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Pseudogap and transport properties in $Fe_{3-x}V_xAl_y$ $(x=0.5-1.05;\ y=0.95,1.05)$

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We have measured the Hall resistivity for the intermetallic compound $Fe_{3-x}V_xAl_y$ $(x=0.5-1.05;\ y=0.95,1.05)$ at room temperature. The Hall coefficient changed its sign from positive to negative around the Heusler composition (i.e., $x=y=1$) with increasing x value or decreasing y value. We have measured the temperature dependence of the Hall coefficient and the electrical resistivity for $Fe_{1.98}V_{1.02}Al$ and quenched $Fe_{1.95}V_{1.05}Al$ in the temperature range of 5–300 K. These two compounds showed very different behavior in the electrical resistivity but the behavior of the Hall coefficient was quite similar. At higher temperatures, the Hall coefficient showed a strong temperature dependence but it approached a constant value at low temperatures suggesting that these compounds are semimetals with a pseudogap. The charge carrier density was found to be less than a few tenths per unit cell. The rise of electrical resistivity at low temperatures is not owing to an energy gap but due to magnetic scattering while the negative temperature coefficient at high temperatures is attributable to pseudogap.

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I. INTRODUCTION

The Heusler-type Fe_2VAl compound was reported at first to be a candidate for the $3d$ heavy fermion material[1] and has attracted a lot of interest so far. The electrical resistivity is semiconducting[1–3] although photoemission measurements suggest a large density of states at Fermi level.[1] The temperature coefficient of resistivity is metallic below the Curie temperature T_c (Refs. 1–3) suggesting a possibility that a strong magnetic scattering is the cause of the semiconducting behavior. However, the negative temperature coefficient of resistivity is observed up to 1300 K,[1] which could not be explained only with magnetic scattering mechanism. The magnetoresistance is negative at low temperatures[4] indicating a strong magnetic scattering, but it becomes positive at higher temperatures where the temperature coefficient of resistivity is still negative. Thus the origin of the negative temperature dependence of the electrical resistivity is not clear so far.

The specific heat C shows an enhancement at low temperatures.[1,2,5,6] The value of C/T increases with decreasing temperature but starts to decrease below about 1 K forming a maximum around 1 K.[5] However, the electrical resistivity does not show any anomaly at the temperature where the maximum of C/T value appears.[5] On the other hand, the specific heat behavior under magnetic fields is well described with a Schottky anomaly which indicates the presence of magnetic clusters having a magnetic moment of $3.7\mu_B$.[6] The NMR measurements[7,8] and the strong heat treatment effects[2] also indicate the presence of magnetic clusters. Thus the origin of the magnetism is considered to be magnetic clusters in this compound.

In band calculations[9,10] Fe_2VAl is a semimental with a carrier density of 0.003–0.012 per one formula unit and is stable against ferromagnetic ordering. In this paper we report, first, the change of the sign of the charge carriers when the values of x and y vary. Then we report the temperature dependence of the electrical resistivity and the Hall coefficient for $Fe_{1.98}V_{1.02}Al$ and for quenched $Fe_{1.95}V_{1.05}Al$. In $Fe_{3-x}V_xAl_y$ compounds, strong anomalous Hall effects are generally observed at low temperatures, which prohibit an accurate evaluation of the Hall coefficient. However, $Fe_{1.98}V_{1.02}Al$ is an exception which does not exhibit the anomalous Hall effect. The quenched $Fe_{1.95}V_{1.05}Al$ showed the anomalous Hall effect but the magnitude was relatively weak compared to that in Fe-rich compounds (i.e., $x \leqq 1$). The two compounds show quite different behavior in electrical resistivity and we suggest the causes bringing about the differences by measuring Hall coefficient and other properties.

