

Transition Metal 3d→2p X-ray Emission Spectra of Al₇₂Ni₁₂Co₁₆ Quasicrystal

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Introduction

A decagonal Al-Ni-Co quasicrystal shows the 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. In order to clarify the origin of the unique structural and physical properties, we have studied the electronic structure, particularly Co 3d and Ni 3d states, of the decagonal quasicrystal by x-ray emission (XES) spectroscopy with use of the synchrotron radiation as an excitation source, which may reduce the experimental errors in the photon energy calibration of the XES spectrum.

Experimental

A single decagonal quasicrystal Al₇₂Ni₁₂Co₁₆ was used for the XES measurement after polishing its surface. The XES measurement was performed at room temperature at BL-2C of Photon Factory. The 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 3d→2p XES spectra of Al₇₂Ni₁₂Co₁₆ recorded at the excitation photon energy of 889.1 eV in comparison with a valence-band x-ray photoelectron (XPS) spectrum, which exhibits a single peak of the transition metal 3d band at the binding energy E_B of 1.7 eV. The present XES results clearly indicate that the 3d band consists of the Ni and Co 3d states and that the Co 3d states are slightly higher in the binding energy than the Ni 3d states, as predicted [1], but they are inconsistent with the results reported so far [2]. This difference might be caused by the energy calibration method in the previous electron-induced XES measurement.

Figure 2 shows the electronic structures calculated by a DV-X α method for Al₆₀Ni₂₀Co₂₀ clusters in the insets. The atomic arrangement in these clusters is based on a model proposed by Hiraga *et al.* [3]; the upper cluster has an innermost Ni ring, while the lower cluster does an innermost Co ring. Although the calculated 3d bands are located at lower binding energies than the experimental results, the comparison with the experimental XES spectra suggests that the Al-Ni-Co quasicrystal may have the atomic arrangement similar to the upper cluster. This is compatible with the calculations for large periodic

approximants with 1276 atoms/cell [1]. These findings imply the importance of the Al-Co interaction in this quasicrystal.

References

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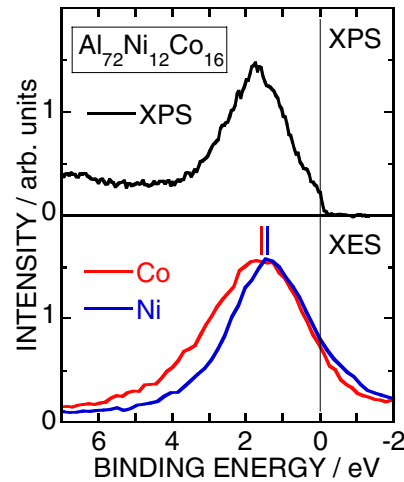


Fig.1 Valence-band XPS and 3d→2p XES spectra of the decagonal quasicrystal Al₇₂Ni₁₂Co₁₆.

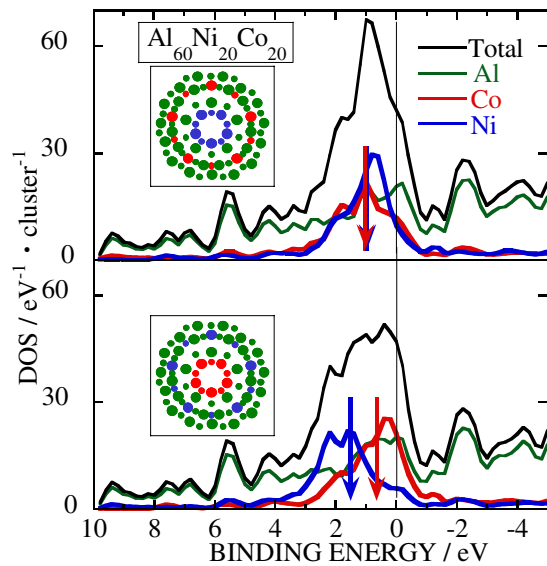


Fig.2 Density of states for Al₆₀Ni₂₀Co₂₀ clusters shown in the insets. Large and small circles in the insets represent atoms (Al: green, Ni: blue, and Co: red) in the upper and lower layers of the cluster, respectively.