A STUDY OF DEFECT IN CRYSTAL STRUCTURE BY ELECTRICAL RESISTIVITY

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ABSTRACT

We measured the electrical resistivity in the temperature range from 2K to 300K to study some information of nano crystal structure for the rare earths. The electrical resistivity follows the Matthiessen's rule with five contributions. The contribution of electron –electron scattering is dominant at low temperature for the strongly correlated electron system. Therefore, the residual resistivity ratio values, ratio of resitivity at room temperature and resitivity at absolute zero, are estimated to know some parameters to indicate the quality of samples. Most of $RRhIn_5$ single crystal compounds show the low defect in crystal structure. The small values of RRR in $RRhIn_5$ (R= Dy, Ho, Tb, Er) indicate that some remained indium metals presented inside of these compounds, which must be taken into account during the measuring process. The resistivity data is also in good agreement with our recent SEM and EDX results.

Keywords*: Nanoscale structure, Crystal defect, Electrical resistivity.*

I. INTRODUCTION

The crystal structure of 115 compounds are studied by the single-crystal X-ray diffraction (XRD) to determine the lattice constants, crystal structure which are well-known methods. These compounds crystallize in $HoCoGa_5$ type-structure. [1,2]. Many interested physical properties of $RRhIn_5$ (R=Ce, Pr) have been investigated [3-5]. To grow the single crystal of the rare earths, we found the Indinium-flux method was also the good method. Recently, H.T. Huy *et al* [6] indicated that the some part of RIn_3 compounds and the remained Indium metal in the surface of $RCoIn_5$ could be found by the photos of SEM and the EDX study. These findings press us to study more the investigation of the crystal structures in nano scale rare earths by the electrical resistivity.

Here, we report the electrical resistivity (ρ) of $RTIn_5$ follows the Matthiessen's rule [7]. The residual resistivity ratio values were estimated to know the quality of crystal structure [8].

II. EXPERIMENTS

The single crystals of $RRhIn_5$ were grown by the self-flux method using In as flux. These single crystal compounds can be grown at the temperature which is lower than their melting points and no required special technique. Many high-quality single crystals of $RRhIn_5$ (*R*: Pr, Nd, Sm, Gd, Tb, Dy, Ho, Er ,Tm and Yb) were obtained. For example, we received several plate like single crystals with dimensions about $10x7x4mm^3$ in $NdRhIn_5$, $GdRhIn_5$,$TbRhIn_5$,… but a few mm^3 in $RRhIn_5$ (R= Tm,Yb).

Their structural parameters were determined by the single-crystal X-ray diffraction experiments. Next, we used the X-ray Laue film to determine the direction of the single crystal structure. Hence, the samples were cut along [100] and [001] axes of crystallography. They were fixed them into sample holder for the standard four-probe DC current method, as shown in Fig. 1. The electrical resistivity were measured from 1.3K to the room temperature.

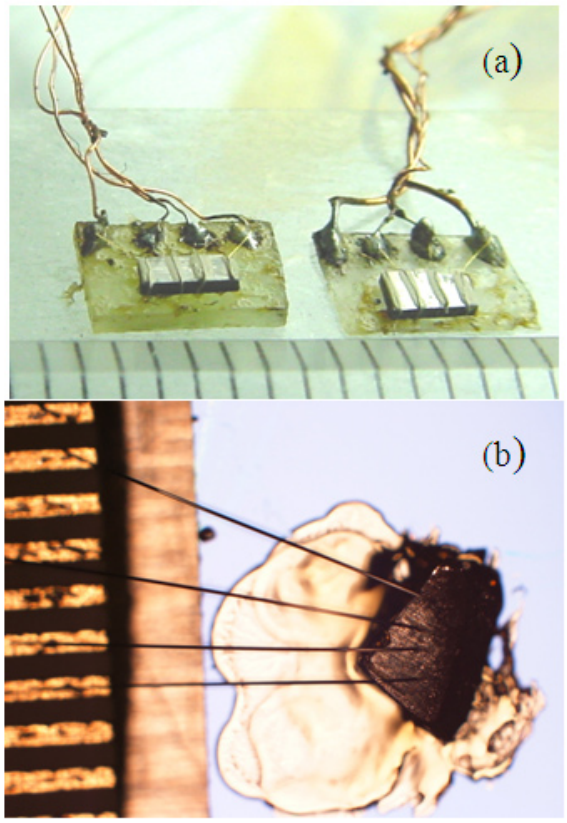

Figure 1. Samples were mounted in the sample holders for resistivity measurements: (a) with larger sample and (b) with less than 1mm dimension sample.

Table 1 is shown the structural parameters of these rare earths.

Igro Pro. Soft ware was used in the analysis process of these data to estimate the RRR values. We can know some information about the nanoscale crystal structure of 115 compounds. Moreover, the results of SEM and EDX were also mentioned in this report.