II. EXPERIMENTAL

Polycrystalline samples of $Fe_{3-x}V_xAl_y$ with $x=0.5-1.05$; $y=0.95,1.05$ were prepared by arc melting the proper amounts of elements for the correct chemical composition. In the course of arc melting a few percent of Al evaporates; the ratio of aluminum after arc melting is smaller by a few percent compared to the starting composition. For convenience, we use the starting composition to refer to the sample in the following. For example, the sample denoted as Fe_2VAl has a real composition close to $Fe_2VAl_{0.96-0.98}$. The samples with $x=0.5$, 0.8, 0.9, and 1.02 were cooled at the rate of 0.017 K/s down to room temperature after a homogenization process of 1273 K×54 ks. We prepared quenched samples of Fe_2VAl and $Fe_{1.95}V_{1.05}Al$. They were quenched

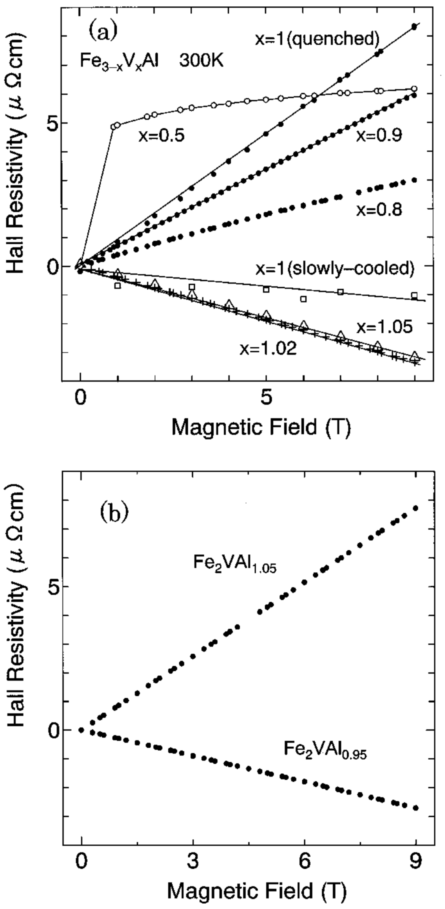

FIG. 1. Variation of Hall resistivity at room temperature with (a) vanadium content and (b) aluminum content.

into water after annealing at 1073 K for 180 ks. We also prepared a slowly cooled sample for Fe_2VAl by cooling at the rate of 0.0017 K/s after the homogenization of 1273 K $\times 54$ ks. No second phase was detected in the powder x-ray diffraction profiles for all samples. We also searched for impurity phase using a scanning electron microscope (SEM) equipped with an energy dispersive x-ray spectrometer (EDS), but found no impurity phase except for a small amount of Al or Al oxide inclusions.

The Hall effect was measured by using the five-terminal method with magnetic fields up to 9 T. Electrical resistivity and magnetoresistance were measured with a conventional four-probe method.

III. RESULTS AND DISCUSSION

A. The sign of Hall coefficient

Figure 1(a) shows the variation of the Hall resistivity ρ_{xy} as a function of magnetic field for the samples with various V concentrations. It was found that the sign of ρ_{xy} is positive for $x<1.0$ while that for $x>1.0$ is negative. For the sample with $x=1.0$, the sign depends on the heat treatment; the quenched sample exhibits a positive Hall resistivity while the slowly cooled sample shows a negative one. The sample with $x=0.5$ exhibits a ferromagnetic transition above room temperature and therefore, it shows strong anomalous Hall effect even at room temperature. In other samples with $x<1.0$, it is clearly seen that the magnitude of the Hall resistivity increases with increasing x. The x dependence is not clear for $x>1.0$ because we could not change the x value over a wide range for the samples with $x>1.0$. These results clearly show that the major charge carriers are holes for $x<1.0$, the concentration of which decreases with increasing x and finally changes its sign from positive to negative at $x=1.0$. Figure 1(b) shows the Hall resistivity for the samples with $y=0.95$ and 1.05, suggesting that the sign of the major charge carriers changes at $y=1.0$ from negative to positive with increasing y value; Al content y has an inverse contribution to the sign of major charge carriers compared to the V content, i.e., x. Thus the Hall resistivity at room temperature shows that this series of compounds has an energy gap or a psudogap and that the Fermi level crosses the gap around the Heusler composition, i.e., Fe:V:Al=2:1:1. The sign change with V content was theoretically predicted by Bansil *et al.*[11] for the Hausler-type disordered alloys $Fe_{3-x}V_xAl$; the Fermi energy E_F moves up relative to the pseudogap with the addition of V, rather than down as in a simple rigid-band picture.

