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BL27SU/c-branch

### Studies of nuclear motion in core-excited $C_2H_2$ molecule by means of high-resolution resonant Auger electron spectroscopy and momentum imaging of fragment ions

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The inner-shell excited states of atoms and molecules normally decay via Auger emission with a lifetime of the order of femto second. In molecular cases, nuclear motion competes with this Auger decay, causing structural deformation in the inner-shell excited states before the Auger decay. These femtosecond nuclear dynamics should be reflected in the resonant Auger electron spectra (RAES) as well as in the momentum spectra (MS) of fragment ions that are produced following the Auger decay. We have initiated the studies of this molecular deformation in the  $C1s$  excited state of linear polyatomic molecule acetylene ( $C_2H_2$ ) using both the high resolution RAES and MS techniques. Here, we report the results of detailed analysis of the RAES studies. Analysis of the MS results is in progress.

The experiments were carried out using the very high resolution electron energy analyzer (Gammadata Scienta 2002) installed on the c branch of beamline BL27SU. High resolution total ion yield spectra (absorption spectra) of acetylene at the  $1s \rightarrow \pi^*$  resonance show a broad peak with poorly resolved structure which can be assigned to

the progression of the symmetric C-H stretching vibration. The RAES spectra were taken at several photon energies across this broad peak and at two detection angles, 0 and 90 degrees, with respect to the electric vector of the linearly polarized incident light within the dipole plane.

Figure 1 shows two examples of such spectra, one (left) taken at 0.3 eV lower and the other (right) at 0.6 eV higher than the peak energy. The spectra represent the binding energy region 11.2-12.8 eV, corresponding to the ground state of the  $C_2H_2^+$  parent ion. The analyzer pass energy was 20 eV. As indicated in the figure, the bending vibrations ( $\nu_4$  and  $\nu_5$ ) were observed in the Auger final state when the photon energy was tuned to the lower side of the absorption peak. This is a direct reflection of the Renner-Teller effect in the doubly degenerate  $C1s^{-1}1\pi_g$  state. On the higher energy side, on the other hand, no bending vibrations were excited and instead anti-symmetric stretching mode  $\nu_3$  was observed. This is a direct evidence for the g-u symmetry breaking due to the pseudo Jahn-Teller coupling between the nearly degenerate  $C1s\sigma_u^{-1}1\pi_g$  and  $C1s\sigma_g^{-1}1\pi_g$  via antisymmetric vibrations.

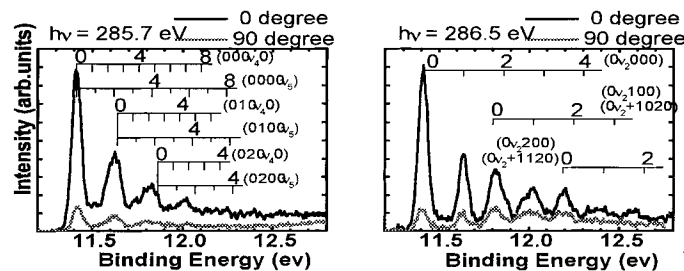


Figure 1. Resonant photoemission spectra to  $C_2H_2^+ X^2\pi_u$  at two photon energies across the  $C1s^{-1}1\pi_g$  band.

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### Angle-resolved photoemission of Ni(110) by soft X-rays

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Angle-resolved photoemission spectroscopy (ARPES) by using high photon energy enable to determine the bulk band structure because of the large escape depth of the photoelectron with the high kinetic energy. However, the validity of this experimental method is still controversial and ARPES study by which determined the band structure has not been reported in 3-dimensional system. Previously, we have performed ARPES of Ni using soft X-rays at R.T. and the spectral structures have been found to show the broadening by the influence of the thermal diffuse scattering.

In this beam time, we have performed the ARPES of Ni by using soft X-rays at 50K to examine the influence of the thermal diffuse scattering on the ARPES and to determine the intrinsic band dispersion of Ni. The excitation energy dependence of the normal emission spectrum has been also investigated, which gives the information about the band dispersion along the surface normal.

Figure 1 shows the temperature dependence of the ARPES excited by 780eV. The thermal diffuse scattering strongly influences the spectra at R.T. and the peaks become drastically sharp at 50K whereas the peak positions are not affected. Thus, the binding energies at the high symmetry points, which are estimated by the spectra at 50K, are consistent with the results of the ARPES by

ultra-violet rays and the estimation by the previous experiment.

The ARPES is clearly depending on the excitation energy, which is well explained by the band structure of Ni along the surface normal direction. It is found that the band dispersion along surface normal can be determined by the dependence of the ARPES on the excitation energy of soft X-rays, which enables to describe the 3-dimensional band structure by the ARPES using soft X-rays.

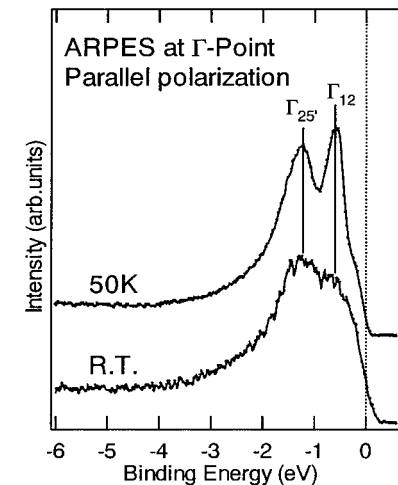


Fig. 1 ARPES of Ni using parallel polarized soft X-rays.