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Co and Ni 3*d* States of $Al_{72}Ni_{12}Co_{16}$ Quasicrystal

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Introduction

Decagonal Al-Ni-Co quasicrystals show the unique two-dimensional atomic arrangement and unusual electric properties [1]. The origin of these features has not been clarified well yet. According to a theoretical calculation [2], a strong Co-Al interaction may cause the large increase in the binding energy E_B of their Co 3*d* states, which is unusually higher than the Ni 3*d* states. Thus, we have investigated the energy distributions of their 3*d* states by the 3*d*-2*p* x-ray emission (XES) spectroscopy, using the synchrotron radiation as an excitation source, which may reduce the experimental errors in the photon-energy calibration of the XES spectrum.

Experimental

The XES measurement was performed at BL-2C of Photon Factory for a single-grain decagonal quasicrystal $Al_{72}Ni_{12}Co_{16}$. The photon energy of the XES spectrum is calibrated with the elastically scattered photons, whose energy is determined by measuring the photoelectron spectrum of Au. The binding energies of the relevant core levels were obtained by the hard x-ray photoelectron measurement at BL47XU of SPring-8.

Results and Discussions

Figure1 shows the Co and Ni 3*d*–2*p* XES spectra of $Al_{72}Ni_{12}Co_{16}$ recorded at the excitation photon energy of 841.43 and 922.96 eV, respectively, in comparison to a valence-band x-ray photoelectron (XPS) spectrum. While the XPS spectrum exhibits a single-peaked transition metal 3*d* band at E_B = 2 eV, the XES spectra clearly show that the band consists of the Ni and Co 3*d* states and that the Ni 3*d* band is located at E_B ~ 2.2 eV, higher than the Co 3*d* one. The present result seems inconsistent with the theoretical prediction [2].

Figure2 shows the electronic structures calculated by a DV-Xα method [3] for $Al_{60}Ni_{20}Co_{20}$ clusters presented in the insets. The atomic arrangement in these clusters is based on a model proposed by Hiraga *et al.* [4]; the cluster consists of two layers separated by 0.2 nm and the innermost atomic ring is composed of Ni and Co in the upper and lower clusters, respectively. Although the calculated electronic bands have ~1eV higher energy than the experimental one, their overall features are consistent with those for the large approximant [1]; a pseudogap near the Fermi level (E_B ~ −1eV in the cluster calculation) for the Al-derived states and a single transition-metal *d* band. The present XES spectra might suggest the atomic arrangement of the lower cluster. However, the Ni and Co 3*d* bands in the cluster are largely separated. Further study is in progress for a cluster with a possible random occupation of Co and Ni at the transition metal site.

References

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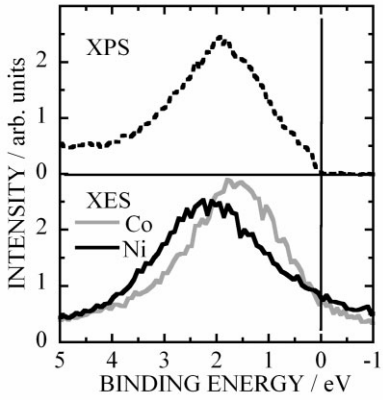

Fig.1 3*d*-2*p* XES and Valence-band XPS spectra of decagonal quasicrystal $Al_{72}Ni_{12}Co_{16}$.

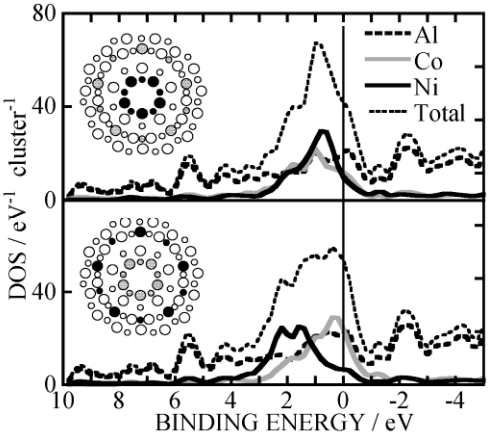

Fig. 2 Density of states for $Al_{60}Ni_{20}Co_{20}$ clusters shown in the insets. Large and small symbols in the insets represent atoms (Al: open circle, Ni: closed circle, and Co: hatched circle) in the first and second layers of the cluster, respectively.