PCP3-1

Synthesis and Physical Properties of New Iridium Oxyfluorides Using Topochemical Reaction Method

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Ruddlesden-Popper (RP) type Iridate Sr_2IrO_4 has been paid much attention due to the interesting physical properties such as J_{eff} = 1/2 Mott insulating state induced by strong spin-orbit interaction[1]. Moreover, the possibilities of unconventional superconductivity in carrier-doped Sr_2IrO_4 has been proposed because it has several similarities with the high-T_c cuprate superconductors such as La_2CuO_4[2]. Carrier doping such as La substitution for Sr site was already attempted[3], but bulk superconductivity has not yet been reported. So far, we have reported synthesis of new iridium oxyfluoride $Sr_2Ir(O,F)_{6-\delta}$ using topochemical reaction method. This compound has more anisotropic structure due to insertion of fluorine layer into rock salt layer, and suppression of the magnetic ordering in Sr_2IrO_4 have been observed with topochemical fluorination. Thus, we utilized topochemical reaction method for other iridates in order to synthesize a novel iridium oxyfluorides.

Ba_2IrO_4 as precursor was synthesized by a conventional solid-state reaction method under high-pressure. Thereafter, it was mixed with various fluorinating argents such as ZnF_2, CuF_2 and PTFE (precursor : fluorinating agents = 1 : 1), and the mixture was heated at 250-550 °C for 12 hours in air. Phase identification was performed by powder X-ray diffraction method. Magnetic susceptibility and resistivity were measured using a SQUID magnetometer and a four-probe method. The valence state of Ir ion was evaluated using XAFS study.The figure shows powder XRD pattern of the compounds and the possible crystal structure. New layered iridium oxyfluoride $Ba_2Ir(O,F)_{6-\delta}$ was successfully synthesized by topochemical fluorination with ZnF_2, CuF_2 and PTFE. This oxyfluoride has the same structure as $Sr_2Ir(O,F)_{6-\delta}$ with largely enhanced *c*-axis length because fluorine layer was inserted in the rock salt layer. The magnetization measurements showed paramagnetic behavior after fluorination. Meanwhile, the electronic transport properties of $Ba_2Ir(O,F)_{6-\delta}$ exhibited semiconducting behavior like $Sr_2Ir(O,F)_{6-\delta}$. Further detail of the compounds such as valence state of Ir will be given in the presentation.

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Keywords: Layered perovskite, Oxyfluorides, Iridates, Topochemical reaction

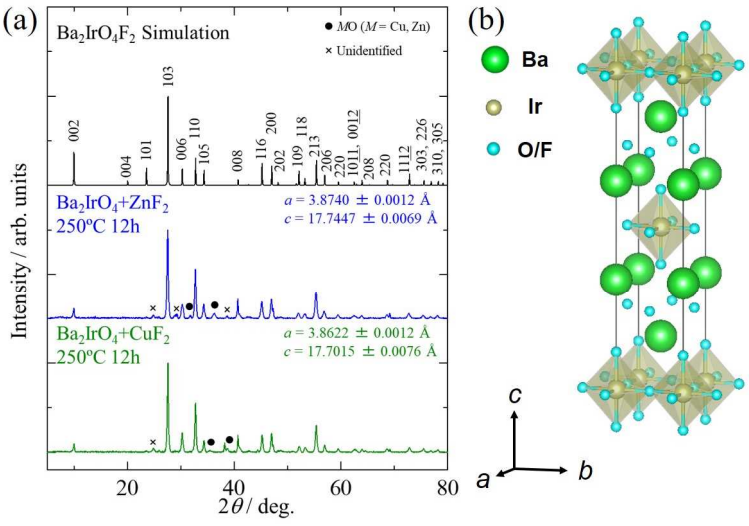

Fig. (a) Powder XRD patterns of $Ba_2Ir(O,F)_{6-d}$ and (b) Crystal structure model of $Ba_2Ir(O,F)_{6-d}$.

PCP3-2

Exploration of New Superconducting Phases in a Scandium Borocarbide System

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Superconducting materials containing light elements are advantageous to emerge the relatively high critical temperature (T_c), because high-frequency vibration of phonons due to the light mass enhances its T_c within the BCS theory. Indeed, there are various superconductors in alkali, alkali-earth, and *d* transition-metal borides and carbides [1-3].

