



HAL
open science

Recent results at the metal-insulator transition of icosahedral AlPdRe

Östen Rapp, Veeturi Srinivas, Joe Poon

► **To cite this version:**

Östen Rapp, Veeturi Srinivas, Joe Poon. Recent results at the metal-insulator transition of icosahedral AlPdRe. *Philosophical Magazine*, 2005, 86 (03-05), pp.655-661. 10.1080/14786430500311758 . hal-00513605

HAL Id: hal-00513605

<https://hal.science/hal-00513605>

Submitted on 1 Sep 2010

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.



Recent results at the metal-insulator transition of icosahedral AIPdRe

Journal:	<i>Philosophical Magazine & Philosophical Magazine Letters</i>
Manuscript ID:	TPHM-05-May-0148.R1
Journal Selection:	Philosophical Magazine
Date Submitted by the Author:	12-Jul-2005
Complete List of Authors:	Rapp, Östen; KTH, Solid State Physics Srinivas, Veeturi; Indian Inst Technology, Physics Poon, Joe; Univ of Virginia, Physics
Keywords:	metal insulator transitions, electronic transport
Keywords (user supplied):	icosahedral AIPdRe, semiconductor-like scaling



Recent results at the metal-insulator transition of icosahedral AlPdRe

Ö. RAPP* §, V. SRINIVAS ¶ and S. J. POON ‡

§Solid State Physics, KTH-Electrum 229, 164 40 Stockholm-Kista, Sweden

¶ Department of Physics and Meteorology, Indian Inst. of Technoloy, Kharagpur 721302 India

‡Department of Physics, University of Virginia, Charlottesville Virginia 22901, USA

The metal-insulator transition, MIT, in icosahedral AlPdRe has been studied from measurements of magnetoresistance and conductivity. Results for the localization length ξ , the characteristic hopping temperature T_0 and their relations at the MIT are discussed. The results indicate important similarities between i-AlPdRe and doped semiconducors.

Key words: icosahedral AlPdRe,
metal-insulator transition,
electronic transport,
semiconductor-like scaling

1. Problems

Although the occurrence of a metal-insulator transition, MIT, in icosahedral (i) AlPdRe has been supported by a number of different experiments, it has remained a somewhat elusive phenomenon due in particular to the unusual and hitherto unexplained electronic transport properties at temperatures below 1 K. One problem is the apparent finite zero temperature conductivity $\sigma(0)$ also in insulators [1-3], which has been found to decrease exponentially into the insulating side [4]. Another problem is that the B^2 region in the magnetoresistance, MR, which is due to shrinking wave functions in variable range hopping (VRH) theories, is displaced with decreasing temperatures towards smaller magnetic fields. This contribution, and the negative component of the MR from interference between forward scattering events [5] become unobservable at temperatures below 1 K. The MR in this temperature region is not understood. On the other hand, if one limits analyses to the temperature dependence of the conductivity one is faced with an expression of the form

$$\sigma(T) = \sigma(0) + \sigma_0 \exp(-[T_0 / T]^\nu) \quad (1).$$

T_0 is a characteristic temperature for the hopping process, and ν is 1/4 for Mott VRH and 1/2 for Efros-Shklovskii VRH. When any temperature dependence of σ_0 in the VRH-term is neglected, and the value of ν is unknown, Eq (1) has 4 free parameters. This is too flexible for a smooth function, and such results for T_0 have not turned out to be reliable.

A third problem is that the nature of a driving parameter for the MIT is not clarified. In samples of the same nominal composition of $\text{Al}_{70.5}\text{Pd}_{21}\text{Re}_{8.5}$ which are phase pure in standard X-ray diffraction, one can produce widely different electronic properties by different annealing conditions. E.g., the resistance ratio $R = \rho(4.2 \text{ K}) / \rho(295 \text{ K})$ can vary from 2 to 300 encompassing an MIT. It is not known which is the relevant effect on the electronic structure. Although R is an empirical parameter which is not accurately controlled in sample preparation, it has nevertheless been useful for characterizing quasicrystals, and since a decade for correlating transport properties [6]. Justification for such a procedure is strengthened by the observation that changes in R in a single AlPdRe sample

can be monitored by neutron irradiation over a range of R -values which encompasses the MIT [7].

In this contribution we use a recently developed method [8] to circumvent some of the problems mentioned. Results for T_0 , and the localization length ξ , and their relations to R and an estimated charge density as driving parameters are discussed for a series of i- $\text{Al}_{70.5}\text{Pd}_{21}\text{Re}_{8.5}$ samples.

