

Local Atomic Arrangement and Electronic Structure of $\text{Al}_{72}\text{Ni}_{12}\text{Co}_{16}$ Quasicrystal

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Introduction

A decagonal Al-Ni-Co quasicrystal shows unique two-dimensional quasiperiodic atomic arrangement and associated unusual electric properties. According to a theoretical calculation [1], its Co 3d states are located unusually in lower energy than Ni 3d states because of a strong Co-Al interaction, which is inconsistent with results on electron-stimulated 2p-3d x-ray emission (XES) [2] and 2p-3d resonance photoemission [3] studies. Thus, we have examined again XES spectra using synchrotron radiation as an excitation source, which may reduce experimental errors in the photon energy calibration of the XES spectrum, in order to clarify the Co 3d and Ni 3d states of the decagonal quasicrystal and the origin of the unique structural and physical properties.

Experimental

A single decagonal quasicrystal $\text{Al}_{72}\text{Ni}_{12}\text{Co}_{16}$ was used for the XES measurement after polishing its surface. The XES measurement was performed at room temperature at BL-2C of Photon Factory with use of a 7 m grating in an XES spectrometer, which brought better energy resolution than the previous measurement [4]. Binding energies of the relevant core levels were obtained by hard x-ray photoelectron measurement at BL47XU of SPring-8.

Results and Discussions

Figure 1 shows the Co and Ni 2p-3d XES spectra of $\text{Al}_{72}\text{Ni}_{12}\text{Co}_{16}$ recorded at the excitation photon energy $h\nu$ of 841.43 and 922.96 eV, respectively, in comparison to a valence-band x-ray photoelectron (XPS) spectrum taken at $h\nu = 851.76$ eV. While the XPS spectrum exhibits a single-peaked transition metal 3d band at the binding energy of $E_B = 1.7$ eV, the present XES results clearly indicate that the band consists of the Ni and Co 3d states and that the Ni 3d band is located at $E_B \sim 2.2$ eV, higher than the Co 3d one at $E_B \sim 1.7$ eV. This agrees well with the above-mentioned experimental results [2, 3].

Figure 2 shows electronic structures calculated by a DV- $X\alpha$ method [5] for clusters shown in the insets. Atomic arrangements in these clusters are based on a model proposed by Hiraga *et al.* [6] and Henley *et al.* [7]. The upper cluster has an innermost Ni ring, while transition metals in the lower cluster are rather randomly arranged. Although calculated 3d bands and pseudogaps for Al-derived states are located at lower binding energies than the experimental one, detailed comparison of calculated results with the present XES spectra suggests a random arrangement of

transition metals in the quasicrystal, which agrees well with recent studies by electron microscopy [8].

References

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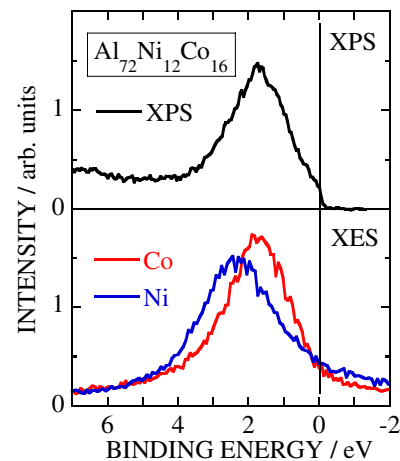


Fig.1 Valence-band XPS and 2p-3d XES spectra.

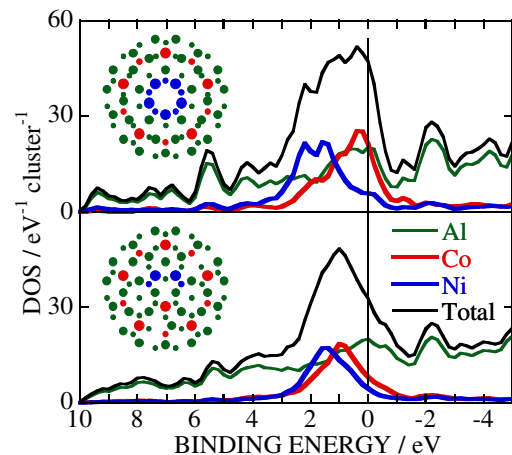


Fig.2 Density of states for clusters shown in the insets. Large and small circles in the insets represent atoms (Al: green, Ni: blue, and Co: red) in the first and second layers, respectively.