B. $Fe_{1.98}V_{1.02}Al$ and quenched $Fe_{1.95}V_{1.05}Al$

In this series of intermetallic compounds anomalous Hall effects were observed. One example is that of $Fe_{2.5}V_{0.5}Al$ shown in Fig. 1. Another example is shown later in Fig. 3 for the quenched $Fe_{1.95}V_{1.05}Al$. The details of the anomalous Hall effects will be reported in a separate paper. These anomalous Hall effects are closely related to the magnetism and prohibit an accurate estimation of the normal Hall effect. Unfortunately all of the samples with $x \leqq 1.0$ show the anomalous Hall effects at low temperatures. In this paper we report the temperature dependence of Hall coefficient for $Fe_{1.98}V_{1.02}Al$ and quenched $Fe_{1.95}V_{1.05}Al$. The former sample did not show the anomalous Hall effect down to 5 K and in the latter sample it is relatively weak compared to this effect in the samples with Fe-rich compositions. Therefore we can investigate the behavior of Hall coefficient down to low temperatures for these compounds. Another reason why we chose these two samples is that they show very different behavior in electrical resistivity. For these reasons we minutely investigated the transport properties in these two compounds. We refer to $Fe_{1.98}V_{1.02}Al$ as V1.02 and the quenched $Fe_{1.95}V_{1.05}Al$ as the quenched V1.05 hereafter.

Figure 2 shows the electrical resistivity for the two compounds. The resistivity of V1.02 is much smaller than that for the quenched V1.05 and exhibits one maximum around 260 K and one minimum around 55 K. By contrast, the resistivity of the quenched V1.05 is semiconducting through the whole temperature range. It should be noted that the temperature dependence of the quenched V1.05 does not seem to be that of a semiconductor with a single energy gap; it is characterized by a steep rise below about 50 K but a somewhat weaker temperature dependence at higher temperatures.

Figure 3 shows the value of $-v/(e\mathbf{R}_H)$ as a function of temperature, where v, e, and $\mathbf{R}_H$ are the volume of the unit cell, the electron charge and the Hall coefficient, respec-

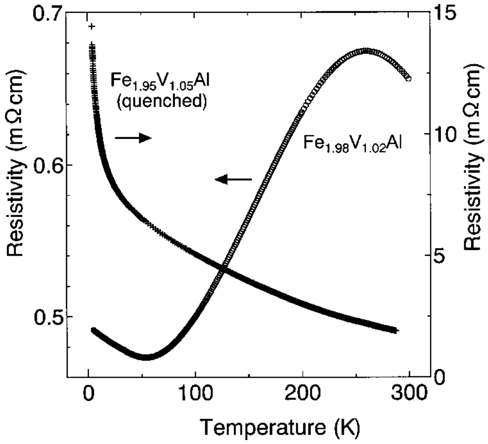

FIG. 2. Electrical resistivity as a function of temperature for Fe$_{1.95}$V$_{1.05}$Al and Fe$_{1.98}$V$_{1.02}$Al.

tively. In the case where the charge carriers consist of only electrons, this value represents the number of electrons in a unit cell. The lattice constant used for obtaining the unit cell volume is that of Fe$_2$Val: $a = 5.77$ Å. The inset in Fig. 3 shows the Hall resistivity as a function of magnetic field at 5 K. The Hall resistivity of V1.02 exhibits a linear dependence on magnetic field while that of the quenched V1.05 shows an anomalous Hall effect. Owing to this anomalous Hall effect we could not obtain the normal Hall coefficients for the quenched V1.05 below about 20 K. The temperature dependence of $-v/(e\mathbf{R}_H)$ has two characteristic features: a rapid increase at higher temperatures but a weak temperature dependence at lower temperatures. These two features are common to both compounds. It should be noted that the value of $-v/(e\mathbf{R}_H)$ for V1.02 approaches a constant value at low temperatures. This tendency is also observed in the quenched V1.05 although the data for this sample is lacking below 20 K owing to the anomalous Hall effect. The temperature coefficient of V1.02 is smaller than that of the quenched V1.05 at low temperatures. This is probably the evidence that the carrier density of V1.02 at the ground state is larger than that of the quenched V1.05 as discussed later.