III. RESULTS AND DISCUSSION

A. Nanoscale crystal structure

The structural parameters of $RRhIn_5$ were determined by the single-crystal x-ray diffraction experiments with the Mo-*K*α radiation. Table 1 is shown the structural parameters of these rare earths. We confirmed that all the $RTIn_5$ compounds crystallize in the tetragonal $HoCoGa_5$-type structure ($P4/mmm$ #123 D^1_{4h}), as shown in Fig. 2.

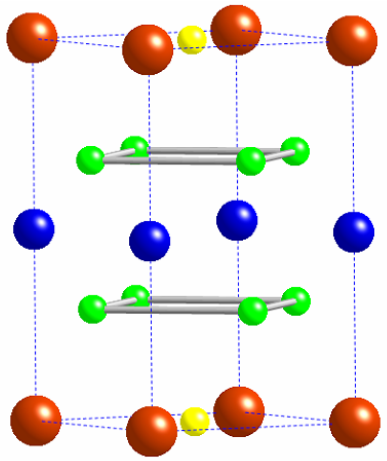

Figure 2. Crystal structure of $RTIn_5$ single crystal compounds in colors (red: Rare earths, blue: Rh, green and yellow: In)

Name of Compounds	Lattice constants (nm)		fractional coordinate
	a	*c*	*z (4 i site)*
$LaRhIn_5$	0.4673	0.7590	0.3078
$CeRhIn_5$	0.4652	0.7544	0.3060
$PrRhIn_5$	0.4642	0.7521	0.3052
$NdRhIn_5$	0.4630	0.7501	0.3045
$SmRhIn_5$	0.4614	0.7459	0.3032
$GdRhIn_5$	0.4606	0.7439	0.3025
$TbRhIn_5$	0.4599	0.7420	0.3017
$DyRhIn_5$	0.4591	0.7394	0.3008
$HoRhIn_5$	0.4590	0.7389	0.3007
$ErRhIn_5$	0.4585	0.7377	0.3000

$TmRhIn_5$	0.4587	0.7360	0.3005
$TmCoIn_5$ [7]	0.4552	0.7398	0.3048
$YbRhIn_5$	0.4604	0.7447	0.3011
$YbCoIn_5$ [7]	0.45875	0.7469	0.3060

The lattice constant data of *a* and *c* reveal the gradual shrink phenomenon from La to Tm, which is identified by the well-known lanthanide contraction.

On the other hand, the lattice constants of $YbRhIn_5$ deviate from the lanthanide contraction, meaning that Yb ion is divalent, while the other rare earth ions are trivalent.

B. The analysis data of electrical resistivity

The electrical resistivity *(ρ)* follows the Matthiessen's rule [10] that include the electron scattering *($ρ_0$)*, the electron - phonon scattering *($ρ_{ph}$)*, the electron-electron scattering *($ρ_{ee}$)* and the electron-magnon scattering *($ρ_{mag}$)*, as shown below:

$$\rho(T) = \rho_0 + \rho_{ph} + \rho_e + \rho_{mag} \quad [1]$$

The $ρ_0$-value, which originates from the electron scattering due to the impurities and defects, is a constant for a variation of the temperature. The $ρ_0$-value is important to know the quality of an obtained sample. If $ρ_0$ is large, the sample contains many impurities or defects. The quality of a sample can be estimated by determining a so-called residual resistivity ratio, $RRR=ρ_{RT}/ρ_0$ where $ρ_{RT}$ is the resistivity at room temperature. Of course, a large value of *RRR* indicates that the quality of the sample is good.

Next, a scattering lifetime t_0 and a mean free path ℓ_0 are also expressed in the viewpoint of the resistivity, which are well-known in the solid state [9]:

$$\rho_0 = \frac{m^*}{ne}\cdot\frac{1}{\tau_0} \quad [2]$$

where *n* is density of carrier and *e* is an electric charge. Then t_0 and i_0 values are:

$$\tau_0 = \frac{m^*}{ne\rho_0} \quad [3]$$

$$\ell_0 = v_F\tau_0 = \frac{\hbar k_F}{ne\rho_0} \quad [4]$$

The temperature dependence of ρ_{ph} which originates from the electron scattering by phonon, changes monotonously. It is proportional to *T* (*temperature*) above the Debye temperature, while it is proportional to T^5 far below the Debye temperature, and will be zero at *T*=0.

