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High-pressure electrical resistivity studies for $\text{Ba}_{1-x}\text{Cs}_x\text{Fe}_2\text{Se}_3$

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Abstract. High-pressure electrical resistance measurements were performed for iron-based ladder material $\text{Ba}_{1-x}\text{Cs}_x\text{Fe}_2\text{Se}_3$ ($x = 0.25$ and $0.65$) using a diamond anvil cell (DAC). Recent high-pressure study revealed that iron-based ladder material $\text{BaFe}_2\text{S}_3$ exhibits an insulator-metal transition and superconductivity, and this discovery would provide important insight for understanding the mechanism of iron-based superconductors. Therefore, it is intriguing to investigate the high-pressure properties for the iron-based ladder material $\text{Ba}_{1-x}\text{Cs}_x\text{Fe}_2\text{Se}_3$ system. The parent compounds $\text{BaFe}_2\text{Se}_3$ and $\text{CsFe}_2\text{Se}_3$ show insulating and magnetic ordering features. For $\text{Ba}_{1-x}\text{Cs}_x\text{Fe}_2\text{Se}_3$ system, no magnetic ordering is observed for $x = 0.25$ and minimum charge gap was estimated for $x = 0.65$. The insulator-metal transitions are observed in both materials.

1. Introduction

The discovery of iron-based superconductors had a considerable impact on condensed matter physics, triggering rapid efforts in studying the interplay between crystal structure, magnetism, and superconductivity [1]. Several kinds of iron-based superconductors have been discovered at this moment. These materials have a two-dimensional (2D) iron lattice as a common feature, despite of having different crystal structures. These compounds exhibit characteristic magnetic phases adjacent to the superconducting phase based on the 2D iron lattice. While a striped magnetic order is observed in the magnetic phases for $1111$ (e.g. $\text{LaFe}_2\text{AsO}$), $122$ (e.g. $\text{BaFe}_2\text{As}_2$), $111$ (e.g. $\text{LiFeAs}$) and $11$ (e.g. $\text{FeSe}$) type iron-based superconductors, a block type magnetic order was revealed in $245$ (e.g. $\text{KFe}_4\text{Se}_5$) type iron-based superconductor. Such a variety has substantial importance to understand the interplay between magnetism and superconductivity [2].

Recently, an iron-based quasi-one-dimensional compound $\text{AFe}_2\text{X}_3$ ($\text{A} = \text{Ba, K, Cs}$, and $\text{X} = \text{S, Se}$) having the spin-ladder arrangement of Fe atoms has attracted much attention. $\text{BaFe}_2\text{S}_3$ is an insulator having the stripe magnetic order, in which the magnetic moments are arranged to form ferromagnetic units along the rung direction, stacking antiferromagnetically along the ladder direction. This stripe-
type magnetic structure is reminiscent of the 1111 and 122 systems found in the iron-based superconductors. Recently, BaFe$_2$S$_3$ was revealed to exhibit pressure-induced superconductivity having $T_c$ of 14 K at 11 GPa [3]. Motivated by this discovery, extensive studies have been carried out for other iron-based ladder materials. In copper-based materials, the superconducting phase emerges not only in square lattice structures but also in ladder structures. The two-leg ladder material Sr$_{14-x}$Ca$_x$Cu$_{24}$O$_{41}$ exhibits superconductivity under high pressures above 4 GPa with $T_c$ of 12 K, which provided great insight to understanding the high-$T_c$ superconductivity [4].

The magnetic structure of BaFe$_2$Se$_3$ is block-type, in which the magnetic moments form Fe$_4$ ferromagnetic units which stack antiferromagnetically along the ladder direction in a one-dimensional analogue of the block magnetism observed in the 245 system [5, 6]. In contrast, the magnetic structure of the CsFe$_2$Se$_3$ is stripe-type, in which the magnetic moments couple ferromagnetically along the rung and antiferromagnetically along the leg direction. This magnetic structure represents a one-dimensional analogue of the stripe magnetism observed in 1111 and 122 systems [7]. Since these ladder materials exhibit magnetic structures similar to those of the iron-based superconductors, they can be considered as potential superconductors.

In this study, high-pressure electrical resistivity measurements are performed for Ba$_{1-x}$Cs$_x$Fe$_2$Se$_3$ ($x = 0.25$ and 0.65). The crystal is composed of a quasi-one-dimensional structure formed by edge-shared FeSe$_4$ tetrahedra with channels occupied by (Ba, Cs) atoms and these materials for $x = 0.25$ and 0.65 have the $Cnmc$ space group, as shown in figure 1, while BaFe$_2$Se$_3$ has the $Pnma$ space group. The crystal structure is depicted by the VESTA software [8]. The block-type magnetism is suppressed by substitution of Ba into Cs, and no magnetic reflection was observed in the powder neutron diffraction measurements for $x = 0.25$ [9]. It is interesting to study electrical properties under high pressure for $x = 0.25$, because the antiferromagnetic ordering of BaFe$_2$S$_3$ is suppressed with applying pressure and superconductivity appears after suppression of magnetic ordering state [10]. On the other hand, the formal valence of Fe is Fe$^{2+}$ and Fe$^{2.5+}$ for BaFe$_2$Se$_3$ and CsFe$_2$Se$_3$, respectively. The material for $x = 0.65$ is chosen for the second material for high-pressure experiment, since the material for $x = 0.65$ shows the minimum charge gap state [9].

