# Isotope effects in $H^+(D^+)$ desorption induced by $4a_1 \leftarrow O$ 1s resonant transition of condensed H,O (D,O)

Akira NAMBU<sup>1\*</sup>, Eiichi KOBAYASHI<sup>1,2</sup>, Kazuhiko MASE<sup>1,3</sup>

<sup>1</sup>KEK-PF, Tsukuba, Ibaraki 305-0801, Japan

<sup>2</sup>Inoue Foundation for Science, 15-15 Nanpeicho, Shibuya-ku, Tokyo 150-0036, Japan

<sup>3</sup>PRESTO, JST, 4-1-8 Honcho Kawaguchi, Saitama 332-0012, Japan

(\* Present Address: Chemistry Department, Brookhaven National Laboratory, Upton, NY 11973-5000)

### **Introduction**

In order to study the interactions between water molecules and photon at  $4a_1 \leftarrow O$  1s resonant transition energy, Auger electron – photoion coincidence (AEPICO) experiments have been performed for condensed water (H<sub>2</sub>O and D<sub>2</sub>O). Several kinds of isotope effect were observed in H<sup>+</sup> (D<sup>+</sup>) desorption. Those isotope effects are successfully explained by a four-step ion desorption mechanism involving O-H (O-D) bond extension within the lifetime of the O 1s core hole.

### **Experimental**

All the experiments were performed with a homemade EICO analyzer which consists of a coaxially symmetric mirror analyzer for electron and a miniature time-of-flight (TOF) mass spectrometer for ions [1]. A soft x-ray beamline of 8A was employed for the experiments.

Water (H<sub>2</sub>O/D<sub>2</sub>O) was purified by the cycles of freezepump-thaw and the liquid-nitrogen-cooled (~80 K) goldplated surface was exposed to 50 Langmuir (1 Langmuir =  $1 \times 10^{-6}$  Torr·s) of H<sub>2</sub>O/D<sub>2</sub>O molecules to form an amorphous condensed layer.

## **Results and Discussion**

The result of AEPICO is shown in Fig. 1. In AEPICO spectrum, at first, the amount of photoion desorbed at the same time (within  $\sim$ 1 ns) of certain energy Auger electron is measured as a TOF spectrum. Next, those amounts of desorbed ion are plotted as a function of (Auger) electron kinetic energy to reproduce the AEPICO spectra. Thus, the AEPICO spectra show the relationship of the Auger-



Fig. 1 AEPICO Spectra of H<sub>2</sub>O and D<sub>2</sub>O.

final-state and ion desorption probability. Also, the analysis of the TOF data allows us to reveal the kinetic energy distribution of desorbed ion (Fig. 2).

As shown in Fig. 1 and Fig. 2, several kinds of isotope effects were observed in AEPICO spectrum and kinetic energy distribution of desorbed ion kinetic energy; (1) peak shifts in AEPICO (Fig.1) and resonant Auger electron spectra (not shown), (2) the relative intensity differences in AEPICO spectra (Fig. 1), (3) the differences in ion kinetic energy for the selected Auger-final-states (Fig. 2) and (4) the intensity difference in prominent peak in ion yield spectra (not shown).

Those effects can be explained by the four-step desorption mechanism which employs three potential energy surfaces and ultrafast O-H (O-D) bond extension within the lifetime of the O 1s core-hole [1]. With this mechanism, when the H is replaced by the D whose mass is as twice as H, the length of ultrafast extension should be shorter than that of H, thus that the desorption is affected by this mass difference [2].

### **References**

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\* akira.nambu@bnl.gov



Fig. 2 Kinetic Energy Distribution of Desorbed Photoion.