scattering**

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Supporting information 1

The spectrometer is composed of two main chambers and a sample manipulator. Each region of the system is pumped by a Pfeiffer (TMU 261) 210 L/s turbomolecular drag pump. These two pumps are backed by another Pfeiffer 60 L/s turbomolecular pump (TMU 071P) and further by a Pfeiffer 3.3 m³/h dry pump (MVP 055). This ensures a hydrocarbon-free environment. An ultimate pressure below 0.5×10^{-10} mbar (limit of the controller) was achieved in both the ionization and scattering chambers after bake-out. All the quadrupoles and control electronics are from Extrel Core Mass Spectrometry. The analyzer quadrupole was kept at a nominal scattering angle of 90° with reference to the incident ion beam. The mass analyzer was operated at a resolution of ± 0.2 Da.

Every experiment begins with the cleaning of the substrate. Polycrystalline copper was used as the substrate material. The heater for the substrate was electrically isolated from the rest of holder by sapphire balls. Volatile impurities were removed by heating the substrate to a temperature of 400 K for 10 min. Then the substrate was rapidly cooled to 110 K and kept at that temperature for 10 min. Before depositing the sample molecule, the substrate was again heated to 220 K for 10-20 seconds to avoid any kind of condensation on the substrate plate during the cooling process. After this procedure, substrate was cooled back to the required temperature for the experiments. Thus the experimental procedures ensured the removal of any kind of impurity

condensing on the substrate. In addition, the surface cleanliness was checked by chemical sputtering. The liquids were purified by several freeze-pump-thaw cycles on each day of the experiment before use. Surfaces for the studies were prepared by the deposition of the corresponding vapors, which were introduced onto the sample chamber through a leak valve. The gas-line was pumped thoroughly to avoid contamination. The distance between the sample source and copper substrate was adjusted in order to obtain uniform sample growth on the substrate.

