

Cluster Model Calculation of Decagonal Al-Co-Ni Quasicrystal

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A decagonal Al-Co-Ni quasicrystal shows unique two-dimensional quasiperiodic arrangement and associated unusual electric properties [1]. Its quasiperiodic arrangement is usually viewed as a special tiling such as the Penrose one with two unit tiles of fat and skinny rhombi [1,2], and it may consist of one unit cluster with an overlap rule [3]. According to a band structure calculation for a large model approximant [4], a Ni ring-like arrangement is preferentially formed in the center of a cluster-like unit at the vertex of its rhombic tiles, and its Co 3d states are located unusually lower in energy than Ni ones because of a strong Co-Al interaction. However, this predicted electronic structure is inconsistent with the experimental partial density of transition-metal 3d states (3d-DOS) studied by x-ray emission (XES) and photoemission (XPS) measurements [5]. New models with Al atoms incorporated in the cluster center have been also proposed by recent electron microscopy [2], where it is still hard to distinguish between the Co and Ni sites. However, the origin of the unique structure and properties has not been well understood yet. Thus we have investigated the electronic structure and atomic arrangement of the Al-Co-Ni quasicrystal by a DV- $X\alpha$ cluster calculation.

In the calculation, we have modified the commercially available code SCAT [6] and our computing system with 64-bit memories for faster calculation with larger cluster than dealt with in the original code. The modified code shows about 20% faster calculating speed for several typical clusters than the original one. As shown in FIG. 1, the cluster size could be extended from a small Al-Co-Ni model cluster to a large one, whose size is almost the same as the 2 nm unit cluster [2]. Atomic arrangements in both the clusters are based on a recent model proposed by the electron microscopy [2]. The small cluster in FIG. 1(a) is composed of two layers, A and B, separated by 0.2 nm, while the large one in FIG. 1(b) has a triple layered structure with hydrogen atoms at the layer edges in the stacking sequence of A-B-A or B-A-B layers with the interlayer distance of 0.2 nm. Large and small symbols in the figure represent the constituent atoms in the A and B layers, respectively.

Densities of states (DOS) of the Al-Co-Ni model clusters are compared with the XES and XPS spectra [5] in FIG. 2 after broadening calculated line spectra with a 0.2 eV Gaussian function. For the large cluster, the DOS was obtained as the sum of the DOS for the central A and B layers calculated for the respective B-A-B and A-B-A clusters. For both the small and large clusters, the Al partial DOS shows the decrease near the Fermi energy, a pseudogap, and the Ni 3d-DOS is located lower in energy than the Co one. These features are shifted towards the high energy for the small cluster, while the DOS for the large cluster agrees considerably well with the experimental results.

In summary, we have modified the code SCAT for the faster and larger cluster calculation and have proposed a new cluster model for the Al-Co-Ni quasicrystal specifying the Co and Ni sites.

References

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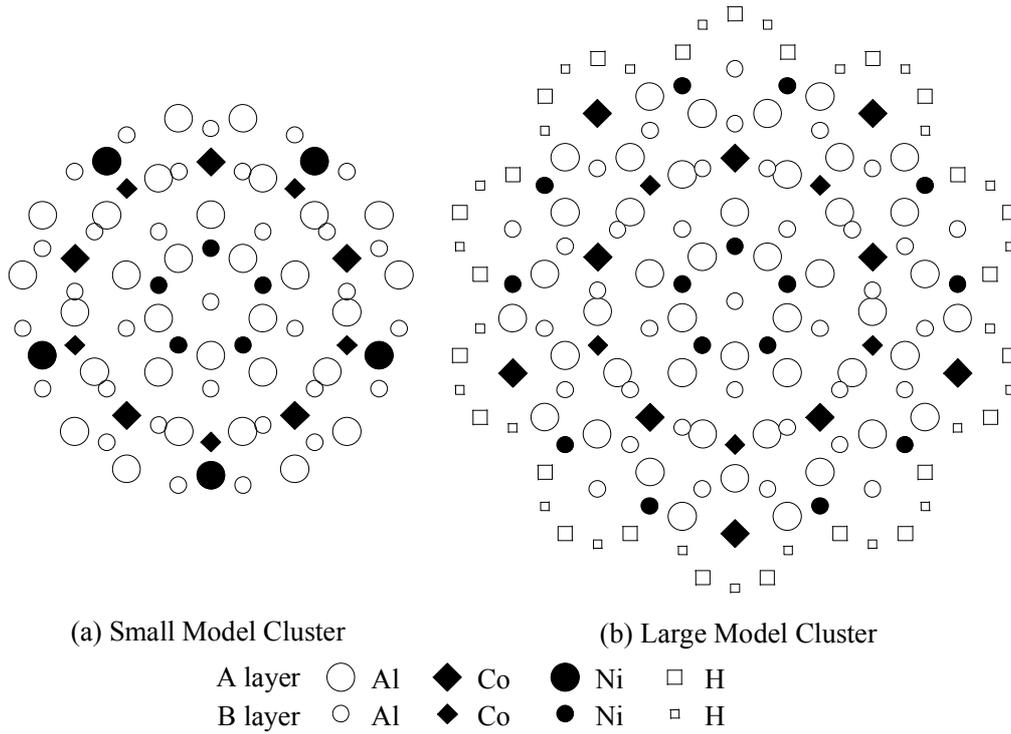


FIG. 1. Al-Co-Ni model clusters. The small cluster (a) has a double layered structure consisting of A and B layers, while the large cluster (b) has an A-B-A or B-A-B triple layered structure with hydrogen atoms at their layer edges.

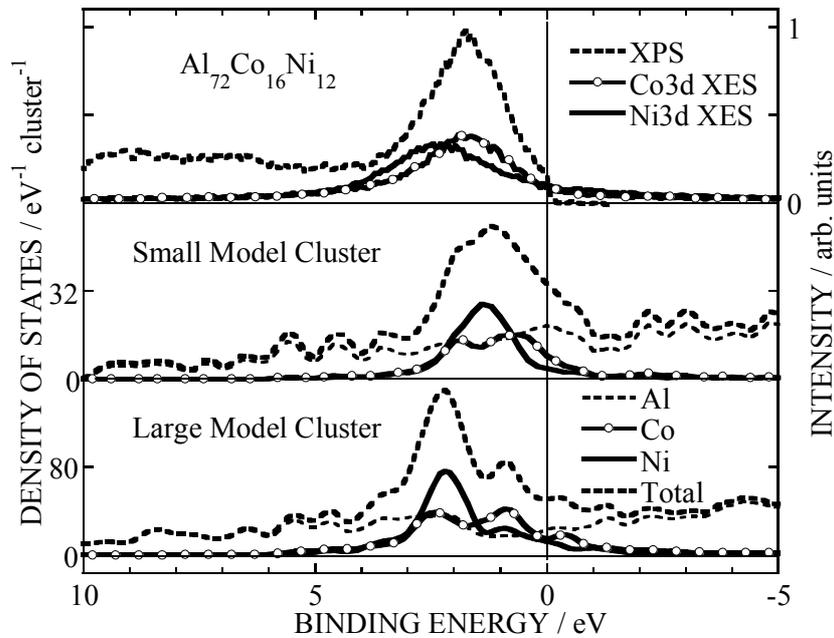


FIG. 2. Density of states calculated for Al-Co-Ni model clusters shown in FIG. 1. Experimental XPS and XES spectra are also shown in the top panel for comparison.