

Covalent Nature in Electronic States of Quasicrystals

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Quasicrystals (QCs) are long-range ordered materials with rotational symmetry incompatible with translational one. Natural questions arising from such aperiodic ordered systems are those concerning motion of quantum particles, such as electrons. Electronic structures of QCs have drawn much attention from the very beginning and been studied from two different points of view. First, quantum-mechanical motion of particles in a quasiperiodic potential is of special interest. Numerical and analytical studies have been done on wave functions and eigenvalue spectra for tight-binding models on Penrose lattice and others. The second point of view concerns the electronic structures of real materials [1]. Questions to be answered are why alloy phases with such complicated structures are stabilized, what novel physical properties are expected in such non-periodic systems, and so on. We shall discuss the electronic structures of QC and related compounds from the second point of view.

The Hume-Rothery (HR) idea is a unique general theory predicting phase stability of intermetallic compounds and has been accepted as plausible stabilization mechanism of QC-related compounds. According to the HR idea, the Brillouin-zone and Fermi-sphere interaction causes additional stabilization for nearly-free electrons near the Fermi surface, and a particular atomic structure of QC can maximize this stabilization. On the other hand, there have been several arguments that covalent bonding plays more important role in QC-related systems. Coexistence of the metallic and covalent bondings in intermetallic compounds is of special interest because it may provide key ideas for stabilization mechanism of QC-related compounds and their unique properties, which are very different from simple pure metals. Al-Li compound, which is related to so-called Bergmann-type QCs, is a typical example where the strong covalent bonding plays an essential role. In Al-Li compounds, a combination of Al and Li leads to a potential landscape for electrons, which is not that of the entire close-packed structure but that of the sparse Al sublattice, favoring covalent bonding between Al's [2]. A similar bond formation in Bergman Al-Li compound is realized in so-called Zintl compound, which is a compound of elements with very different electro-negativities. In this talk, we try to emphasize how chemistry of constituent elements leads to phase stability of QC-related compounds and discuss a role of the covalent nature in electronic states for other compounds including Cd-based QCs.

[1] Y. Ishii and T. Fujiwara, in "Quasicrystals", ed. T. Fujiwara and Y. Ishii (Elsevier, Amsterdam) (2008), chap.6, pp.171-208.

[2] K. Nozawa and Y. Ishii, Phys. Rev. Lett. **104** (2010), 226406.