Soft X-ray Emission User Group

Spectroscopic study on bond energy and atomic arrangement of transition metals in Co-rich Al-Co-Ni quasicrystal

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Preferred occupation of Co and Ni at the transition metal (TM) sites in the building unit cluster of a two-dimensional Co-rich Al-Co-Ni quasicrystal has been investigated by comparing its Co and Ni $L\alpha$ x-ray emission (XES) spectra with the electronic structure calculated by the discrete variational $X\alpha$ (DV-$X\alpha$) method [1]. The Co and Ni $L\alpha$ XES spectra show that the Co 3*d* states are lower than the Ni 3*d* ones [2]. This TM 3*d* energy distribution is not consistent with those of the model clusters which possess the highly chemical order of the constituent TM's but agrees fairly well with the TM 3*d* energy distribution averaged over the chemically ordered model clusters, which implies the random occupation of Co and Ni at the TM sites [3]. Because the present discrete variational method does not have enough accuracy in estimating the core-level binding energy for the total energy calculation, we have estimated the bonding character and TM's bond energy for local clusters around the TM sites instead. Here, the bond energy is defined as an energy gain in the formation of the valence band of the cluster: a sum of the binding energy of the occupied valence band states relative to the binding energy of the relevant occupied states of the isolated TM atoms [4]. The difference in the bond energy is very small (about 0.06 eV / atom) between the Ni and Co occupations at the TM sites, which also suggests the easy occurrence of the chemical disorder of TM's [5]. Thus, despite the observation of sharp Bragg peaks in electron diffraction for the Co-rich Al-Co-Ni quasicrystal [6], the present study might show a possible contribution of an entropic term to the structural stabilization of the Co-rich Al-Co-Ni quasicrystal.

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