Two-Magnetization Nordheim Model of Randomly Distributed Co Local Sites for the Anomalous Residual Resistivity at the Magnetic Phase Boundary of \( Y_{1-x}R_xCo_2 \) System (R: Rare Earth)

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Abstract. The electrical resistivity \( \rho \) of the Laves phase \( Y_{1-x}R_xCo_2 \) compound system has been measured in magnetic fields up to 10 T and under pressures up to 8 GPa at temperatures from 1.5 to 300 K. The anomalous behavior of residual resistivity has been observed in a region \( x < x_{a} \), where \( x_{a} \) is a critical concentration between inhomogeneously and homogeneously ordered phases, and which has a maximum at \( x_{c} \) where \( T_C \approx 0 \) with a mean field acting on Co sub-lattice is equal to the itinerant Co metamagnetic critical field \( B_c \). In \( x_{c} < x < x_{a} \), the magneto-resistivity and pressure resistivity are anomalously large with positive sign. However, in the paramagnetic region for \( x < x_{c} \), they are anomalously large but with negative sign.

The anomalous behavior is attributed to the s-d scattering of conduction electrons due to statistically disordered Co magnetization. Those phenomena can be explained by a new scattering model of [Two magnetization Nordheim model for randomly distributed Co sites] introduced by us.

1. Introduction
The cubic Laves phase compound of \( YCo_2 \) is known as a strongly enhanced Pauli paramagnet whose itinerant 3d-electron subsystem undergoes a metamagnetic transition into the ferromagnetic at external magnetic field \( B_c \approx 70 \) T \[^1\]. The metamagnetism of \( YCo_2 \) was deduced from the calculated electronic structure, with a sharp peak in the density of states (DOS) \( N(\varepsilon) \) mainly due to the 3d states of Co near the Fermi energy \[^2\]. In \( RCo_2 \) compounds with a nonzero rare-earth 4f magnetic moment, the 3d-4f exchange field to Co, based on an antiferromagnetic coupling between 3d spin and 4f spin \[^3\], exceeds \( B_c \) and drives the Co subsystem into the ferromagnetic state.

Since Co is present commonly in all \( Y_{1-x}R_xCo_2 \) compounds, it is reasonable to assume that \( N(\varepsilon) \) has the same general properties throughout these series. The 3d spin fluctuation makes a main contribution to the high-temperature electrical resistivity \( \rho \) and thermopower \( S \) of both
paramagnetic and magnetic RCo$_2$ compounds [4, 5]. At low temperatures (below 30 K) the electrical resistivity $\rho(T)$ reveals $T^2$ variation for the paramagnetic YCo$_2$, LuCo$_2$, and ScCo$_2$, which indicates that in this temperature range the resistivity is also dominated by the scattering of conduction electrons by spin fluctuations.

Strong enhancement of the residual resistivity in the inhomogeneously ferrimagnetic phase and paramagnetic phase were found in the Y$_{1-x}$R$_x$Co$_2$ [6, 7, 8, 9, 10, 11, 12, 13]. The anomalous behavior can be understood by the interplay of the metamagnetic instability of Co 3d itinerant electrons and disorder of atomic position of Y or R in the (Y, R) sub-lattice, which induces a random distribution of regions of high and low 3d magnetization. Our model named as [Two-Magnetization Nordheim Model] is based on $s-d$ scattering by randomly distributed Co local sites at the magnetic phase boundary of Y$_{1-x}$R$_x$Co$_2$ system (R: heavy rare earth), although the mean field approximation can be applied to cooperative phenomena as magnetic ordering. In order to confirm the validity of our theoretical model, we have investigated Y$_{1-x}$R$_x$Co$_2$ system in detail on the effects of substitution, an external magnetic field and high pressure on the low-temperature electronic transport of these compounds.

2. Results

As resistivity results, we use the normalized resistivity $\rho(T)/\rho(300)$ to compare the properties of different samples, as a large number of pores or micro-cracks exist in these samples of RCo$_2$. Figure 1 presents the temperature dependence of the normalized resistivity, and composition dependences of Curie temperature $T_C$, residual resistivity and magneto-resistance (MR) of the Y$_{1-x}$Tb$_x$Co$_2$ compounds, where MR is defined as $\Delta\rho/\rho = (\rho(B,T) - \rho(0,T))/\rho(0,T)$.

For compounds with a magnetically ordered ground state ($x > 0.2$), $\rho(T)/\rho(300)$ shows a sharp increase at temperatures just below $T_C$ with increasing temperature, owing to relieve spin fluctuations in the Co 3d subsystem. The resistivity of diluted compounds ($0.05 < x < 0.20$) reveals a minimum in $\rho(T)/\rho(300)$ at low temperatures, suggesting that there is additional scattering mechanisms different from the ordered compounds. For YCo$_2$, it increases monotonically.

