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Study on Electronic Structure and Physical Properties of Layered Nitride Compounds
(層状窒化物の電子構造と物性に関する研究)

SEHOON JEONG

1. General Introduction

Low-dimensional compounds have attracted attention for theoretical and experimental studies because of their unique physical and electronic properties, as well as for their practical applications.

Especially, layered compounds have special characteristic properties, i.e., it is easy to intercalate or embed a layered matrix into their interlayer spaces. From the present physical science view of layered compound research, the 2D electronic structure has been one of the great interesting research fields as represented by the representative high-temperature superconductor cuprate, MgB_2, and Fe-based superconductors are commonly consisted of layered structure. In fact, since the discovery of superconductivity in $(La, Ba)_2CuO_4$ and iron-based superconductor, much works on layered compounds have focused on understanding high-temperature superconductivity.

Chapter 2 Superconductivity of Ca_2InN with a Layered Structure Embedding Anionic Indium Chain Array

This chapter describes the emergence of superconductivity in Ca_2InN consisting of a 2-dimensional (2D) array of zigzag indium chains embedded between Ca_2N layers. A sudden drop of resistivity and a specific-heat (C_p) jump attributed to the superconducting transition were observed at 0.6 K. The Sommerfeld coefficient $\gamma =$ 4.24 mJ/mol K^2 and Debye temperature Θ_D = 322 K were determined from the C_p of the normal conducting state and the superconducting volume fraction was estimated to be ~80% from the C_p jump, assuming a BCS-type weak coupling. Density functional theory calculations demonstrated that the electronic bands near the Fermi level (E_F) are mainly derived from In 5*p* orbitals with π and σ bonding states and the Fermi surface is composed of cylindrical parts, corresponding to the quasi-2D electronic state of the In chain array. By

integrating the projected density of states of In-*p* component up to E_F, a valence electron population of ~1.6 electrons/In was calculated, indicating that the partially anionic state of In. The In 3*d* binding energies observed in Ca_2InN by x-ray photoemission spectroscopy were negatively shifted from that in In metal. The superconductivity of Ca_2InN is associated with the *p*-*p* bonding states of the anionic In layer.

Chapter 3 Crystal Structure and Physical Properties of New Transition Metal Based Pnictide Compounds: La*TM*$_2$AsN (*TM* = Fe, Co and Ni)

This chapter describes the synthesis and crystal structure analysis of transition metal-based mixed-pnictides: La*TM*$_2$AsN (*TM* = Fe, Co and Ni). New 3*d* transition metal-based mixed-pnictide compounds, La*TM*$_2$AsN (*TM* = Fe, Co and Ni) are synthesized by solid state reactions under a high pressure of 2.5 GPa. These compounds crystalize with an orthorhombic structure (space group *C*mcm) containing four formula units per unit cell. The crystal structure consists of an anisotropic network of *TM*As_3N tetrahedra sharing As-As edges along the in-plane *ac* direction and N corners along the *b*-direction, forming a *TM* honeycomb lattice with a boat-shape conformation bridged by *TM*-N-*TM* linear bonds. The temperature dependences of the electrical resistivity and magnetic susceptibility indicate that these crystals are itinerant antiferromagnets exhibiting parasitic ferromagnetism with transition temperatures of 560, 260 and 410 K for *TM* = Fe, Co and Ni, respectively. These compounds are expected to be parent materials for new superconductors.

Chapter 4 Magnetic and Electronic Structure of Iron-based Mixed-pnictide: $LaFe_2AsN$

This chapter describes magnetic and electronic structures of $LaFe_2AsN$ by neutron powder diffraction and density functional theory calculation. The magnetic structure of $LaFe_2AsN$ was determined as a stripe-type antiferromagnetic ordering state, with ferromagnetic interaction between first nearest neighbor and antiferromagnetic interaction between second nearest neighbor of Fe spin. The electronic bands near the Fermi energy level was mainly made up of Fe 3*d* orbitals, and which were highly hybridized with As 4*p* and N 2*p* orbitals around –5 eV. Since $LaFe_2AsN$ and LaFeAsO have a similarity in stripe type AFM ordering state and electronic structure, the $LaFe_2AsN$ compounds would be considerable as new kind candidate parent compound

for iron-based superconductor.

Chapter 5 General Conclusions

From this Ca_2InN and $LaTM_2AsN$ compounds, the modifications of chemical (oxidation or ligand state) and structural features lead to changes in intrinsic electronic structure and/or physical properties, and imply the possibility for superconducting behavior. If an appropriate element is embedded or partially substituted into these both nitride layered compounds, the resulting compound would also exhibit superconductivity.