![Figure 1](image_url)

Figure 1. The Crystal structure of Ba$_{1-x}$Cs$_x$Fe$_2$Se$_3$, consisting of edge-shared FeSe$_4$ tetrahedra extending along the c axis and of channels occupied by Ba or Cs atoms, in which Fe atoms form a ladder structure.
2. Experimental

High-pressure electric resistance measurements for single crystalline $\text{Ba}_{1-x}\text{Cs}_x\text{Fe}_2\text{Se}_3$ were performed by a standard d.c. four-probe method using a diamond anvil cell (DAC). Detail of the sample preparation is described elsewhere [9]. The electric currents of 1.0, 0.1 and 0.05mA were made to flow to samples. The sample chamber of DAC was filled with powdered NaCl at the pressure-transmitting medium, using a rhenium gasket, and thin (10µm thick) platinum ribbons were used as leads for the standard d.c. four-probe analysis. The anvils having culet size of 0.5mm were used. The samples are rectangular in shape of about 0.1mm×0.1mm×0.3mm. A thin BN layer acted as electric insulation between the leads and the rhenium gasket and finely ground ruby powder scattered in the sample chamber was used to determine the pressure by the standard ruby fluorescence method.

3. Results and Discussion

3.1. $\text{Ba}_{0.75}\text{Cs}_{0.25}\text{Fe}_2\text{Se}_3$ ($x = 0.25$)

Figure 2(a) and (b) show the temperature dependence of the electrical resistance of $\text{Ba}_{0.75}\text{Cs}_{0.25}\text{Fe}_2\text{Se}_3$ under high pressure up to 12 GPa on a logarithmic scale and 13GPa to 18 GPa on a linear scale, respectively. This material has the $\text{Cmcm}$ space group and no magnetic reflection was observed in the powder neutron diffraction measurements for $x = 0.25$. The electric resistance decreases with applying pressure. It shows metallic temperature dependence above 12 GPa. However, the upturn of resistance is observed up to the maximum pressure below 50 K. The double-digit reduction of room-temperature resistance is observed from ambient pressure to 18 GPa. Since about triple-digit reduction of room-temperature resistance was reported for $\text{BaFe}_2\text{S}_3$ at 11 GPa where the metal insulator transition takes place and superconductivity appears [3], the pressure of 18 GPa might be not enough pressure to induce superconductivity for $\text{Ba}_{0.75}\text{Cs}_{0.25}\text{Fe}_2\text{Se}_3$.

![Figure 2](image.png)

Figure 2. (a)Temperature dependence of the electrical resistance of $\text{Ba}_{0.75}\text{Cs}_{0.25}\text{Fe}_2\text{Se}_3$ up to 12GPa on a logarithmic scale. (b)Electrical resistance up to 18.2GPa on a linear scale.
3.2. $\text{Ba}_{0.35}\text{Cs}_{0.65}\text{Fe}_2\text{Se}_3$ ($x = 0.65$)

Figure 3(a) and (b) show the temperature dependence of the electrical resistance of $\text{Ba}_{0.35}\text{Cs}_{0.65}\text{Fe}_2\text{Se}_3$ under high pressure up to 19 GPa on a logarithmic scale and 20 GPa to 30 GPa on a linear scale, respectively. This material has the Cmcm space group and shows the minimum charge gap state. The electric resistance decreases with applying pressure. It shows metallic temperature dependence above 14 GPa. No upturn of resistance is observed up to the maximum pressure in the low temperature range. About 1.5 digit reduction of room-temperature resistance is observed from ambient pressure to 30 GPa. Though this material shows metallic behaviour, the pressure of 30 GPa might be still not enough to induce superconductivity for $\text{Ba}_{0.35}\text{Cs}_{0.65}\text{Fe}_2\text{Se}_3$. It is necessary to carry out the electrical resistance measurement at much higher pressure.

Figure 3. (a)Temperature dependence of the electrical resistance of $\text{Ba}_{0.25}\text{Cs}_{0.65}\text{Fe}_2\text{Se}_3$ up to 19.2 GPa on a logarithmic scale. (b)Electrical resistance up to 30.0GPa on a linear scale.

4. Summary

High-pressure electrical resistance measurements were performed for iron-based ladder material $\text{Ba}_{1-x}\text{Cs}_x\text{Fe}_2\text{Se}_3$ ($x = 0.25$ and 0.65) using a diamond anvil cell (DAC). These samples exhibit the insulator-metal transition at about 12GPa and 14 GPa for $x = 0.25$ and $x = 0.65$, respectively. Superconductivity could not be observed in these experimental pressures. It has to be needed to perform higher pressure experiment for these materials.

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