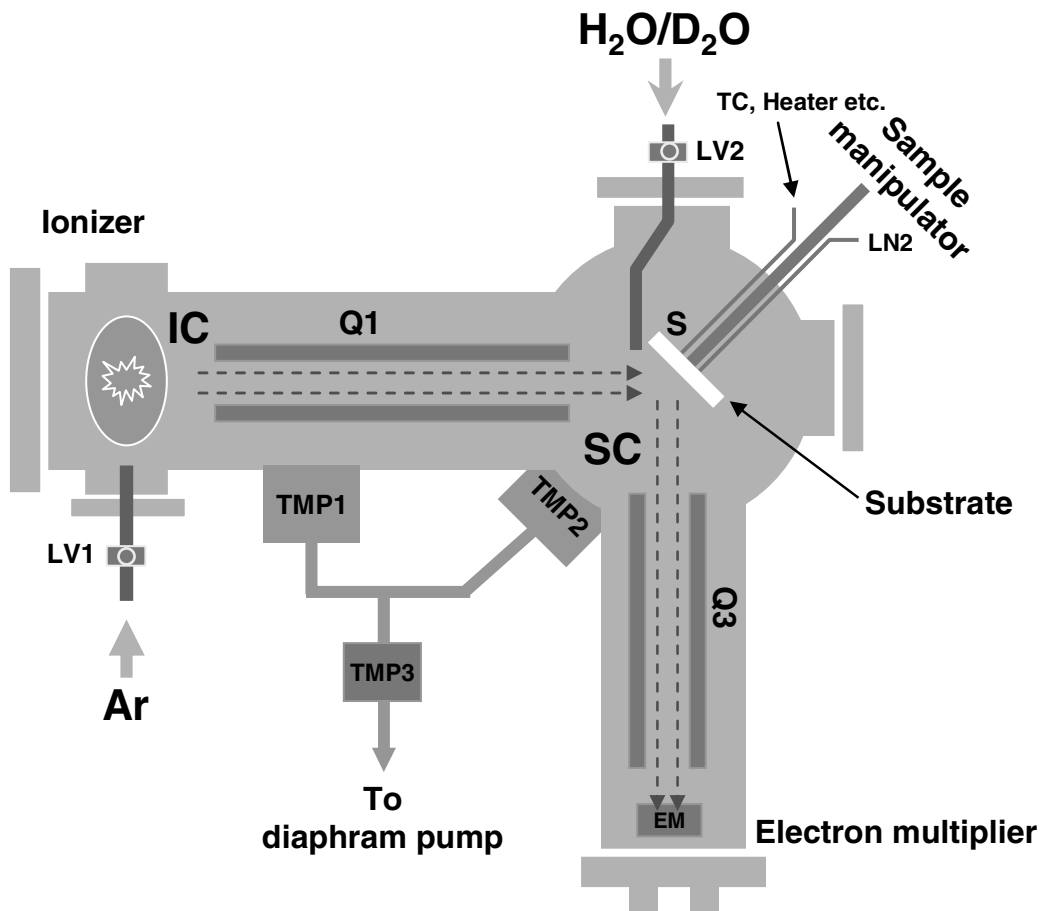


Figure S1. Schematic of the vacuum chamber and ion scattering set-up. TMP1, TMP2 and TMP3 are two 210 and a 60 L/s turbomolecular pumps, respectively. Q1 is the mass filter quadrupole and Q3 is the analyzer quadrupole. LV1 and LV2 are the leak valves on the sample line. Scattering chamber and ionization chamber are represented as SC and IC, respectively. TC corresponds to thermocouple leads. S is the polycrystalline copper substrate. EM represents the electron multiplier assembly of the system. The manipulator is perpendicular to Q1 and Q3, but shifted in the schematic for clarity.

Supporting information 2

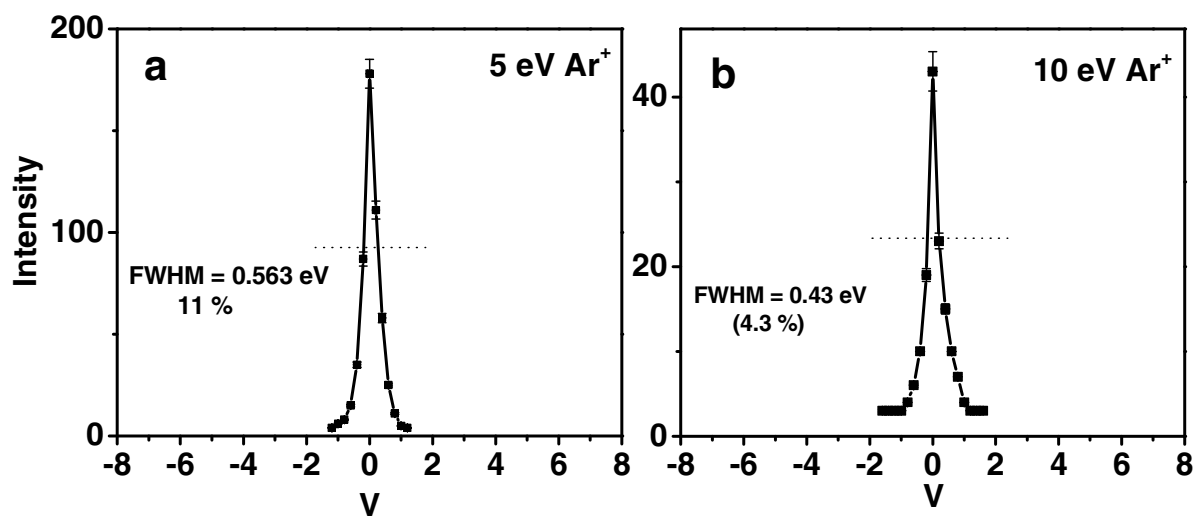


Figure S2. Plot of ion intensity as a function of retarding/accelerating potential at 5 and 10 eV collision energy. Experiments were done at room temperature after floating the Cu substrate. The x-axis scale is the same as that of Figure 1.