2. Method to extract information on T_0 and ξ

To evaluate parameters at the MIT from electronic transport data for i-AlPdRe, one first determines the exponent ν of the VRH expression for $\sigma(T)$, and estimates $\sigma(0)$. This eliminates two parameters in Eq (1), and T_0 can be determined from $\sigma(T)$ in a single parameter fit. ξ is then calculated from the MR.

The magnetoresistance in the B^2 region follows $\Delta\rho(B,T)/\rho(0,T) \cong +B^2/B_0^2$. Here B_0 is the field for which one flux quantum, $\phi_0=e/h$, passes through the interference area $(r^3\xi)^{1/2}$. r is the hopping distance, which for Mott VRH is given by $r_M \sim \xi(T_0/T)^{1/4}$ and for ES VRH by $r_{ES} \sim \xi(T_0/T)^{1/2}$. The

MR in the B^2 region then becomes

$$\left[\frac{\Delta\rho(B,T)}{\rho(0,T)}\right]_M \approx c_M (e/\hbar)^2 \xi^4 T_0^{-3/4} B^2 T^{-3/4} \quad (2a), \quad \left[\frac{\Delta\rho(B,T)}{\rho(0,T)}\right]_{ES} \approx c_{ES} (e/\hbar)^2 \xi^4 T_0^{3/2} B^2 T^{-3/2} \quad (2b).$$

for Mott and ES VRH respectively. For ES VRH the constant was found to be $c_{ES}=0.0015$ [5]. We use this value to obtain an estimates of ξ . Numerical constants in VRH theories are often uncertain, which affects actual values of parameters. In the present case however, errors in ξ are much reduced due to the power of 4 in Eq (2). Furthermore, the main results in the paper are not affected, since they are obtained from slopes in double logarithmic diagrams.

Panel a) of Fig. 1, shows the T-dependence of $\Delta\rho(B,T)/\rho(0,T)$ at constant B in the B^2 region of an $R=220$ sample. ES-VRH in the B^2 region is obeyed over a temperature range which decreases with increasing B , since for large B the magnetic length $\ell_B = \sqrt{\hbar/eB}$ will violate the condition $\ell_B > \xi$. This is accompanied by a gradual cross-over from a B^2 region into a $B^{2/3}$ behavior [5], observed at low temperatures and high fields [9]. Deviations are also seen in the left end of Fig 1 a), where for increasing T , one approaches the region of the initial negative magnetoresistance.

1
2 Similar observations have been made for all $\text{Al}_{70.5}\text{Pd}_{21}\text{Re}_{8.5}$ samples studied by us.

3
4 By restricting measurements to the temperature range 1-10 K the problems with $\sigma(T)$ and MR at

5
6 -4-

7
8
9
10 lower temperatures are avoided. $\sigma(0)$ was taken from measurements to below 15 mK [9].

11
12
13 [Insert Fig 1 about here]

14 15 16 17 18 **3. Results for T_0 and ξ**

19
20 A sample $R=160$ was previously excluded in analyses [8]. $\log[\sigma(T)-\sigma(0)]$ vs $T^{-1/2}$ in this case is
21 described by a straight line over a much reduced range of conductivity variations compared to
22 other samples. However, using the constraints that such a fit should be limited to the range of the
23 MR measurements, 1-10 K, and must not extend above a temperature T^{\max} well below T_0 , limited
24 errors are nevertheless found. The full line in Fig. 1 b) illustrates a best fit to data with $T_0=24.8$ K.
25 The dashed line gives $T_0=21.4$ K. In both cases T^{\max}/T_0 is about 0.3. An error bar of $\pm 15\%$ has
26 been marked for this datum in subsequent graphs.

27
28 Analyses of measurement results were made in regions where $T < T_0$. In the relation r_{ES}
29 $\sim \xi(T_0/T)^{1/2}$ given above, one then finds $r_{\text{ES}} > \xi$, in qualitative agreement with a basic condition for
30 variable range hopping. It can be noted however, that with the more restrictive relation $r_{\text{ES}} = 0.25$
31 $\xi(T_0/T)^{1/2}$, this condition is not fulfilled in all cases. As mentioned, numerical coefficients in the
32 ES model may be uncertain. This problem merits further investigations. It is not unique for
33 quasicrystals but has been frequently observed also in doped semiconductors [10].

34
35 T_0 as a function of R is shown in Fig. 2a). It is seen to increase slightly slower than linearly into
36 the insulator. In this figure, no assumption has been made about a value R_c of R at the MIT, nor
37 has any quantitative information from the magnetoresistance been used. A linear extrapolation of
38 data to $T_0 = 0$ K would suggest a lower limit of $R_c \approx 10$. From the magnetoresistance results,
39 quoted in Ref. [8], a more plausible value is $R_c \approx 20$ K.