The residual resistivity is enhanced strongly below the border Tb content $x_c$ between inhomogeneously and homogeneously ordered phases and takes a maximum at $x_c$. As seen in Fig. 2, the residual resistivity $\rho_{res}/\rho(300)$ rapidly increases with $x$ and attains a maximum near the critical composition of the phase boundary between paramagnetic and magnetically ordered phases $x_c$. The MR is negative for $x < x_c$ and positive for compounds with $x > x_c$. It should be noted the absolute value of MR is largest near the composition $x_c$ where the $\rho_{res}/\rho(300)$ takes maximum [7, 9, 11] as seen in Fig. 1. The MR exhibits almost the same properties for all the measured heavy rare earth compound systems in Y$_{1-x}$R$_x$Co$_2$. The pressure resistance: $\Delta\rho/\rho = (\rho(P,T) - \rho(0,T))/\rho(0,T)$, where $P$ is high pressure, also shows the same properties as MR for all the systems.

The enhancement of the residual resistivity suggests that the $s-d$ scattering of conduction electrons due to the static disorder of internal magnetic field acting on Co atoms, which is higher or smaller than the metamagnetic critical field, gives the main contribution to the low-temperature electronic transport of these compounds.

3. Discussion

The anomalous enhancement of the residual resistivity and the anomalous changing the sign of large MR (and pressure resistivity) shown in Fig. 1 are common features in all of the measured Y$_{1-x}$R$_c$Co$_2$. Especially it is important that $\rho_{res}/\rho(300)$ takes a maximum at the concentration $x_c$, where the magnetic ordering is arising as shown in Fig. 2. Here the averaged internal magnetic field acting on Co sub-lattice is the same as the critical field of metamagnetic transition in the
The properties of $Y_{1-x}Tb_xCo_2$ system. (Top) Temperature dependence of the normalized resistivity. (Second) Concentration dependence of the magnetic ordering temperature $T_C$ and inhomogeneously ordered (or freezing) temperature $T_f$. The vertical dashed line indicates the magnetic phase boundary $x_c$. (Third) The residual resistivity $\rho_{res}/\rho(300)$. (Bottom) The magneto-resistance MR at $B = 10$ T and $T = 2$ K.

Concentration dependence of $\rho_{res}$, the Curie temperature $T_C$ and inhomogeneously ordered (or freezing) temperature $T_f$ for all of the systems of $Y_{1-x}R_xCo_2$, where, $R = Gd$, Tb, Dy, Ho, and Er.

mean field approximation. This suggests that the half of the Co atoms are in high magnetic state and the other half are in low magnetic state at the $\rho_{res}/\rho(300)$ maximum. Such a condition offers a Nordheim-like scattering model for these anomalous enhancement of the residual resistivity in these systems[7, 9]. The local field acting on individual Co atom depends on environmental rare earth (Y or R) distribution as indicated in left figure in Fig. 3. When $x=1$ the local field is uniform, however, Y-substituted compound makes a distribution of Co local field. During all of the local field is higher than the metamagnetic critical field, the compound keeps simple ferrimagnetic. If a part of the local field is less than the critical field, then the compound is inhomogeneously ordered ferrimagnetic, and if the center peak of distribution function is less than the critical field, the compound is paramagnetic or freezing phase. The resistivity anomaly arises when the distributed local field extends across the critical field.

As seen in Fig. 3, the local field acting on Co atoms is distributed, where $y$ is the volume fraction of the high-magnetization component of the Co 3d subsystem. The $s$-$d$ scattering due to 3d magnetic state guide us to a modulated Nordheim’s law as follows: $\rho_{res}/\rho(300)$ is proportional to $(1-y)y$. The function $f(B)$ is the distribution function of the effective field on Co atoms, and $B_c$ is the critical field for the metamagnetic transition of the 3d subsystem. Since the exchange field of aligned 4f moments on Co site is antiparallel to an external field, the external field results in a uniform reduction of the effective field acting on the 3d system: $f(B) \rightarrow f(B-B_{ext})$. The
pressure dependence of $y$ is related to that of the critical field $B_c$ for the metamagnetic transition of the 3$d$ band under high pressures; $B_c$ increases with pressure [14]. On the other hand, pressure does not change the distribution function $f(B)$. Therefore, $y$ decreases under pressure. Thus the value of $y$ depends on the compound content $x$, external field $B_{ext}$, and pressure $P$. In our basic estimation [9], relations between these factors can be obtained as follows:

$$
\Delta x = -\frac{dB_c}{dP} (n_{fd}M_R)^{-1} \Delta P,
$$
$$
\Delta B_{ext} = \left( \frac{dB_c}{dP} \right) \Delta P,
$$

(1)

where $n_{fd}$ is molecular field factor and $M_R$ is rare earth magnetic moment.

The experimental fitting value, $\frac{dB_c}{dP} \approx 25 \text{T/GPa}$, is in good agreement with the theoretical estimation [14] ($\frac{dB_c}{dP} \approx 20 \text{T/GPa}$ by Yamada). Thus we can conclude that our new model of [Two-Magnetization Nordheim Model] is a reasonable approximation for this anomaly.

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