In this study, we searched for a new superconductor in the ternary Sc–B–C system using an arc-melting method. Although a moderately high-T_c superconductor is expected in combination with the comparatively small ionic radius of Sc and potentially high Debye frequencies originating from B and C, this system remains unexplored.

We attempted to synthesize the Sc–B–C compounds under various conditions of the starting composition, and found that a superconducting transition was observed at around 7.7 K only when the B-poor sample (e.g. nominal composition of Sc:B:C=37:2:61) was prepared [4]. Note that neither B-free nor B-excess samples exhibited the superconductivity down to 2 K. The structural refinements through the Rietveld analysis demonstrated that the compound belongs to the tetragonal space group of *P*4/*ncc*. By using the density functional theory calculations, the precise atomic positions of a small amount of B were examined. As a result, a chemical formula of the present superconducting phase was found to be expressed as $Sc_{20}C_{8-x}B_xC_{20}$(x=1 or 2).

The sample exhibited the typical type-II superconductivity below T_c=7.7 K. Our specific-heat measurements revealed that $Sc_{20}C_{8-x}B_xC_{20}$ was classified as an intermediately coupled superconductor. The electronic structure studies by first principles calculations proposed that the contribution of Sc-3*d* orbitals was mainly responsible for the superconductivity.

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Keywords: New material, Superconductor, Borocarbide, Electronic structure

PCP3-3

Crystal Growth and Superconducting Properties of a Chiral Compound $TaSi_2$

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Superconductivity was reported, long time ago, in MX_2 (M = Nb, Ta; X = Si, Ge) [1,2]. Though the reported superconducting transition temperature, T_c, was as high as 16 K for $NbGe_2$, there have been only a few follow-up experiments. It is noted that the measurements of superconducting properties under magnetic fields are lacking, and T_c for each compound remains controversial. The difficulty of establishing the superconductivity in these compounds may be attributed to the fact that it is difficult to synthesize single-phase pure samples. This is because high purity Nb and Ta are not readily available and the melting-points (T_m) and reaction-temperatures of the raw materials are very high (e.g. T_m ~ 3000°C for Ta).

We are interested in these compounds from the viewpoint of electronic structures. As shown in Fig. 1 (a), MX_2 has a hexagonal crystal structure with the space group $P6_222$, which belongs to the chiral symmetry. It is expected that the spin band splitting occurs in the electronic states when strong spin-orbit interaction (SOI) is present in the chiral symmetry. In fact, by the first principles calculations, we confirmed such spin band splitting in these compounds. Therefore, it became increasingly important to examine and establish the superconductivity in these chiral compounds.

Using Ta (6N) and Si (5N) grains, single-phase polycrystalline samples of $TaSi_2$ were successfully synthesized by the arc-melting method in a tetra-arc furnace (Fig. 1 (b)). Residual resistivity at 2 K and residual resistivity ratio of the obtained $TaSi_2$ pellet were 0.22 μΩcm and 143, respectively, indicating the high quality of the sample. The temperature dependence of resistivity was measured using a dilution refrigerator down to 55 mK. Below 0.7 K, the resistivity suddenly dropped, indicating a superconducting transition. Although the onset T_c ~ 0.7 K is lower than the previously reported value (4.4 K [1], which is very close to T_c for Ta), we believe this is the intrinsic superconductivity in $TaSi_2$.

