# Photostimulated ion desorption from H<sub>2</sub>O dissociatively adsorbed on Si(111) studied using photoelectron photoion coincidence spectroscopy [1]

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### **Introduction**

When a core-level of a surface molecule is ionized, an ion desorption may be stimulated by an Auger process leaving multiple valence holes (Auger stimulated ion desorption (ASID)). Since core-level photoelectron spectroscopy can distinguish two atomic sites whose chemical shifts are different, the coincidence measurement of photoelectrons photoions and (photoelectron photoion coincidence, PEPICO) is an ideal technique to study ion desorption at a specific site [2]. Furthermore, site-specific ion desorption is a potential tool for analyzing geometry and properties at specific surface sites. We selected water (H<sub>2</sub>O) adsorbed on Si(111) (H<sub>2</sub>O/Si(111)) as a target, because it is important for fundamental science, and for understanding the mechanisms of wet etching in semiconductor device processing. Tanaka et al. have investigated ASID mechanism of  $H^+$  desorbed from  $H_2O/Si(100)$  in the O Kedge region using PEPICO and Auger electron photoion coincidence (AEPICO) spectroscopy, and concluded that n-valence-hole states (n > 2) are responsible for  $H^+$ desorption [3]. In the present paper we report a study of  $H^+$  desorption from H<sub>2</sub>O/Si(111) in the Si L-edge region using an improved electron ion coincidence (EICO) analyzer.

#### **Experimental**

Clean Si(111) was exposed to 1000 L (1 L =  $1 \times 10^{6}$ Torr s) of water at room temperature. H<sub>2</sub>O is known to be dissociatively adsorbed on Si(111) forming Si-OH and Si-H surface species. Synchrotron radiation at hv = 130 eV was used for photoelectron and PEPICO spectroscopy.

#### **Results and Discussion**

Figure 1 shows the Si 2p - H<sup>+</sup> PEPICO data and Si 2p photoelectron spectrum of a H<sub>2</sub>O/Si(111) surface at hv = 130 eV. The accumulation time was 3900 sec for each PEPICO data. The H<sup>+</sup> PEPICO peak was observed at a relative binding energy of +1.5 eV, corresponding to the Si<sup>+</sup> and Si<sup>2+</sup> sites. We estimated the H<sup>+</sup> desorption probability per Si 2p ionization ( $P_D$ ) by the following equation:

$$P_D = \frac{C_{PEPICO}}{C_{PE} \times R_{Si2p} \times E_{PI}},$$

where  $C_{\text{PEPICO}}$  and  $C_{\text{PE}}$  denote Si 2p – H<sup>+</sup> PEPICO, and the photoelectron counts measured with the EICO analyzer simultaneously at a specific photoelectron kinetic energy. The latter is the same as the number of the trigger for the MCS during the coincidence measurement.  $R_{\text{si2p}}$  is the ratio of the Si 2p photoelectron counts to the electron counts at a specific electron kinetic energy.  $E_{\text{PI}}$  is the photoion detection efficiency of the TOF-MS, given by the following equation:

$$E_{PI} = (T_{Mesh})^3 \times E_{MCP},$$

where  $T_{\text{Mesh}}$  is the transmittance of one mesh in the TOF-MS ( $T_{\text{Mesh}} = 0.77$ ) and  $E_{\text{MCP}}$  is the photoion detection efficiency of the MCPs ( $E_{\text{MCP}} = 0.6$ ). The values of  $P_{\text{D}}$ were estimated to be  $<4 \times 10^{6}$ ,  $5 \cdot 7 \times 10^{6}$  and  $2 \cdot 4 \times 10^{5}$ for the Si<sup>0</sup>, Si<sup>+</sup> and Si<sup>2+</sup> sites, respectively. We assigned the Si<sup>+</sup> and Si<sup>2+</sup> sites responsible to the H<sup>+</sup> desorption to the Si-OH and Si(O)-OH sites, respectively.

We also carried out Si  $2p - H^+$  PEPICO measurements of Si(111) exposed to H<sub>2</sub>O of about 5 L, on which Si-OH and Si-H sites exist. The H<sup>+</sup> PEPICO signal, however, was below the detection limit of our apparatus ( $P_D < 4 \times 10^{-6}$ ). The results show that H<sup>+</sup> desorption probability is quite small at the Si-OH and Si-H sites.



Fig. 1. Si  $2p - H^{\dagger}$  PEPICO (filled circles) and Si 2p photoelectron (solid line) spectra of H<sub>2</sub>O/Si(111) at hv = 130 eV. Both spectra are normalized by the ion counts simultaneously measured with the EICO analyzer

## **References**

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