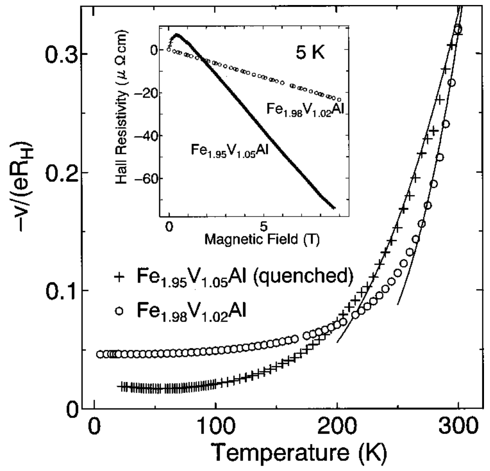

FIG. 3. $v/(e\mathbf{R}_H)$ as a function of temperature for Fe$_{1.98}$V$_{1.02}$Al and quenched Fe$_{1.95}$V$_{1.05}$Al. $v/(e\mathbf{R}_H)$ approximately represents the carrier density multiplied by a constant value. See the text for an explanation of the fitted curve.

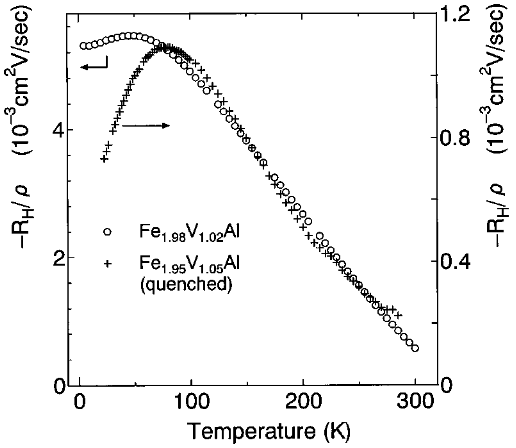

FIG. 4. $\mathbf{R}_H/\rho$ as a function of temperature for Fe$_{1.98}$V$_{1.02}$Al and quenched Fe$_{1.95}$V$_{1.05}$Al. $\mathbf{R}_H/\rho$ approximately represents the mobility of the carrier multiplied by a constant value.

We plot the value of $-\mathbf{R}_H/\rho$ as a function of temperature in Fig. 4. The value of $-\mathbf{R}_H/\rho$ corresponds to the mobility μ in the case of free electrons. The magnitude of $-\mathbf{R}_H/\rho$ is almost one order different between the two compounds, but the essential temperature dependence is basically the same; it increases with decreasing temperature, becomes a maximum and then decreases below a certain temperature T_m.

Figures 5(a) and 5(b) show the magnetoresistance for V1.02 and V1.05, respectively. Both of the magnetoresistances are negative at low temperatures suggesting the presence of magnetic scattering. The magnitude of the negative magnetoresistance of V1.02 is one order smaller than that of V1.05 suggesting that the magnetic scattering of V1.02 is much smaller than that of V1.05. In V1.02 the magnitude of the negative magnetoresistance rapidly increases below about 30 K. On the other hand, the large negative magnetoresistance is observed below 40 K for the quenched V1.05. Thus the temperature range in which the negative magnetoresistance is observed agrees well with the temperature range where the value of $-\mathbf{R}_H/\rho$ shows a positive temperature coefficient (Fig. 4). Both compounds show the Curie-Weiss-like behavior in magnetic susceptibility but the magnitude of the magnetic susceptibility of V1.02 is much smaller than that of V1.05. Thus the magnitude of magnetic scattering is closely related to the Curie-Weiss-like behavior.