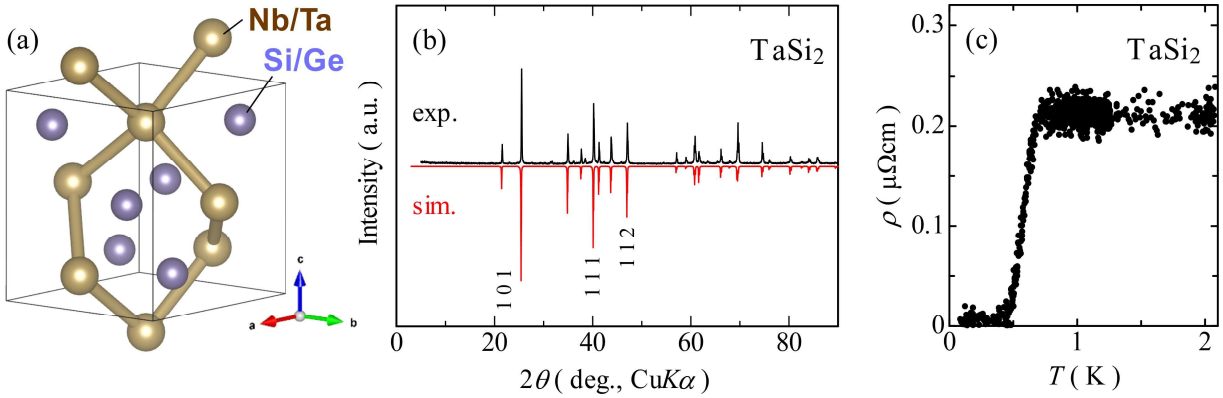

Fig. 1 (a) Crystal structure of MX_2 (M = Nb, Ta; X = Si, Ge). (b) XRD patterns of $TaSi_2$ (experiment vs. Simulation). (c) Temperature dependence of resistivity in the $TaSi_2$ pellet.

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Keywords: Chiral Compound, Crystal Growth, Spin-orbit Interaction

PCP3-4

Superconductivity in a Topological Dirac Nodal-Line Semimetal

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Topological electronic materials, especially Dirac nodal-line semimetals (DNLSs), have been attracting attention in condensed matter physics. DNLSs have gapless nodal-line Dirac dispersions along the specific momentum-directions in the electronic band structures, which are protected by the nonsymmorphic symmetry of the crystal structures even under the strong spin-orbit-interaction (SOI). ZrSiS and InBi are the DNLSs, belonging to the nonsymmorphic space group P4/nmm. They are known to exhibit large magnetoresistance (MR) due to the existence of the Dirac line node. $LaAgBi_2$ (shown in Fig. 1(a)) was reported to exhibit large MR [1]. Recently, we found that $LaAgBi_2$ was also the DNLS [2] from the fact that it belongs to the same P4/nmm space group and has strong SOI from Bi. As shown in Fig. 1 (b), it should be noted that the Dirac dispersion exactly crosses at the Fermi energy in $LaAgBi_2$. In this study, we explored the possibility of superconductivity in $LaAgBi_2$ as a DNLS. High-quality single crystals of $LaAgBi_2$ were obtained by the self-flux method. As shown in Fig. 1 (c), our sample of $LaAgBi_2$ exhibited the higher residual resistivity ratio of 131 and the larger magnetoresistance of 2400% at 2 K and 9 T than those of previous studies (10 and ~1200%, respectively [1]). Furthermore, we found that the resistivity dropped rapidly below 2 K (inset of Fig. 1 (c)). As increasing the applied magnetic fields, the resistivity-drop was suppressed, indicating the resistivity behavior below 2 K is due to superconductivity. We will report the details of superconducting properties, including anisotropy, at lower temperatures.

