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論文 / 著書情報
Article / Book Information

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種別(和文)	論文要旨
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（博士課程）
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論 文 要 旨

THESIS SUMMARY

専攻： Department of	材料物理科学　専攻	申請学位（専攻分野）： Academic Degree Requested	博士 Doctor of　（　工学　）
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要旨（英文 800 語程度）
Thesis Summary（approx.800 English Words ）

Layered 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 high-temperature superconductor cuprate, MgB_2, and Fe-based superconductors, which 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 transition temperature superconductivity. Therefore, this thesis has reported an electronic structure and physical properties of two kinds of layered nitride compounds. First, superconductivity in Ca_2InN is composed of a 2D array of zigzag indium (In) chains and Ca_2N layers. Moreover, the strong ionicity of $[Ca_2N]^+$ layer could be applied to stabilize the anionic In layers. From this compound, I found BCS type superconductivity. 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 $\Theta_D = 322$ 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 calculation results demonstrated that the superconductivity arisen from the In layer [–($In^{0.6-}$)–] which was formed by In 5*p* orbitals with *pσ* and *pπ* bonding states. Second, a crystal structure and physical properties of a new 3*d* transition metal based mixed pnictide compounds, LaTM_2AsN (*TM* = Fe, Co, and Ni), were reported. LaTM_2AsN (*TM* = Fe, Co and Ni) were synthesized by solid state reactions under a high pressure of 2.5 GPa. These compounds were crystalized with an orthorhombic structure (space group *C*mcm) containing four formula units per unit cell. The crystal structure was consisted of an anisotropic network of $TMAs_3N$ 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. From the close-up view of adjacent $TMAs_3N$ tetrahedra, which shared As-As edge along *a* direction. Each tetrahedron had C_s point group symmetry with a mirror plane perpendicular to *a* direction containing *TM*, N and one of the three As sites. Thus, there were two types of *TM*-As bonds with one *TM*-N bond tilted from *b* direction. Additionally, due to the mirror plane perpendicular to *a* direction, the direction of *TM*-N bond in the adjacent tetrahedra was anticlinal each other and there was no inversion symmetry. The temperature dependences of the resistivity shown that all of the compounds were shown the positive temperature dependences with room temperature resistivities of 1.16, 0.51 and 0.35 mΩ·cm for *TM* = Fe, Co and Ni, respectively. Moreover, the temperature dependences of the magnetic susceptibility were indicated that while a monotonic increase in the FC susceptibility is typical in ferromagnetic (FM) states, the peak and shoulders in the ZFC curves are typical in AFM states, indicating that AFM and FM transitions simultaneously occurred just below the magnetic transition temperature T_M of 560, 260 and 410 K for *TM* = Fe, Co and Ni, respectively. The magnetic structure of $LaFe_2AsN$ was demonstrated 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 along to a direction and antiferromagnetic interaction between second nearest neighbor of Fe spin along to c direction. In other word, the type of each Fe-spin pair was predicted to be a stripe-type ordering along the in-plane of *ac* direction, which commonly observed for 1111-type iron arsenide. 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. In the present studies, I found the potential of the new type of superconductor system from nitride layered compounds such as Ca_2InN and $LaTM_2AsN$. The modifications of chemical, i.e., oxidation of ligand state, and structural features could be led to changes in intrinsic electronic structure and/or physical properties to favor a superconducting behavior. If an appropriate elemental is embedded or partially substituted into these both nitride layered compounds, I expect that the resulting compound would also exhibits superconductivity.

備考 ： 論文要旨は、和文 2000 字と英文 300 語を 1 部ずつ提出するか、もしくは英文 800 語を 1 部提出してください。
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