C. Discussion

The fact that the value of $-v/(e\mathbf{R}_H)$ approaches a constant value with decreasing temperature (Fig. 3) means that V1.02 does not have an energy gap. Considering that the sign of carriers changes around the Heusler composition Fe$_2$VAl (Fig. 1), we may conclude that V1.02 and the quenched V1.05 are semimetals. For the case where the charge carriers consist of holes and electrons, the Hall coefficient in the drift velocity approximation is[12]

$$\mathbf{R}_H = \frac{1}{e}\frac{p - nb^2}{(p + nb)^2}, \tag{1}$$

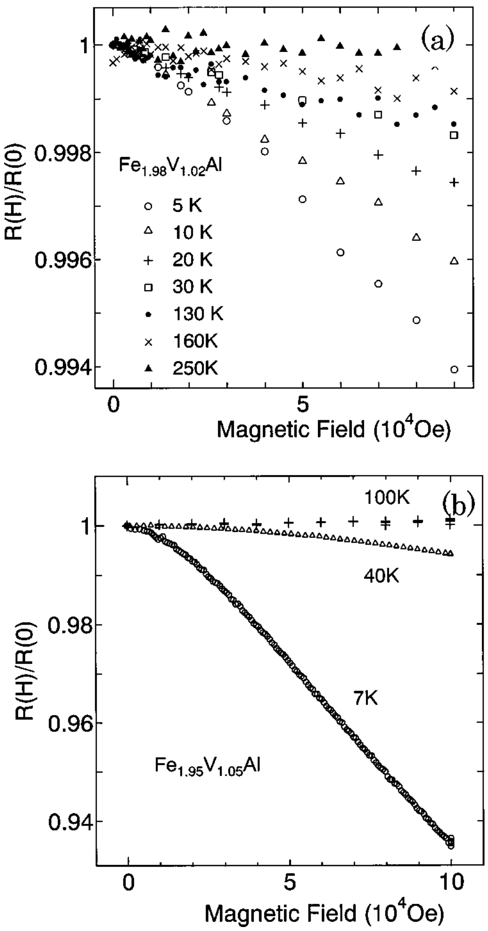

FIG. 5. Magnetoresistance for (a) $Fe_{1.98}V_{1.02}Al$ and (b) quenched $Fe_{1.95}V_{1.05}Al$.

where p, n, and b are the density of holes, the density of electrons and the ratio of the mobility of electrons to that of holes μ_e/μ_h, respectively. From this expression we may say that the value of $-v/(e\mathbf{R}_H)$ overestimates the real carrier density in the case that electrons and holes coexist. As shown in Fig. 3, the value of $-v/(e\mathbf{R}_H)$ is less than 0.1 in the ground state suggesting that the carrier number per unit cell is far less than unity confirming the earlier conclusion that these compounds are semimetals. The strong temperature dependence at higher temperatures suggests that there is a conduction band with larger density of states above a certain energy separation.

Here we compare the values of the Hall coefficient with those estimated from the band calculations. According to the local spin density approximation calculation carried out by Singh and Mazin,[9] the density of electrons is 0.012 electrons f.u., compensated by an equal number of holes in the stoichiometric compound Fe_2VAl. The effective mass for the hole band (m_h) and that for the electron band (m_e) are $\sim 0.5m_{\mathrm{bare}}$ and $\sim 0.31m_{\mathrm{bare}}$, respectively, where m_{bare} is the bare electron mass. We substitute the value of m_h/m_e for an approximate value of b in Eq. (1) assuming that the scattering probability is same between holes and electrons. Thus we obtain $-v/(e\mathbf{R}_H)\sim 0.05$. On the other hand, Weht and Pickett[8] obtained smaller density of electrons of 2.9 $\times 10^{-3}$/f.u. (and same amount of holes) by making generalized gradient corrections to the local density band structure. They also give an effective mass $\sim m_{\mathrm{bare}}$ for holes and $\sim 0.41m_{\mathrm{bare}}$ for electrons. With these values we obtain $-v/(e\mathbf{R}_H)\sim 0.007$. These values estimated from the band calculations are in fairly good agreement with those in Fig. 3. Thus real carrier density is speculated to be $\sim$0.01 or less in Fe_2VAl.

In the case of semimetals, there is no energy gap between a hole band and an electron band. Consequently holes and electrons are thermally generated even at low temperatures. Thus the carrier density in semimetals may gradually increase with increasing temperature even at low temperatures. However, the temperature coefficient would depend on the magnitude of the overlap between the hole band and the electron band. For example, if the overlap is large enough, the number of thermally activated carriers is small compared to that at the ground state and hence the temperature dependence is expected to be small in this case. The V1.02 shows weaker temperature dependence than the quenched V1.05 at low temperatures as shown in Fig. 3. This difference suggests that the carrier density in V1.02 is larger than that in the quenched V1.05, which is consistent with the result that the magnitude of resistivity of V1.02 is almost one order smaller than that of the quenched V1.05 (Fig. 2).