Supporting information 3

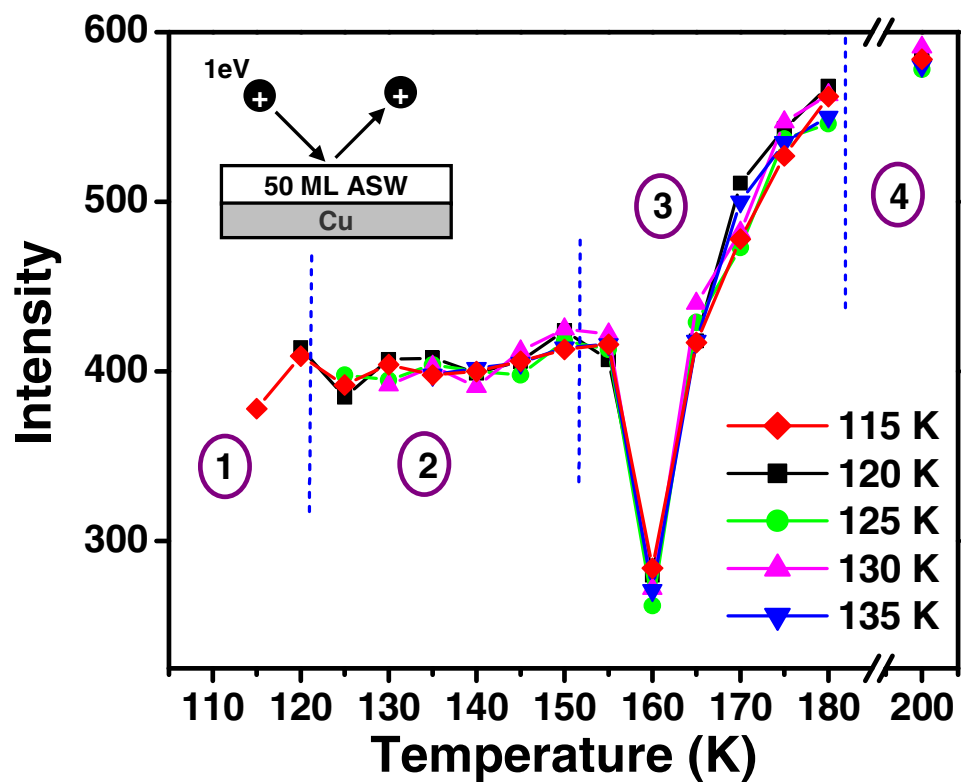


Figure S3. The intensity variation as a function of temperature for 50ML ice surface prepared by depositing water vapor at various temperatures. Deposition temperature is mentioned on each trace. The transition is not seen for samples prepared above 120 K, but all other features are identical to those in Figure 1. The error bars have been omitted for clarity.

Supporting information 4

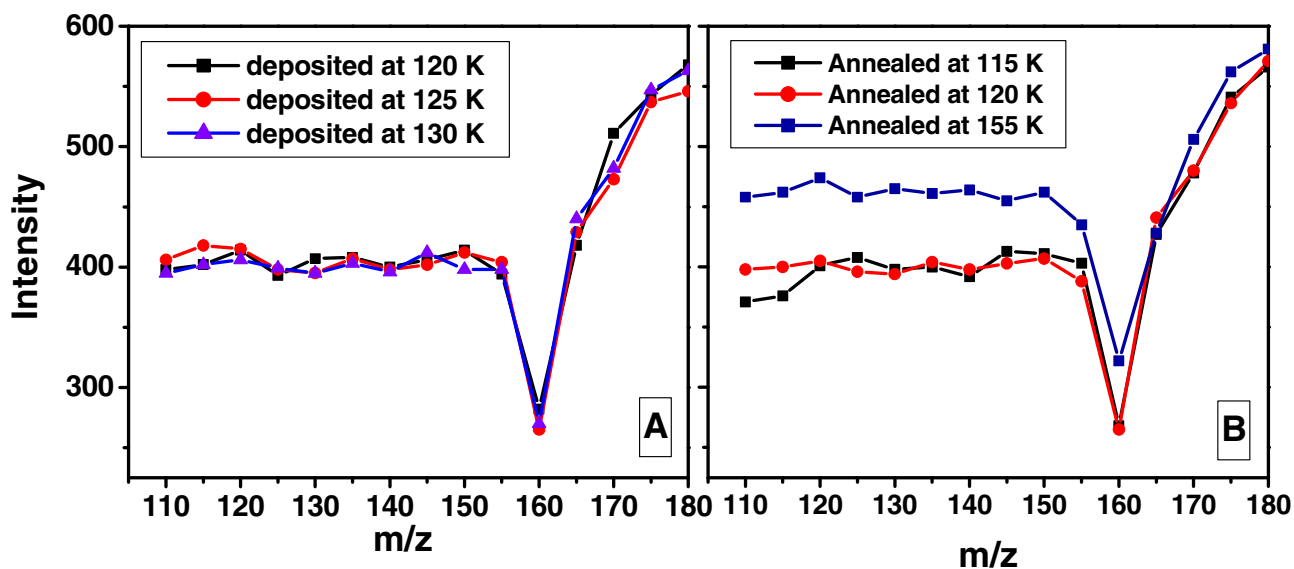


Figure S4. (A) The intensity variation as a function of temperature for 50ML ice surface prepared by depositing water vapor at three different temperatures; 120 125 and 130 K. Samples were cooled back to 110 K before starting the experiment. (B) The intensity variation as a function of temperature for 50ML ice surface prepared at 110 K and annealed at 115, 125 and 155 K and further cooled back to 110 K to start the experiment. The error bars have been omitted for clarity. Trace for 155 K annealed sample is significantly different as part of the ice layers have desorbed. The data suggest that the transition is not reversible.