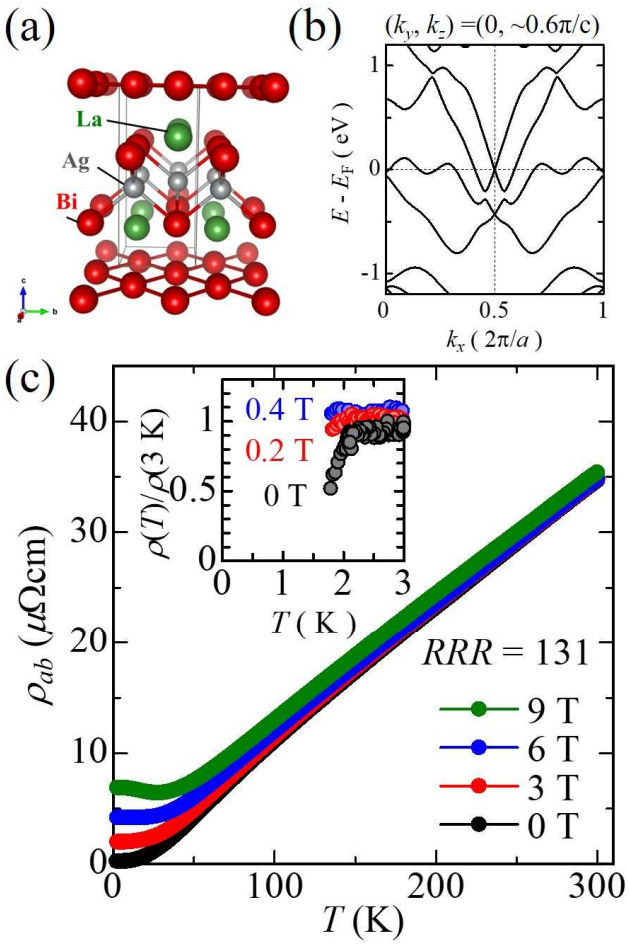

Fig. 1 (a) The crystal structure of $LaAgBi_2$. (b) The electronic dispersions plotted along the k_x direction at the fixed (k_y, k_z) = (0, ~0.6π/c). (c) Temperature dependence of resistivities under various magnetic fields. Inset: The plot of $\rho(T)/\rho(3\ K)$ versus temperature below 3 K.

PCP3-5

Effect of non-magnetic rare earth substitution for *A*site on mixed anion *APX*superconductors

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Non-magnetic rare earth atom substitution effect for *A*site in *APX*-based Zr(P, S)$_2$system, Hf(P, Se)$_2$and Hf(P, S)$_2$superconductors (see Fig. (a)) for improvement of superconducting transition temperature (T_c) have been examined.

In Zr (P, Se)$_2$[1], the $T_c$improvement with partial substitution of an non-magnetic rare earth Lu atom for Zr site and the doping behavior by partial substitution were discussed [2, 3]. By partially substituting an non-magnetic rare earth Lu atom for Zr site in ZrPS, the lattice constants *a*and *c*decrease monotonically with increasing nominal substitution *y*in contrast to the case of non-magnetic rare earth substitution of Zr sites in Zr (P, Se)$_2$[1]. It is shown that the maximum $T_c$for ZrPS was increased from 3.70 K [1] to 6.36 K (see Fig. (b)). In $HfP_{1.55}Se_{0.45}$, lattice constants *a*decrease and *c*increasing monotonically with increasing nominal substitution *y*when Lu atoms are partially substituted for Hf atoms. $T_c$was also increased from 4.88 K [1] to 5.89 K. In $HfP_{1.45}S_{0.55}$, lattice constants *a*decrease slightly and *c*increasing monotonically with increasing nominal substitution *y*when Lu atoms are partially substituted for Hf atoms. $T_c$was also increased from 3.16 K [1] to 5.86 K. In this presentation, the doping behavior by partial substitution and the increase of $T_c$is discussed.

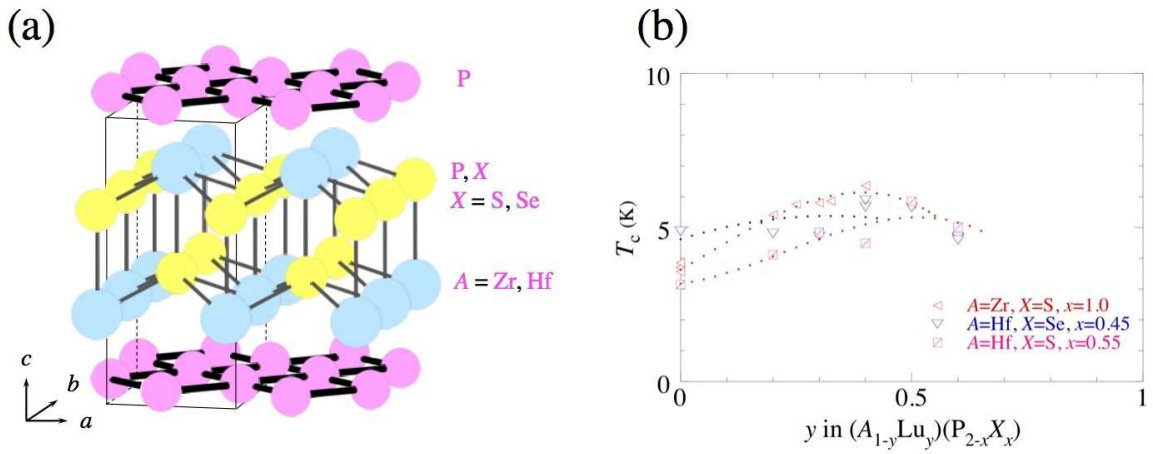

Fig. (a) The crystal structure for PbFCl-type $AP_{2-x}X_x$(*A*=Zr, Hf; *X*=S, Se), (b) $T_c$dependence on substitution nominal amount *y*for $(A_{1-y}Lu_y)(P_{2-x}X_x)$ (*A*=Zr, Hf;*X*=S, Se).