We cannot explain the steep rise of $-v/(e\mathbf{R}_H)$ above about 200 K in Fig. 3 if we assume a simple semi-metal situation in which only two parabolic energy bands overlap each other. We must consider other energy bands which are separated by a certain energy gap, i.e., pseudogap, to explain the steep rise at high temperatures. Here we assume a simple formula to describe the temperature dependence of carrier density n and p:

$$n(T)=n_0(T)+n_1T^{3/2}\exp(-E_g/2k_BT),$$

$$p(T)=p_0(T)+p_1T^{3/2}\exp(-E_g/2k_BT). \tag{2}$$

The first terms n_0 and p_0 express the low energy excitation around the Fermi energy. The temperature dependence of these terms are expected to be weak. The second terms express the thermal activation across the pseudogap, where we assume that holes and electrons have the same activation energy. This assumption would be correct if the electronic structure is symmetric with respect to the Fermi energy. At low temperatures, the first terms n_0 and p_0 would dominate the other terms while the second terms would become dominant at higher temperatures. Here we ignore the first terms n_0 and p_0 to roughly estimate the value of E_g. With this assumption, the value of $-v/(e\mathbf{R}_H)$ is proportional to $T^{3/2}\exp(-E_g/2k_BT)$ from Eq. (1). We can fit the data at higher temperatures using this expression. The result of data fitting is shown in Fig. 3. The fit is not very good owing to the excessively simplified model used for fitting. The deduced values for E_g are 0.14 eV for the quenched V1.05 and 0.26 eV for V1.02. We need the data above room temperature to evaluate the value of E_g more precisely. The magnitude of the psuedogap for Fe_2VAl has been reported to be 0.1 eV from electrical resistivity[1] and 0.27 eV from NMR measurement.[8] The values estimated in this study are consistent with these previous results.

The temperature dependence of the electrical resistivity is very different for V1.02 and the quenched V1.05, although the behavior of $-v/(e\mathbf{R}_H)$ is very similar. Here we seek the causes which make the difference. The electrical resistivity is expressed as

$$\rho=\frac{1}{e(n\mu_e+p\mu_h)}. \tag{3}$$

From Eqs. (1) and (3), $-\mathbf{R}_H/\rho$ is written as

$$-\mathbf{R}_H/\rho=\mu\frac{n-p}{n+p}, \tag{4}$$

where we assume $\mu_e=\mu_h=\mu$. From Eq. (2) and above discussion, at low temperatures, we obtain $-\mathbf{R}_H/\rho\approx\mu(n_0-p_0)/(n_0+p_0)$. The mobility μ should have temperature dependence. However, as discussed before, the values of p_0 and n_0 are also expected to have weak temperature dependence although they approach constant values in the ground state. Therefore, the variation of $-\mathbf{R}_H/\rho$ may reflect both temperature dependences. In the special case where p_0 and n_0 have the same temperature dependence, the temperature dependent factor would cancel out and $-\mathbf{R}_H/\rho$ would show the temperature dependence of μ except for a constant factor at low temperatures. Since the terms p_0 and n_0 may be expected to have almost the same temperature dependence, we may expect that the temperature dependence of the term $(n_0-p_0)/(n_0+p_0)$ is weak. At least this term would approach a constant value at low temperatures since both n_0 and p_0 should approach constant values. As shown in Fig. 4, the value of $-\mathbf{R}_H/\rho$ of the quenched V1.05 exhibits strong temperature dependence even at the lowest temperatures. Therefore, for the quenched V1.05, we conclude that the temperature dependence below T_m may be attributed to that of the mobility μ. On the other hand, the value for V1.02 shows weaker temperature dependence below T_m. However, we attribute the drop of $-\mathbf{R}_H/\rho$ value in V1.02 to the mobility μ to consistently explain the magnetoresistance and resistivity behavior as explained later. At high temperatures we ignore the term p_0 and n_0 and obtain $-\mathbf{R}_H/\rho\approx\mu(n_1-p_1)/(n_1+p_1)$ from Eqs. (2) and (4). Thus, with this approximation, the value of $-\mathbf{R}_H/\rho$ is equal to the value of μ multiplied by a constant value which is smaller than unity. Therefore we may consider that the $-\mathbf{R}_H/\rho$ at higher temperatures in Fig. 4 reflects the temperature dependence of the mobility. Above 100 K the mobility decreases as increasing temperature. This behavior may be attributed to phonon scattering although the characteristic T^{-1} dependence was not observed. The reason for the absence of T^{-1} dependence is not clear at the present, but we suspect that the mobility may be changing as the characters of the charge carriers change from those within the pseudogap to those thermally excited outside the pseudogap.

