Raman Scattering and Electronic Structure of $Al_{72}Co_{16}Ni_{12}$ Qasicrystal

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Introduction

We have studied the atomic arrangement of the constituent transition-metals in decagonal quasicrystals from the energy distribution of their transition-metal 3*d* states in order to understand the origin of their unique arrangement and physical properties in terms of building clusters [1, 2]. The atomic arrangement of two-dimensional quasicrystals may be viewed as consisting of a single unit cluster with overlap rules [3], although it is usually regarded as a special tiling of two unit tiles, fat and skinny rhombi, with 5-fold rotational but no translational symmetry [4]. So far we have investigated the occupied 3*d* energy distribution of an Al-Co-Ni quasicrystal by the Co and Ni *L*α x-ray emission (XES) and resonance photoemission measurement [1]. In this study, we have measured the resonance XES (RXES) spectra near the Co and Ni *L* edges for clarifying the excited states of the quasicrystal in particular the unoccupied 3*d* electronic structure.

Experimental and Calculating Procedures

A single decagonal quasicrystal of $Al_{72}Co_{16}Ni_{12}$ 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(2*p*) of the relevant 2*p* core levels were obtained by hard x-ray photoelectron measurement at BL47XU of SPring-8.

Results and Discussion

Figure 1 shows the Co and Ni RXES spectra (solid curves) of Al_{72} $Co_{16}Ni_{12}$ recorded at the photoexcitation just below their L_3 thresholds in comparison with the *L*α XES spectra (broken curves) recorded at the excitation far from their L_3 thresholds. Here, the XES spectra are shown in terms of the binding energy so as to present the transition-metal 3*d* partial density of occupied states, while the RXES spectra is plotted inversely in energy so that their so-called elastic peaks are aligned to the peaks of the relevant XES spectra. As already reported [1, 5], the Ni 3*d* band is lower in energy than the Co 3*d* one, which is consistent with the observation in the 2*p*-3*d* resonance photoemission.

The RXES spectra are mainly composed of the so-called elastic peak and a band with the energy loss of about 3 eV (E_B ~ -1 eV in Fig.1). The elastic peak has asymmetric line shape, which may be caused by the low-energy excitation of the free carriers. As seen in Fig.1, the energy-loss bands are located above the Fermi level, the origin of the binding energy. Thus we have assigned this energy loss to the excitation from the occupied 3*d* bands to the unoccupied 3*d* states. Hence the *d*-*d* energy-loss bands in the RXES spectra may present approximately the 3*d* partial density of unoccupied states (UPDOS), more precisely a joint density of states in the *d*-*d* excitation. In the figure, curves with open circles are drawn as the UPDOS after subtracting the symmetric part of the elastic peak from the measured RXES spectrum. There is no prominent peak recognized as an anti-bonding band in the Co and Ni UPDOS. Both the Co and Ni 3*d* partial densities of states show single-peaked profile as a whole, which may indicate the interaction between the relatively localized 3*d* states and the metallic itinerant states. The Co 3*d* partial density of states is wider than the Ni one, implying the larger interaction with the metallic states. A shoulder found in the high binding energy side of the Co *L*α XES spectrum might suggest the predicted strong interaction with Al [6].

References

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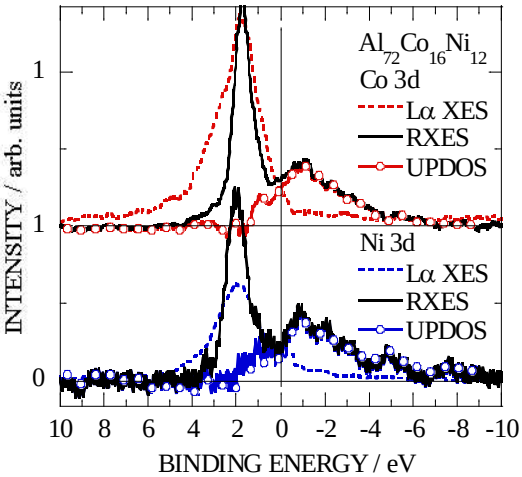

Fig.1 Co and Ni X-ray emission spectra of $Al_{72}Co_{16}Ni_{12}$.