X-ray Photoelectron Studies of Decomposition of 2-iodoethanol on Cu(100)

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To understand whether the C-I bond of ICH_2CH_2OH on Cu(100) breaks at low temperatures, the I 4d x-ray photoelectron was investigated. The binding energy of I 4d is sensitive to the iodine chemical bonding. For example, the I $4d_{3/2}$ of iodobenzene on Pd(110) appears at 52.2 eV, in contrast to the adsorbed atomic iodine at 51.4 eV. Due to the interaction between neighboring iodine atoms, the 51.4 eV I $4d_{3/2}$ may shift to 50.4eV at higher coverages. Figure 1 shows the I 4d photoelectron spectra for the Cu(100) exposed to 1L ICH_2CH_2OH at 100K, followed by brief heating of the surface to the temperatures indicated. The spectra are similar from 100 to 250K and the I $4d_{3/2}$ and $4d_{5/2}$ are located at 51.5 and 49.8 eV, respectively. The I $4d_{3/2}$ binding energy is close to that of I on Pd(110), indicating that ICH_2CH_2OH dissociates by C-I bond rupture upon adsorption on Cu(100) at 100K. Figure 2 shows the I 4d spectrum of Cu(100) exposed to 6L ICH_2CH_2OH at 100K. The I $4d_{3/2}$ of adsorbed ICH_2CH_2OH appears at 52.6 eV and that of atomic iodine shifts to 50.8 eV due to the iodine-iodine interaction.

The results of XPS together with those of temperature-programmed reaction/desorption and reflection-absorption infrared spectroscopy performed in our UHV system reveal the reaction routes of ICH_2CH_2OH on Cu(100). ICH_2CH_2OH can dissociate on Cu(100) at 100K, forming a $-CH_2CH_2OH$ surface intermediate. Density functional theory calculations predict that the $-CH_2CH_2OH$ is most probably adsorbed on atop site. $-CH_2CH_2OH$ on Cu(100) further decomposes to yield C_2H_4 below 270K. No evidence shows the formation of $-CH_2CH_2O-$ intermediate in the reactions of ICH_2CH_2OH on Cu(100) in contrast to the decomposition of $BrCH_2CH_2OH$ on Cu(100) and ICH_2CH_2OH on Ag(111) and Ag(110), exhibiting the effects of carbon-halogen bonds and metal surfaces.

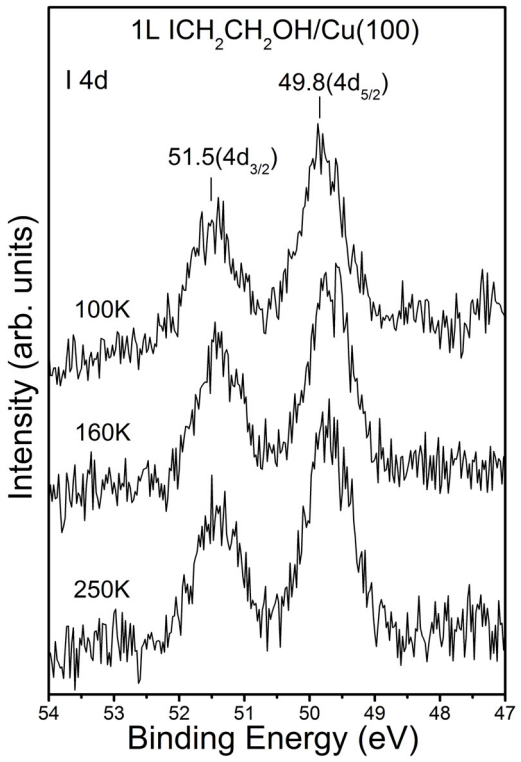

Figure 1. Variation of I 4d photoelectron spectra with annealing temperature. The Cu(100) was initially exposed to 1L ICH_2CH_2OH at 100K. These spectra were taken at different spots on Cu(100).

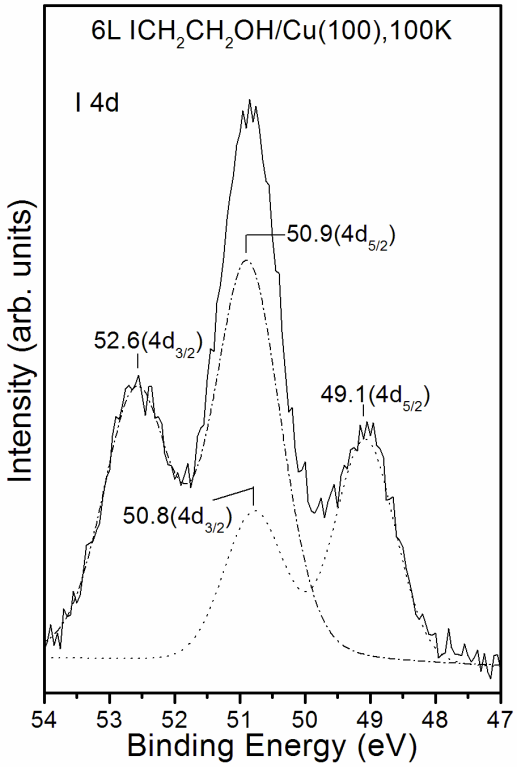

Figure 2. X-ray photoelectron spectrum of 6L ICH_2CH_2OH on Cu(100) at 100K.