AMTC Letters
Vol. 2 (2010)

Cluster Model Calculation of Ni-rich Al-Co-Ni Quasicrystal

Kazuo Soda[1], Manabu Inukai[2], Masahiko Kato[1], Shinya Yagi[1]

[1]Department of Quantum Engineering, Graduate School of Engineering, Nagoya University, Nagoya, 464-8603, Japan
[2]Venture Business Laboratory, Nagoya University, Nagoya 464-8603, Japan

Decagonal phases of Al-Co-Ni alloys have been investigated extensively with electron microscopy as a typical two-dimensional quasicrystal (QC) [1], where quasiperiodic planes are stacked periodically along a tenfold axis, and the atomic arrangement in the plane may be viewed as consisting of one unit cluster with an overlap rule or constructed by a special tiling such as the Penrose one with two unit tiles of fat and skinny rhombi. Various structural modifications have been also observed as a function of the Co/Ni ratio [2]. Decagonal Al-transition metal (TM) mixed ring-like arrangement is found for the unit cluster center of the Co-rich Al-Co-Ni QC [1], while the symmetry breaking of the decagonal cluster center is recognized for the Ni-rich one [3]. However, it is still challenging to clarify the unique atomic arrangement and its formation mechanism because of the lack of periodicity and of the difficulty in distinguishing between the constituent TM's by electron microscopy. Thus we have studied the TM arrangement by calculating the electronic structure of the model unit cluster based on the microscopic observation [4-7] and comparing it with the spectroscopic data. In this letter, we will show results calculated for the Ni-rich QC.

The electronic structure was calculated by the discrete variational $X\alpha$ method [8] with a commercially available code SCAT modified [5]. The cluster used for the calculation is made up of two types of the layers A and B, as shown in FIG. 1, and has a triple-layered structure in the stacking sequence of A-B-A or B-A-B layers. The atomic arrangement in each layer is based on a theoretical study by use of interatomic pair potentials for a Ni-rich approximant $Al_{70}Co_9Ni_{21}$ [9]. In FIG. 1, an underlying Penrose tiles and hexagon-boat-star (HBS) tiles are shown by broken and solid lines, respectively. The electronic structure of the unit cluster for the Ni-rich QC was obtained as the sum of the density of states for the central A and B layers calculated for the respective B-A-B and A-B-A clusters in order to avoid the so-called surface effects.

In FIG. 2, obtained energy distribution of the TM 3*d* states, *i.e.* its partial density of states (DOS), of the Ni-rich model cluster is compared with the DOS of the Co-rich mixed model cluster [6] as well as the TM $L\alpha$ x-ray emission (XES) and x-ray photoelectron (XPS) spectra of a Co-rich QC [4], which may present the TM 3*d* and total DOS's, respectively. In the Co-rich mixed model, Co and Ni are regarded as occupying the TM sites randomly. As already reported [4-7], fairly good agreement between the calculated and observed TM 3*d* DOS's suggests the large chemical disordering between Co and Ni in the Co-rich QC. For the Ni-rich cluster, the Ni 3*d* DOS has double-peaked distribution, which is caused by the Ni-Ni bond formation, while the Co 3*d* DOS has a single peak due to the large Al-Co interaction. These distributions are different from those for the Co-rich cluster and can be clarified by the

XES and XPS measurements.

References

[1] K. Hiraga, Adv. Imaging and Electron Phys. **122** (2002) 1.
[2] S. Ritsch *et al*., Phil. Mag. Lett **78** (1998) 67.
[3] E. Abe *et al*., Phys. Rev. Lett. **84** (2000) 4609.
[4] M. Inukai *et al*., Phil. Mag. **87** (2007) 3003.
[5] M. Inukai *et al*., Adv. Microsc. Theor. Calc. Lett. 1 (2008) 156.
[6] M. Inukai *et al*., Z. Krist. 223 (2008) 851.
[7] M. Inukai *et al*., J. Phys.: Conf. Ser. *in press*.
[8] H. Adachi *et al*., J. Phys. Soc. Jpn., **45** (1978) 875.
[9] M. Mihalkovič *et al*., Phys. Rev. B **65** (2002) 104205.

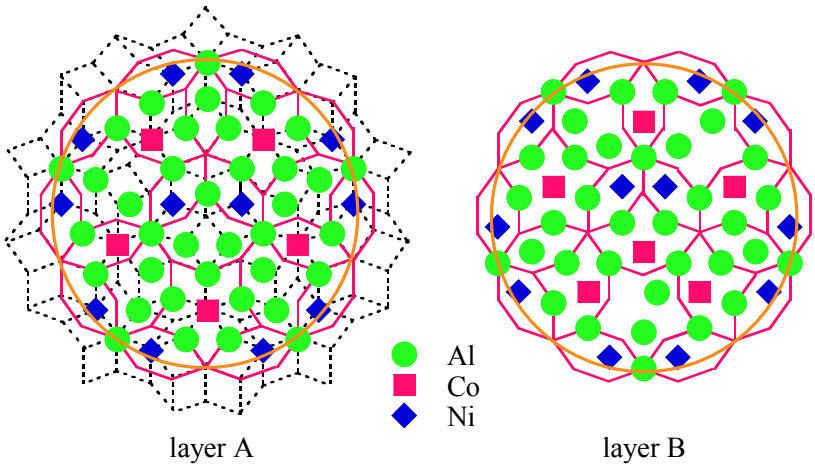

FIG. 1. Model unit cluster $Al_{72}Co_{11}Ni_{24}$ of Ni-rich Al-Co-Ni quasicrystal (approximant $Al_{70}Co_9Ni_{21}$). A large circle represents the diameter of a unit cluster (~2 nm).

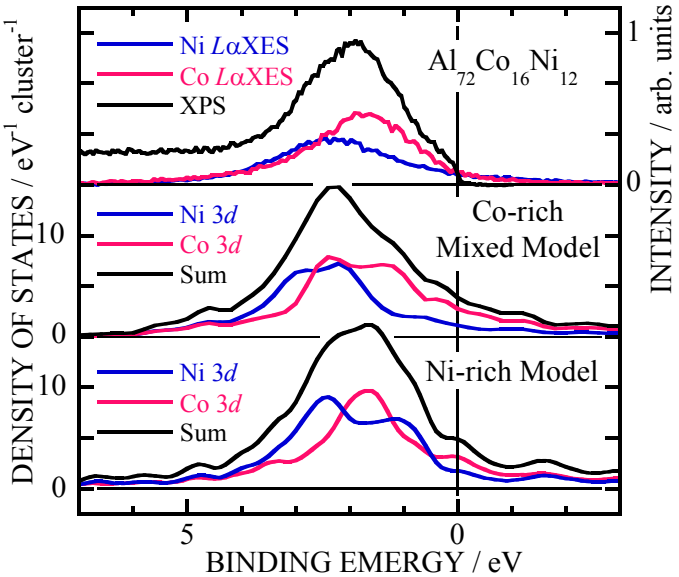

FIG. 2. Energy distributions of transition metal 3*d* states of Al-Co-Ni quasicrystal.