Ion Desorption Induced by Core-Electron Transitions of Surface Molecules Studied with Energy-Selected Electron-Ion Coincidence Spectroscopy

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Energy-selected electron ion coincidence (EICO) spectroscopy combined with synchrotron radiation is a novel and powerful tool for study of ion desorption induced by core-electron transitions of surface molecules [1]. We have developed an EICO apparatus, which consists of a cylindrical mirror electron energy analyzer and a time-of-flight ion mass spectrometer [1-3]. The Auger electron photoion coincidence (AEPICO) spectroscopy is powerful for elucidating mechanism of ion desorption induced by Auger transitions, because it provides ion mass spectra for the ion desorption channels related to the selected Auger final states [1-3]. A study of condensed H₂O using AEPICO spectroscopy showed that H⁺ desorption is stimulated by O KVV Auger processes leaving two-hole states. The H⁺ desorption probability is found to depend on the bonding character of the orbitals where holes are created and on the effective hole-hole Coulomb repulsion. H⁺ desorption induced by $4a_1 \leftarrow O$ 1s and $3p \leftarrow O$ 1s resonant transitions of condensed H₂O is also investigated using AEPICO spectroscopy. For H⁺ desorption at $4a_1 \leftarrow O$ 1s the results were explained by a four-step mechanism, that is, 1) the $4a_1 \leftarrow O$ 1s transition, 2) expansion of the HO-H distance, 3) a spectator-Auger transition, and 4) H⁺ desorption. For H⁺ desorption at $3p \leftarrow O 1s$, on the other hand, the results were explained by a three-step mechanism, that is, 1) the $3p \leftarrow 0$ 1s transition, 2) a spectator-Auger transition, and 3) H⁺ desorption. The difference in the ion desorption mechanism was attributed to the difference between the characters of the 4a1 and 3p orbitals, that is, 4a₁ is O-H anti-bonding while 3p is O-H non-bonding. Photoelectron photoion coincidence (PEPICO) spectroscopy, on the other hand, is a novel method to measure the chemical shift at the ion desorption site. In a study of condensed H₂O using PEPICO spectroscopy, the peak position of oxygen 1s photoelectron was observed to be shifted by 0.7 eV from that in PEPICO yield spectrum. This result was attributed to the difference of chemical environment between the surface H_2O responsible for H^+ desorption and the bulk H_2O .

References

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