Supporting information 5

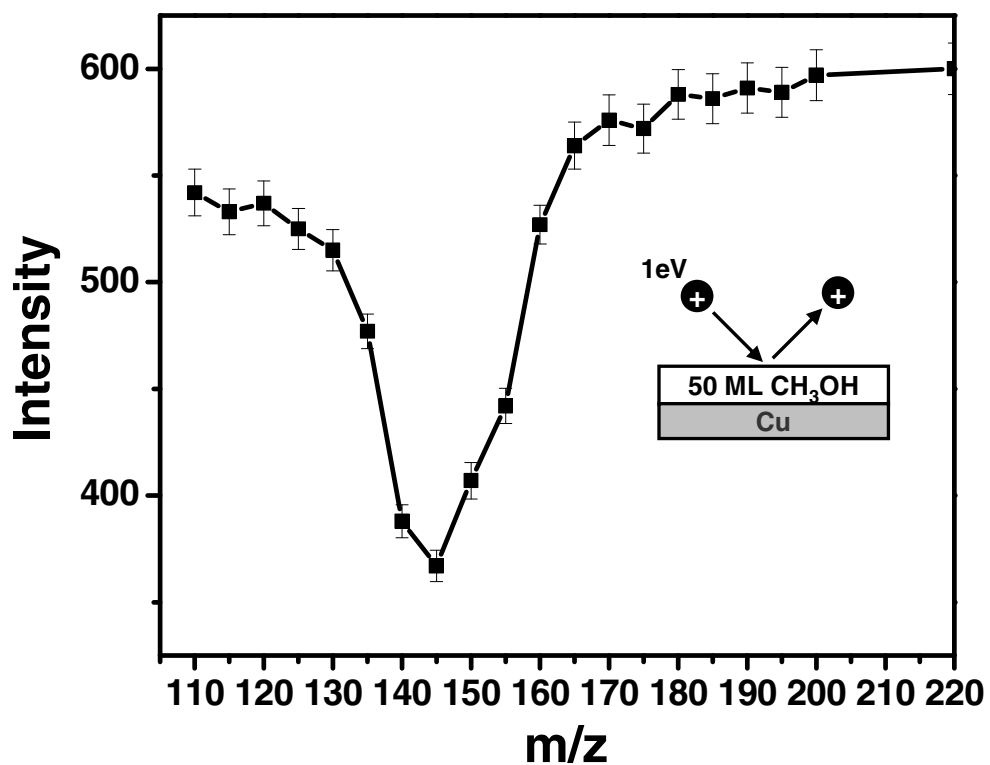


Figure S5. The intensity variation as a function of temperature for 50ML CH₃OH surface. Onset of desorption is ~130 K and the temperature window for CH₃OH desorption is larger compared to water.

Supporting information 6

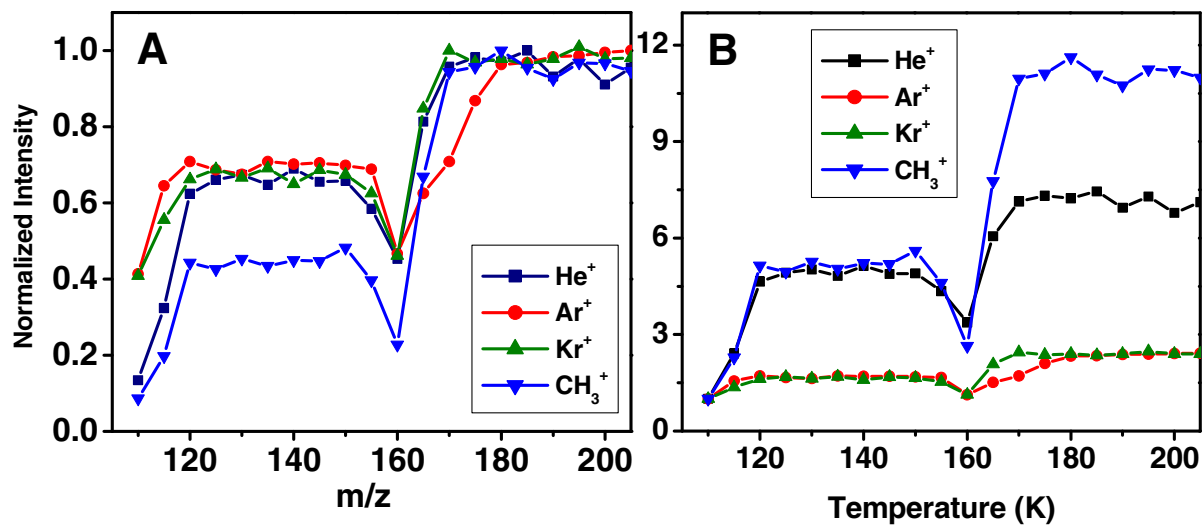


Figure S6. The normalized intensity variation as a function of temperature for 50ML ASW for different ions at 1 eV collision energy. In A, intensities are normalized to the value of Cu substrate at 200 K, for each ion and in B intensities are normalized to the value at 110 K from ASW for each ion.