40
41 From T_0 and the slopes of the straight lines in Fig 1a, ξ can be calculated from Eq. (2b). In
42 practise, accuracy is improved by evaluating instead the temperature dependence of the slope of
43 $\Delta\rho/\rho$ vs B^2 . In all measurements, the results for ξ and T_0 were evaluated at temperatures and

magnetic fields where the forms of Eqs (1) and (2b) were obeyed. The magnetoresistance of the R=160 sample has been described previously [11].

-5-

$T_o(\xi)$ is shown in Fig 2b) on the form T_o vs ξ^{-1} , in order to compare with the relation

$$T_o = \frac{const}{N(\epsilon_F)\xi^3} \quad (3).$$

[Insert Fig 2 about here]

Eq (3) is often used with a constant density of states $N(\epsilon_F)$. However, it is seen from Fig. 2 b) that T_o increases more slowly than ξ^{-3} into the insulator, and rather as $\xi^{-2.6}$. Eq (3) and this result thus suggest that in addition to the decrease of ξ into the insulator, there is a contribution to the increase of T_o from a slow decrease of $N(\epsilon_F)$. Independent evidence for such a decrease of $N(\epsilon_F)$ is obtained from the observation for quasicrystals that $N(\epsilon_F)$ from the specific heat decreases as the slowly decreasing $1/\sqrt{\rho(295K)}$ into the insulator [12,13]. In the latter of these references this correlation included also i-AlPdRe.

It is also interesting to note that the exponent of ξ of -2.6 in Fig 2b is close to -8/3. When the second derivative, β , of the MR with respect to B^2 and $T^{-3/2}$ is the same for all samples, one finds from Eq 2b that $T_o \sim \xi^{-8/3}$. This was found previously [8] with β within 10% of $0.0167 T^{-2} K^{3/2}$.

The R=160 sample again falls somewhat outside this behavior with a 20% smaller β . The general trend of the results is not affected by this discrepancy.

4 Comparison with doped semiconductors

To compare with doped semiconductors it is preferable to transform R to a driving parameter related to charge density n . Although there is no straightforward experimental control, as in semiconductors, of a charge density, we assume that the change of n can nevertheless be estimated in a similar way. With n_c the value of n at the MIT, taken to occur at $R_c = 20$ [8], we then take

$$\frac{n(R)}{n_c(R=20)} = \frac{\sigma(R, 295K)}{\sigma(20, 295K)} \quad (4).$$

1
2
3
4
5
6
7
8
9
10
11
12
13
14
15
16
17
18
19
20
21
22
23
24
25
26
27
28
29
30
31
32
33
34
35
36
37
38
39
40
41
42
43
44
45
46
47
48
49
50
51
52
53
54
55
56
57
58
59
60

-6-

In this equation any R dependence in the relaxation time, $\tau(295\text{K})$, has been neglected, and this relation is therefore approximate. Nevertheless, this approach is related to methods often used for doped semiconductors, where e.g. R is used for calibration of the charge scale n [14,15].

On ingot samples in the form of parallelepipeds cut from ingots, the dimensions were carefully determined under microscope, with corrections applied for voids in the samples [16], likely reducing the experimental error in n to below 5%.

The critical behavior of T_0 and ξ as a function of $1-n/n_c$ is shown in Fig 3. T_0 follows a relation $T_0 \sim [1-n/n_c]^{1.2}$ while for ξ we find $\xi \sim [1-n/n_c]^{-0.46}$. For T_0 the exponent is significantly smaller than 2.0 obtained with similar methods from $\sigma(T)$ and MR of GaAs doped by neutron irradiation [17]. Our result for the exponent γ of ξ is close to $-1/2$. For GaAs, γ was found to be -0.6 [17].

[Insert Fig 3 about here]

In doped semiconductors, a common result for the exponent, μ , of the vanishing zero temperature conductivity on the metallic side is $1/2$. In 3-D scaling one expects $\gamma = -\mu$, since the conductivity then scales as the inverse of a characteristic length. Furthermore, critical exponents are expected to be the same on both sides of a phase transition. One can hence compare the localization length on the insulating side of $i\text{-AlPdRe}$ with the conductivity of doped semiconductors on the metallic side.

The similarity between these exponents in $i\text{-AlPdRe}$ and a large class of semiconductors suggests that the MIT of $i\text{-AlPdRe}$ is of the same universality class as for doped semiconductors. This confirms a disorder driven MIT in $i\text{-AlPdRe}$, long expected from transport results on the metallic side [18,19].