[1] H. Kitô *et al.* J. Phys. Soc. Jpn. 83 (2014) 074713.
[2] H. Kitô *et al.* J. Phys. Conf. Ser. 1054 (2018) 012003.

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Keywords: substitution effect, Mixed anion superconductor, AP2-xXx (A=Zr, Hf; X=S, Se)

PCP3-6

Electronic Structure of novel Superconductor doped-ZrPSe

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Recently found superconductor $ZrP_{2-x}Se_x$ has the same structure with iron-based superconductor LiFeAs. $ZrP_{1.25}Se_{0.75}$ already has T_c ~ 5.8K, and the substitution of non-magnetic rare-earth elements for Zr even increases T_c [1-3]. Moreover, these doped-ZrPSe are also isostructural to ZrSiS, which has Dirac cone protected by non-symmorphic symmetry and three-dimensional Dirac line nodes [4-6].
Therefore, doped-ZrPSe can give a promising platform for investigating the interplay between the Dirac line nodes and the superconductivity. In order to study these points, it is necessary to clarify the electronic structure of doped-ZrPSe.

In this paper we report the results of the first-principles calculations for cation and anion co-doped system $(Zr_{1-y}Y_y)P(As_{0.25}Se_{0.75})$ using virtual crystal approximation. We found that the density of states at the Fermi level (=$D(E_F)$) shows a dome-shape with respect to the doping concentration y, as shown in the Figure. This result qualitatively explains the observed y dependence of T_c, especially for $(Zr_{1-y}Y_y)P_{1.25}Se_{0.75}$. We also found the similarity of the band structure between ZrSiS and doped-ZrPSe. Characteristic band crossing near E_F along M-G axis, which is found to be the Dirac line node in ZrSiS, is also found in doped-ZrPSe. This result strongly suggests that the superconductivity and the Dirac line node are co-existed in doped-ZrPSe.

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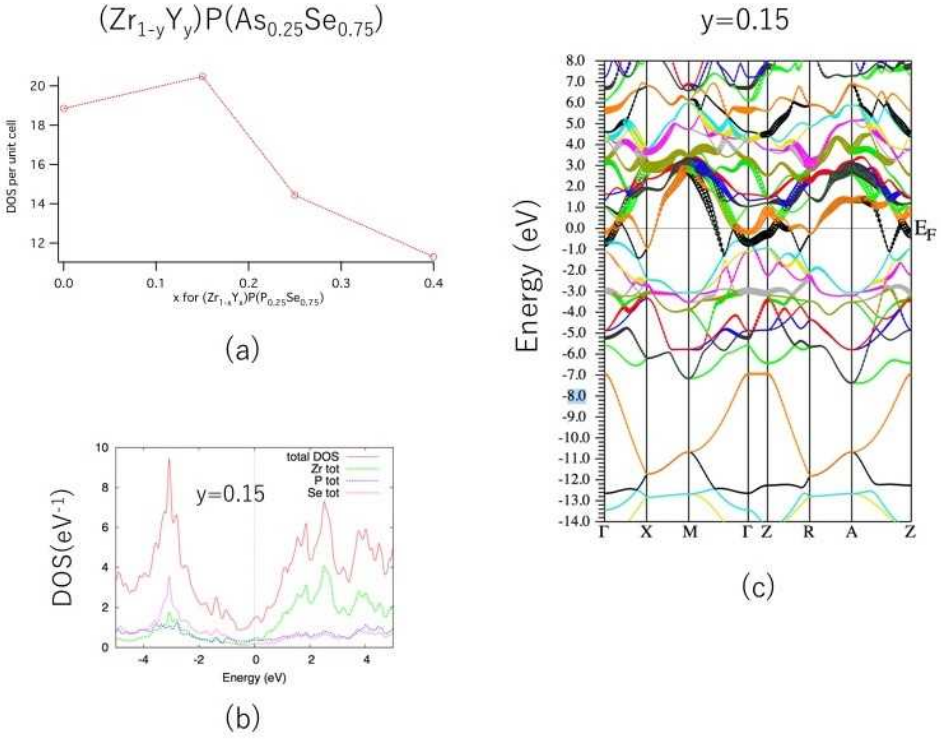