The magnitude of the negative magnetoresistance rapidly increases with decreasing temperature below 30 K for V1.02 and below 40 K for the quenched V1.05. The magnitude in V1.02 is almost one order smaller than that for the quenched V1.05. The negative magnetoresistance is considered as the evidence of strong magnetic scattering which may decrease the mobility of charge carriers. Thus the decrease of $-\mathbf{R}_H/\rho$ value shown in Fig. 4 is consistently explained that the mobility decreases because of the magnetic scattering. In conclusion the mobility of charge carriers forms a maximum at 50–80 K due to a crossover between the phonon scattering and the magnetic scattering; the scattering mechanism is considered to be basically the same for both samples.

The resistivity is a function of both mobility and carrier density as shown in the Eq. (3). It should be emphasized that the essential features of both carrier density and mobility are the same for both V1.02 and the quenched V1.05 as shown in Figs. 3 and 4 regardless of the large apparent differences in the resistivity behavior. The steep rise of resistivity at low temperatures observed in the quenched V1.05 (Fig. 2) is not owing to an energy gap but due to a temperature-dependent magnetic scattering while the negative temperature coefficient of resistivity observed above 100 K is due to a pseudogap of more than 1500 K. In this sample the shift from the former temperature region to the latter one is so smooth that the boundary is not so clear. In V1.02 the upturn of the resistivity at low temperatures is owing to the magnetic scattering and the negative temperature coefficient of resistivity above the resistivity maximum is due to the pseudogap. The positive temperature coefficient between these two temperature regions is attributable to the phonon scattering. A cusp of resistivity has been observed at the Curie temperature in this series of compounds.[1–3] From our results this is probably owing to a suppression of the magnetic scattering. We speculate that the semiconducting behavior at high temperatures generally observed in $\mathrm{Fe}_{3-x}\mathrm{V}_x\mathrm{Al}_y$ could be attributed to the pseudogap.

In $\mathrm{Fe_2VAl}$ the Curie-Weiss-like magnetic behavior has been considered to originate from the Fe clusters.[6–8] The Fe clusters are imperfections in the crystal lattice, such as substitution of Fe for V sites. There is a correlation between the negative magnetoresistance and the Curie-Weiss-like magnetic susceptibility suggesting that the Fe clusters cause the strong magnetic scattering. It is interesting that the small amount of defects have great influences on the transport properties. Unfortunately the detailed properties of the magnetic clusters are not clear so far. Investigations on the magnetic clusters are necessary to fully understand the transport properties.

In summary, we have shown, first, that the sign of major charge carriers changes at the Heusler composition with respect to both V and Al contents. Secondly, we revealed, for V1.02 and quenched V1.05, that the density of charge carriers rapidly decreases with decreasing temperature, but finally approaches a constant value at low temperatures. The carrier number per unit cell was considered much less than unity. These results clearly show that these compounds are semimetal with a pseudogap as expected with band calculations. The electrical resistivity of the quenched V1.05 shows negative temperature dependence through the whole temperature range while that of V1.02, by contrast, shows one minimum and one maximum. However, we found that the essential mechanisms are the same for the two compounds; both sets of results can be attributed to three factors: a pseudogap, phonon scattering and magnetic scattering. It should be noted that the rise of resistivity at low temperatures is not owing to an energy gap, but due to magnetic scattering while the negative temperature coefficient at high temperatures is attributable to pseudogap. Thus these compounds are *magnetic* semimetals with a pseudogap. It is necessary to investigate the mechanism of magnetic scattering to fully understand the transport properties.

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