MS02.O04

Observations of Local Electronic States in Al-based quasicrystals by STEM-EELS

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Most quasicrystals (QCs) reveal pseudogaps in their density of states around Fermi level, and hence the stability of QCs have been discussed in terms of energetic gains in electron systems. In fact, many QCs have been discovered by tuning valence electron density based on Hume-Rothery rule. Therefore, understanding electronic structures in QCs may provide an important clue for their stabilization mechanism. Generally, it has been frequently discussed based on an interaction between Fermi surface and Brillouin zone boundary within the framework of nearly free electron model, which is believed to be an underlying physics of a Hume-Rothery's empirical criteria. However, the electronic structures of QCs have not yet been fully understood, particularly being in microscopic-macroscopic relations. In the present work, we investigate local electronic states in Al-based QCs using electron energy loss spectroscopy (EELS) combined with scanning transmission electron microscopy (STEM), by which EELS spectra with sub-Å probe and atomic structure can be obtained simultaneously. We report STEM-EELS results on AlCuIr decagonal phases [1]. Principal components analysis clearly shows up the atomic-site dependence of plasmon loss spectra in a two-dimensional map. Qualitatively, there seems to be certain correlations between the plasmon peaks and the core-loss edges, Al L_1, Ir O_{23}, Ir N_{67} and Cu L_{23}, all of which reveal different behaviours at the cluster centers and the edges. All results indicate the cluster centers have metallic states and the cluster edges have covalent states in comparison. First-principles calculations confirm the unusual electronic state. We analyse a distribution of covalent electrons by Fourier transformation of electron localization function. The distribution seems like a 10-fold charge density wave with Fermi wave length. It suggests that the Hume-Rothery mechanism is important even when hybridization effect mainly contributes to pseudogap formation. The cluster centers can be regarded as the regions which are unable to contribute to the Hume-Rothery mechanism. It may be origin of the unusual electronic states. This work was conducted in Research Hub for Advanced Nano Characterization, The University of Tokyo, supported by the Ministry of Education, Culture, Sports, Science and Technology (MEXT), Japan. It is acknowledged that T. Seki is a research fellow of Japan Society for the Promotion of Science.

[1] *P. Kuczera, J. Wolny, W. Steurer, Acta Crystallographica, 2012, B68, 578-589*

Keywords: Quasicrystal, Electronic structure, STEM-EELS