Fig. (a) Density of states at the Fermi level of $(Zr_{1-y}Y_y)P(As_{0.25}Se_{0.75})$ as a function of y. (b) Density of states curve of $(Zr_{0.85}Y_{0.15})P(As_{0.25}Se_{0.75})$. (c) Energy dispersion of $(Zr_{0.85}Y_{0.15})P(As_{0.25}Se_{0.75})$. The width of the band represents the contribution of Zr d-e_g orbitals.

Keywords: doped-ZrPSe, band structure calculation, doping dependence, Dirac line nodes

PCP3-7

Index theorem, skyrmions and the Witten effect in topological quantum systems

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Topological materials have attracted much attention from both physicists and mathematicians recently. Topological properties are closely related to the index theorem. The index theorem known as the Atiyah-Singer index theorem is formulated on a manifold without boundary. An interesting phenomenon will appear when considering the index theorem for manifolds with boundaries. We discuss such interesting phenomena in topological systems including a topological superconductor that emerge from the boundary effect. The boundary effect will result in fractional quantization of charges (that is, the existence of magnetic and electric charges). The Witten effect will also be very attractive when the Dirac electron exists, for example, on the surface of topological materials.

Keywords: topological materials, index theorem, monopoles, Witten effect

PCP3-8

Many-variable variational Monte-Carlo studies of superconductivity with incipient bands in two-band Hubbard models

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The ``incipient'' band, which is not within, but close to the Fermi level, can contribute significantly to spin-fluctuation-mediated pairing [1,3,4]. The incipient band pairing can achieve both strong pairing interactions and light electron mass, possibly resulting in extremely high T_c. The previous studies argued that superconductivity with incipient bands can be induced by engineering of band structures and carrier concentrations in the weak coupling regime [2]. On the other hand, in the case of the strong coupling regime, the pairing mechanism continues to be a matter of debate. Using a many-variable variational Monte-Carlo method [5] for two-band Hubbard models, we find a possible evidence for a correlation-driven Lifshitz transition at the emergence of superconductivity with incipient bands. We also find that in the presence of large Fermi surfaces in the weak coupling limit, incipient bands tend to stick to the Fermi level when the electron correlation is increased.

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Keywords: Strongly correlated electron systems, Unconventional superconductivity, Incipient bands, Correlation driven Lifshitz transition

PCP3-9

Characterization of rice hull magnetic activated carbon and a rotary drum type magnetic separator with ferromagnetic mesh filters

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We have developed rice hull magnetic activated carbon (RH-MAC) and studied its adsorption properties for heavy and valuable metal ions in water and magnetic separation properties using a rotary drum type magnetic separator with ferromagnetic mesh filters. RH-MAC was synthesized by impregnating rice hull with an iron nitrate solution and heat-treatments in nitrogen and carbon dioxide atmosphere. In those processes, a lot of meso-pores and nano-size magnetite were generated inside the activated carbon. The magnetization of RH-MAC increased with increasing concentration of iron nitrate solution. The maximum magnetization of RH-MAC3 made from 1.6 mol/L iron nitrate solution reached 22.2 Am^2/kg at 1 T. RH-MAC had excellent properties for metal ions especially for Cd and Rb ions. To evaluate the magnetic separation properties for RH-MAC, a rotary drum type magnetic separator with the multiple magnetic mesh filters wrapped around a permanent magnet drum was used. It was conformed that capacity rate of RH-MAC increased by multiplying magnetic mesh filters, and the capture rate of RH-MAC3 reached 94% at the flow rate about 900 ml/min with 0.5T and the capture rate reached 98.2% by using triple magnetic mesh filter at the flow rates of 250 ml/min. We also simulated the magnetic particle trajectory by the finite element method for magnetic separation. The simulation results qualitatively matched up to the experimental results. To realize a high speed water processing, we proposed a high magnetic field rotary drum type magnetic separator using a superconducting magnet.

Keywords: Rice hull magnetic activated carbon, High gradient magnetic separation