Search for Ga-based icosahedral quasicrystal

Takanobu Hiroto^{1,2}, Kazuya Honda¹, Kazue Nishimoto³, Koichi Kitahara¹,

Tsutomu Ishimasa⁴, Kaoru Kimura¹

¹ Graduate School of Frontier Sciences, The University of Tokyo, Kashiwano-ha 5-1-5, Kashiwa 277-8561, Japan

² National Institute for Materials Science, 1-2-1 Sengen, Ibaraki 305-0047 Japan
³Institute of Multidisciplinary Research for Advanced Materials, Tohoku University, Sendai 980-8577, Japan

⁴Toyota Physical and Chemical Research Institute, Yokomichi 41-1, Nagakute 480-1192, Japan HIROTO.Takanobu@nims.go.jp

Introduction

Quasicrystals are defied as a solid which has the sharp Bragg peaks as a conventional crystal but loses the lattice translational symmetry in physical space. Recently, some interesting behaviours in quasicrystals (and its related approximants) such as superconductivity [1], quantum critical phenomena [2] as well as various magnetic transitions [3] *etc.* are demonstrated. However, such properties are still limited in quasicrystals. Thus, new icosahedral quasicrystals (*i*-phases) in novel alloys may open a new research field of quasicrystal society.

Since the discovery of the stable quasicrystal in ternary Al-Cu-Fe [4] alloy, Al-transition metals (TMs)-based stable *i*-phases have been reported. These *i*-phases were discovered by the Hume–Rothery rules, which is a tendency for a specific crystal structure to form at a characteristic ratio of the number of itinerant electrons per atom (e/a) [5], as a guide. In the case of Al-TM type *i*-phases, this e/a values are known around 1.8. Recently extensively studied or discovered quasicrystals, which may be classified as Tsai-type *i*-phases, the e/a values are known around 2.0. Our motivation is to search for the Ga-based *stable i*-phase similar to those in Al-TM systems as well as number of alloy systems of Tsai-type systems.

We chose the Ga-Ru-Cu system and the Ga-Ni-(Hf, Zr, and Sc) systems to search for the Ga-based *stable i*-phase. The former is the counterpart of Al-Ru-Cu alloy, which has the widest formation range of the stable *i*-phase of all known Al-TM alloys [6]. The latter is known to form the 1/1 approximant phase in the literature [7].

To clarify the presence or absence of a stable *i*-phases (or the possibility of new intermetallic phases), we construct the isothermal section of the ternary diagram of Ga-Ru-Cu system and the Ga-Ni-(Hf, Zr, and Sc) system in experimentally.

Experimental

High-purity elements with appropriate amount were melted by an arc-melting on a watercooled Cu hearth. The obtained mother ingot was then sealed inside a quartz tube under a pure Ar atmosphere and annealed at appropriate temperature for typically 48 - 72 hours in an electronic furnace. The phase constitutions / compositions were studied by powder X-ray diffraction (XRD) as well as scanning electron microscopy/energy dispersive X-ray spectroscopy (SEM/EDX) measurements. Some alloys were also examined by the transmission electron microscopy (TEM).

Results and discussion

Figure 1 show the ternary phase diagram of Ga-Cu-Ru system at 1073 K determined by our experiments. No *i*-phase (as well as its approximant phase) are not discovered. However, we found only one ternary phase namely τ -phase [8] with the ideal composition of Ga₅₀Ru_{37.5} Cu_{12.5}, which have the *C*-centered orthorhombic lattice with a = 11.80 Å, b = 6.04 Å and c = 3.07 Å. This intermetallic phase is strongly related to the GaRu phase.



Figure 1. Ternary diagram of the Ga-Ru-Cu system at 1073 K determined by our experiments [8].

Ga-Ni-(Sc, Zr, and Hf) systems were reported to form 1/1 approximant (classified as Tsai-type approximant), however, its formation condition as well as the possibility of the formation of *i*-phase are not fully discussed. In this presentation we will demonstrate the phase diagram of Ga-Ni-(Sc, Zr, and Hf) and also discuss the possibility of *i*-phases.

- K. Kamiya, T. Takeuchi, N. Kabeya, N. Wada, T. Ishimasa, A. Ochiai, K. Deguchi, K. Imura, and N. K. Sato, *Nature Comm.* 9, (2018), 154.
- K. Deguchi, S. Matsukawa, N. K. Sato, T. Hattori, K. Ishida, H. Takakura, and T. Ishimasa, *Nature Materials*, 11, (2012), 1013-1016.
- R. Tamura et al., Phys. Rev. B, 82, (2012), 220201(R); T. Hiroto et al., J. Phys.: Condens. Matter., 25, (2013), 426004; T. Hiroto et al., J. Phys.: Condens. Matter., 26, (2014), 216004; A. Ishikawa et al., Phys. Rev. B, 93, (2016), 024416.
- 4. A. P. Tsai, A. Inoue and T. Masumoto, CJpn. J. Appl. Phys. 26, (1987), L1505-L1507.
- 5. U. Mizutani, Hume-Rothery Rules for Structurally Complex Alloy Phases, CRC Press, (2011), Chapter 1.
- 6. B. Grushko and T. Velikanova, CALPHAD, 31, (2004), 125-145.
- V.Ya. Markiv and N.M. Belyavina, Dopovidi akademii nauk ukrainskoi RSR, seiya B, 12, (1983) 30; T. Ishimasa, S. Kashimoto, R. Maezawa, Mater. Res. Soc. Symp. Proc., 805, (2003), 3.
- 8. T. Hiroto, K. Honda, K. Nishimoto, K. Kitahara, and K. Kimura, Materials Transactions, 59, (2018), 575-579.

This work was supported by a Grant-in-Aid for Scientific Research (KAKENHI (JP16H04489)) from the Japan Society for the Promotion of Science (JSPS) and a Grant-in-Aid for JSPS fellows (15J04682).