Finally, we can regard the total resistivity in non-magnetic compounds at low temperatures as follows:

$$\rho(T) = \rho_0 + \rho_{ee}(T) = \rho_0 + AT^2 \quad [5]$$

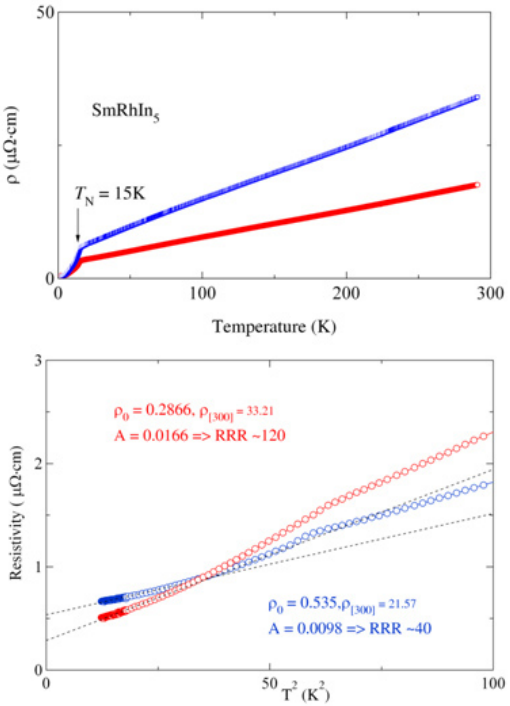

Fig. 3. The resistivity data for J//[100] and [001] in $SmRhIn_5$: (up) the temperature dependence of the electrical resistivity and (down) below 10K in T^2 scale. The dotted line are fitting curves for guide eyes.

Where, the coefficient $A^{1/2}$ is proportional to the effective mass. Yamada and Yosida [7] obtained the rigorous expression of $\rho_{e\text{-}e}$ in the strongly correlated electron system on the basis of the Fermi liquid theory.

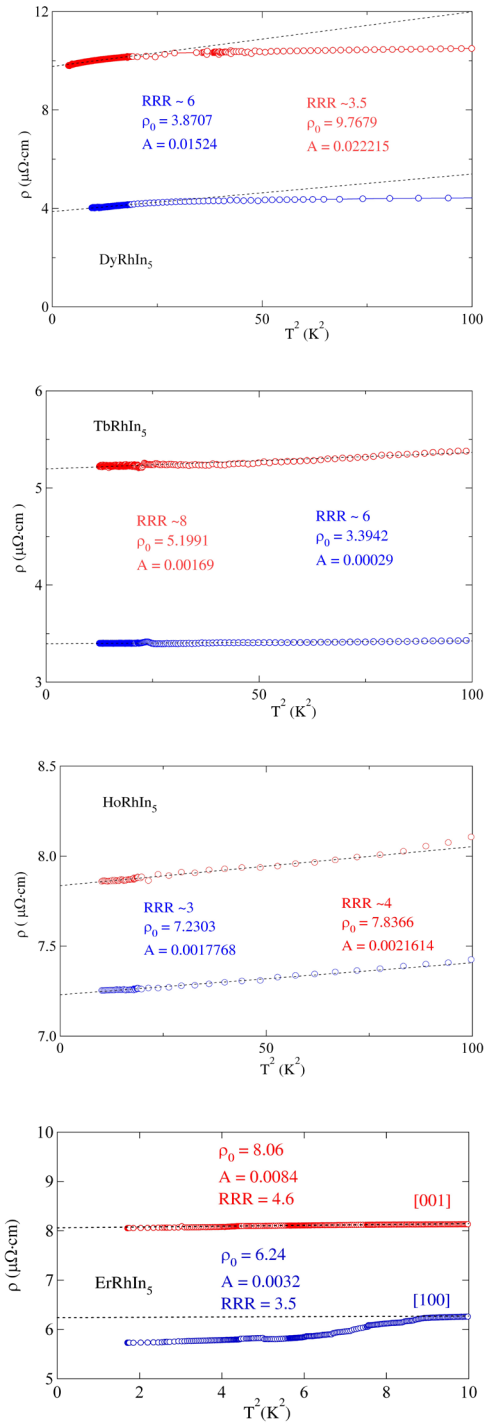

Fig. 4. The T^2 dependence of the electrical resistivity in $RRhIn_5$ (R= Dy, Tb, Ho and Er from up to down). The dotted line are fitting curves for guide eyes.

Almost $RTIn_5$ showed anti-ferromagnetic ordering, besides the rare earths of Ce, Pr, Yb. The Neel temperature, T_N, indicate the anti-ferromagnetic phase. $TbRhIn_5$ is the highest T_N of 47.3K, while $GdRhIn_5$ is 38.9K. The lowest T_N of 2.9K is $ErRhIn_5$. Moreover, $RRhIn_5$ (R=Sm, Er) showed two T_N transitions.

