Synthesis and characterization of intermetallic compounds with anti-PbFCl type structure

Takahiro YAMADA¹

¹ Institute of Multidisciplinary Research for Advanced Materials, Tohoku University, Japan

Intermetallic compounds composed of multiple elements with large electronegativity differences are known as Zintl phases or polar intermetallics, and they possess both ionic and covalent bonding. This leads to unique crystal structures and a range of electronic structures exhibiting metallic, semi-metallic, and semiconducting behavior. Some metallic compounds show superconductivity, while some semimetals and semiconductors exhibit thermoelectric, photovoltaic, and catalytic properties, and therefore are useful in materials science. Furthermore, intermetallic compounds with special electronic band structures, in which the conduction and valence bands cross each other near the Fermi level, have attracted growing attention in condensed matter physics as they exhibit topological quantum properties. Therefore, the exploration and characterization of Zintl phases and polar intermetallics have become very important active fields from both theoretical and experimental perspectives.

NaAlSi is an *sp* electron superconductor that crystallizes in an anti-PbFCl-type layered structure with a transition temperature T_c of about 7 K (Fig. 1) [1–3]. Recently, the electronic state calculations predicted the presence of topological nodal lines in the semimetallic band structure, and the relation between the topological property and superconductivity is attracted much attention [3–5]. NaAlGe, which is isomorphous with NaAlSi and has a similar electronic structure, has been reported not to exhibit superconductivity above 1.8 K [1, 2]. The experimental information on the physical properties including the superconducting of NaAlSi and NaAlGe is still limited mainly because all the

experiments were performed on polycrystalline samples.

In the present study, we successfully prepared NaAlSi and NaAlGe single crystals by a Na–Ga flux method (Fig. 2). The transport and thermodynamic properties of the nodalline semimetals were investigated. NaAlSi forms a superconducting gap below 6.8 K, whereas NaAlGe forms a pseudogap below 100K, despite the fact that their calculated band structures and physical properties at elevated temperatures are equivalent. In

comparison to the electron-phonon instability in NaAlSi, we suggest that excitonic instability-related fluctuations are responsible for the pseudogap formation in NaAlGe [6, 7].

References:

- [1] S. Kuroiwa, et al., Physica C 466, 11 (2007)
- [2] H. B. Rhee, et al., Phys. Rev. B 81, 245114 (2010)
- [3] L. Schoop, et al., Phys. Rev. B 86, 174522 (2012),
- [4] L. Muechler, et al., APL Mater. 7, 121103 (2019)
- [5] L. Jin, et al., J. Mater. Chem. C 7, 10694 (2019).
- [6] T. Yamada, *et al.*, *JPSJ*. **90**, 034710 (2021).
- [7] T. Yamada, et al., JPSJ. 91, 074801 (2022).



Fig. 1. Crystal structure of NaAlSi/Ge (anti-PbFCl-type structure).



Fig. 2. Electrical resistivity along the *a*-axis of the single crystals of NaAlSi and NaAlGe.