# Atomic Arrangement and Electronic Structure of $Al_{72}Co_{16}Ni_{12}$ Quasicrystal Studied by X-ray Emission Spectroscopy and Cluster Calculation

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## Introduction

A decagonal quasicrystal Al-Co-Ni shows unique two-dimensional quasiperiodic atomic arrangement and associated unusual electric properties [1]. The atomic arrangement is usually regarded as a special tiling of two unit tiles, fat and skinny rhombi, with 5-fold rotational but no translational symmetry [1, 2]. It may be also viewed as building from a single unit cluster with overlap rules [3]. A band structure calculation for model approximants shows that the energy distribution of their transition-metal 3*d* states depends considerably on the transition-metal arrangement [4]. Thus, we have studied the electronic structure and atomic arrangement of the Al-Co-Ni quasicrystal by the Co and Ni $L\alpha$ x-ray emission (XES) measurement and DV-$X\alpha$ cluster calculation, in order to clarify the origin of the unique structure and physical properties.

## Experimental and Calculating Procedures

A single decagonal quasicrystal $Al_{72}Co_{16}Ni_{12}$ was used for the XES measurement after polishing its surface. The XES spectra were measured at room temperature at BL-2C of Photon Factory. Binding energies $E_B$ of the relevant core levels were obtained by hard x-ray photoelectron measurement at BL47XU of SPring-8.

The DV-$X\alpha$ calculation was performed by a code SCAT [5] for a model cluster, which is based on a recent model proposed by the electron microscopy [2], specifying the Co and Ni sites. An example of the cluster is illustrated in the inset of Fig.1. The cluster has a triple-layered structure of two unit layers A and B with hydrogen atoms at their layer edges in the stacking sequence, for example, of A-B-A, which may be regarded as a 2 nm unit cluster of the decagonal quasicrystal [2].

## Results and Discussion

Figure 1 shows the Co and Ni $L\alpha$ XES spectra of $Al_{72}Ni_{12}Co_{16}$ recorded at the excitation photon energy $h\nu$ of 841 and 923 eV, respectively, in comparison to a valence-band x-ray photoelectron spectrum (XPS) taken at $h\nu$ = 852 eV and a calculated density of states (DOS) for the model cluster. Here, the DOS is the sum of the DOS of the central layers A and B in the B-A-B and A-B-A stacking sequences, respectively, in order to reduce the surface effects. The XES spectra clearly show that a single-peaked band observed at $E_B$ = 2 eV in XPS consists of the Ni and Co 3*d* states and that the Ni 3*d* states are located lower in energy than the Co 3*d* ones, which is inconsistent with the prediction by the band structure calculation for the approximant [4].

As seen in Fig.1, the calculated DOS agrees fairly well with the XES results, although the Co 3*d* states are rather bimodal. The transition-metal 3*d* bands and a pseudogap *i.e.* the reduction of the Al partial DOS, across the Fermi energy are located lower in energy as a whole than calculated for previous small model clusters [6]. The calculated Co 3*d* bands, however, are still incompatible with the experimental results. The Co 3*d* bands at the high and low binding energies are ascribed to Co atoms in the second-inner and peripheral part, respectively, of the model cluster. The previous study suggests rather random occupation of the transition-metal sites by Co and Ni [6]. Thus, further detailed study on the arrangement, including the improvement of the peripheral part of the model cluster, and chemical interaction of the transition-metals is now in progress and will be reported elsewhere.

## References

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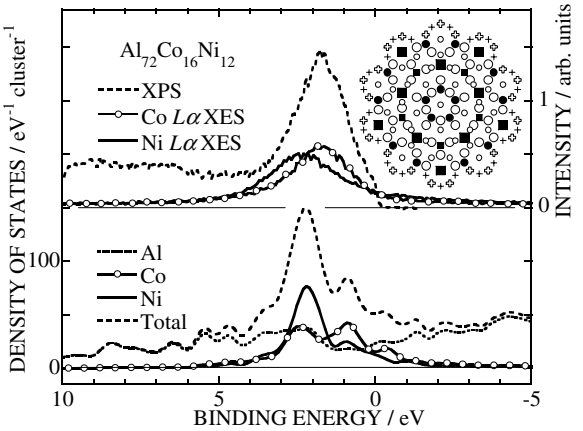


Fig.1 Co and Ni $L\alpha$ XES spectra of $Al_{72}Co_{16}Ni_{12}$. A valence-band XPS spectra and calculated density of states are shown for comparison. A model cluster for the calculation is shown in the inset, where large and small symbols represent atoms in the A and B layers of the cluster, respectively: Al by open circles, Ni by closed circles, Co by squares, and H by crosses.