The resistivity curves of $SmRhIn_5$ for the current along [100] and [001] direction of crystal structure are shown in Fig. 3. The below show the T^2 dependence of the electrical resistivity in below 10K, where the contribution of ρ_{ee} is dominant in the strongly correlated electron system. We used the Igro Pro to make measuring curves and estimated RRR values.

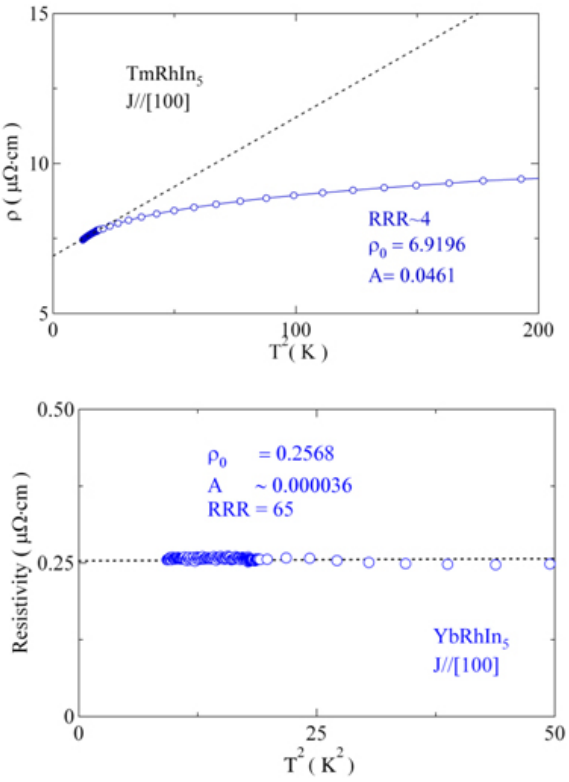

Fig. 5. The T^2 dependence of the electrical resistivity: (up) $TmRhIn_5$ and (down) $YbRhIn_5$. The dotted line are fitting curves for guide eyes.

The value of ρ_0 and A can be obtained by the fitting curve as a linear function. The residual resistivity ratio RRR (ρ_{300K}/ρ_{0K}) of $SmRhIn_5$ are

120 and 40 for *J*//[001] and [100], respectively.

As same method, other *RRR* values of $RRhIn_5$ (R= Dy, Tb, Ho and Er) were also estimated, as shown in Figure 4 from up to down, respectively.

Due to the thin dimensional samples, the electrical resistivity only were measured along [100] for $TmRnIn_5$ and $YbRhIn_5$, as shown in Figure 5, respectively.

C. The RRR values and their defect in crystal structures

Figure 3 indicates that $SmRhIn_5$ has low defect in crystal structure because of large values of RRR (40 for *J*// [100] and 120 for *J*// [001]). We got high quality sample of $SmRhIn_5$ by this flux method. However, the small values of RRR (6 for *J*//[100] and 8 for [001]) in $TbRhIn_5$ indicate the high defect in crystal structure.

The RRR values of $PrRhIn_5$ are 250 for *J*// [100] and 260 for *J*//[001], which indicate the high quality sample. For $NdRhIn_5$ compound, these values are smaller than $PrRhIn_5$ as 64 and 180. $GdRhIn_5$ indicated the small value of 13 for J//[100], but it is 125 for RRR in [001]. The other $RRhIn_5$ are (6;13) for $DyRhIn_5$, (3;3) for $HoRhIn_5$, (6;4) for $ErRhIn_5$, (4; no data) for $TmRhIn_5$ and (65; no data) in $YbRhIn_5$. The small values of RRR mean that many impurities were in crystal structure of these compounds.

We note that the electrical resistivity of some compounds could not study in the case of the current along [001] direction because of thin samples. The high value of *RRR* in $RRhIn_5$ (*R*=Pr, Nd, Sm, Gd, Tm, Yb) mention us these samples are good quality. The ρ_0-value, which originates from the electron scattering due to impurities and defects, is constant for a variation of the temperature which is small.

By the results of SEM and EDX data for $RRhIn_5$ (*R*= Nd, Tb, Dy, Ho, Er) [9], we found that $TbRhIn_5$, $HoRhIn_5$, $ErRhIn_5$,$TmCoIn_5$, $YbCoIn_5$ are not high quality samples.

Finally, RRR values inform directly the quality of sample or the defect inside crystal structure. These resistivity data are in good agreement with the results of SEM and EDX.

IV. CONCLUSION

The RRR values by the electrical resistivity measurements reflected the remained indium metals in side of rare earths compounds, which must be taken in account during the measuring process. The surface of sample must be well-polished for the obtained good results. Moreover, the error in anisotropic physical property experimental results can be taken in account if we know how is the defect of sample. Therefore, the electrical resistivity in low temperature is a good survey to evaluate the defect of crystal structure of samples. It will be one of the useful technique to study some information of the nano crystal structure.

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