Theoretically disorder in quasicrystals has been studied in various different models. Burkov et al

1
2 introduced a fractional multicomponent Fermi surface in a model for real dirty quasicrystals, and
3
4 found that some general properties of quasicrystals could be described [20]. Olenev et al
5
6 calculated electron spectra and wave functions in a tight binding approximation on a model
7
8 structure
9

10
11
12
13
14
15 -7-
16
17

18
19 corresponding to a three dimensional analogue of the Penrose tiling [21]. It was found that
20
21 disorder

22 led to a tendency for electron localization. These models focussed on general quasicrystalline
23
24 properties. Experimentally it is now known that a metal-insulator transition has not been observed
25
26 in other quasicrystals besides i-AlPdRe. In a recent investigation, using local-density-functional
27
28 techniques to calculate ab-initio electronic structures for a series of quasicrystalline
29
30 approximants to i-AlPdRe, it was suggested that substitutional disorder would create localized
31
32 states in a semiconducting band gap [22]. Our finding that i-AlPdRe is semiconductor-like is
33
34 consistent with these results. The failure to observe a gap in real i-AlPdRe would in this picture be
35
36 due to disorder induced localized states filling the band gap.
37
38

39 40 41 **5. Brief conclusions.**

42
43 The scheme described for evaluating parameters at the MIT in i-AlPdRe from electrical transport
44
45 results appears to be fairly robust with respect to deviations in properties which occur between
46
47 different samples. Results for T_0 and ξ in the vicinity of the MIT have been illustrated. The
48
49 divergence of ξ suggests that the MIT of i-AlPdRe is semiconductor like.
50
51
52
53
54
55
56
57
58
59
60

References

- [1] Q. Guo and S. J. Poon, Phys. Rev. B **54**, 12793 (1996).
- [2] M. Rodmar, F. Zavaliche, S.J. Poon, and Ö. Rapp, Phys. Rev. B **60**, 10807 (1999).
- [3] T.I. Su, C.R. Wang, S.T. Lin, and R. Rosenbaum, Phys. Rev. B **66**, 54438 (2002).
- [4] Ö. Rapp, V. Srinivas, P. Nordblad, and S. J. Poon, J. Non Cryst. Solids **334&335**, 356 (2004).
- [5] B.I. Shklovskii and B.Z. Spivak, in *Hopping Transport in Solids*, edited by M. Pollak and B. Shklovskii, (North Holland, Amsterdam 1991), pp 271-348.
- [6] M. Ahlgren et al., Czechoslovak J Phys. **46**, 1989 (1996).
- [7] A. Karkin et al., Phys. Rev. B **66**, 92203 (2002).
- [8] Ö. Rapp, V. Srinivas, and S. J. Poon, Phys. Rev. B **71**, 12202 (2005).
- [9] V. Srinivas et al., Phys. Rev. B **65**, 94206 (2002).
- [10] E.g. T. G. Castner in Ref [5], pp 1-47.
- [11] V. Srinivas, M. Rodmar, S. J. Poon, and Ö. Rapp, Phys. Rev. B **63**, 172202 (2001).
- [12] U. Mizutani, J. Phys. Condens. Matter, **10**, 4609 (1998).
- [13] Ö. Rapp, in *Physical Properties of Quasicrystals* (edited by Z. M. Stadnik, Solid State Sciences, Vol 125, Springer, Berlin 1999), p. 127.
- [14] H. Stupp et al., Phys. Rev. Lett. **71**, 2634 (1993).
- [15] S. Bogdanovich, P. Dai, M. P. Sarachik, and V. Dobrosavljevic, Phys. Rev. Lett. **74**, 2543 (1995).
- [16] M. Rodmar et al., Phys. Rev. B **60**, 10807 (1999).
- [17] A. N. Ionov, I. S. Shlimak, and M. N. Matveev, Solid State Commun. **47**, 763 (1983).

- 1
2 [18] M. Rodmar, F. Zavaliche, S. J. Poon, and Ö. Rapp, Phys. Rev. B **61**, 2926 (2000).
3
4 [19]. J. Delahaye and C. Berger, Phys. Rev. B **64**, 94203 (2001).
5
6 [20] S. E. Burkov, A. A. Varlamov, and D. V. Livanov, Phys. Rev. B **53**, 11504 (1996).
7
8 [21] D. V. Olenov, E. I. Isaev, and Yu. Kh. Vekilov, JETP, Journal of Experimental and
9
10 Theoretical Physics **86**, 550 (1998).
11
12

13
14 -9-
15
16
17
18
19

- 20 [22] M. Krajč ^v i and J. Hafner, Phys. Rev. B **68**, 165202 (2003).
21
22
23
24
25
26
27
28
29
30
31
32
33
34
35
36
37
38
39
40
41
42
43
44
45
46
47
48
49
50
51
52
53
54
55
56
57
58
59
60

-10-

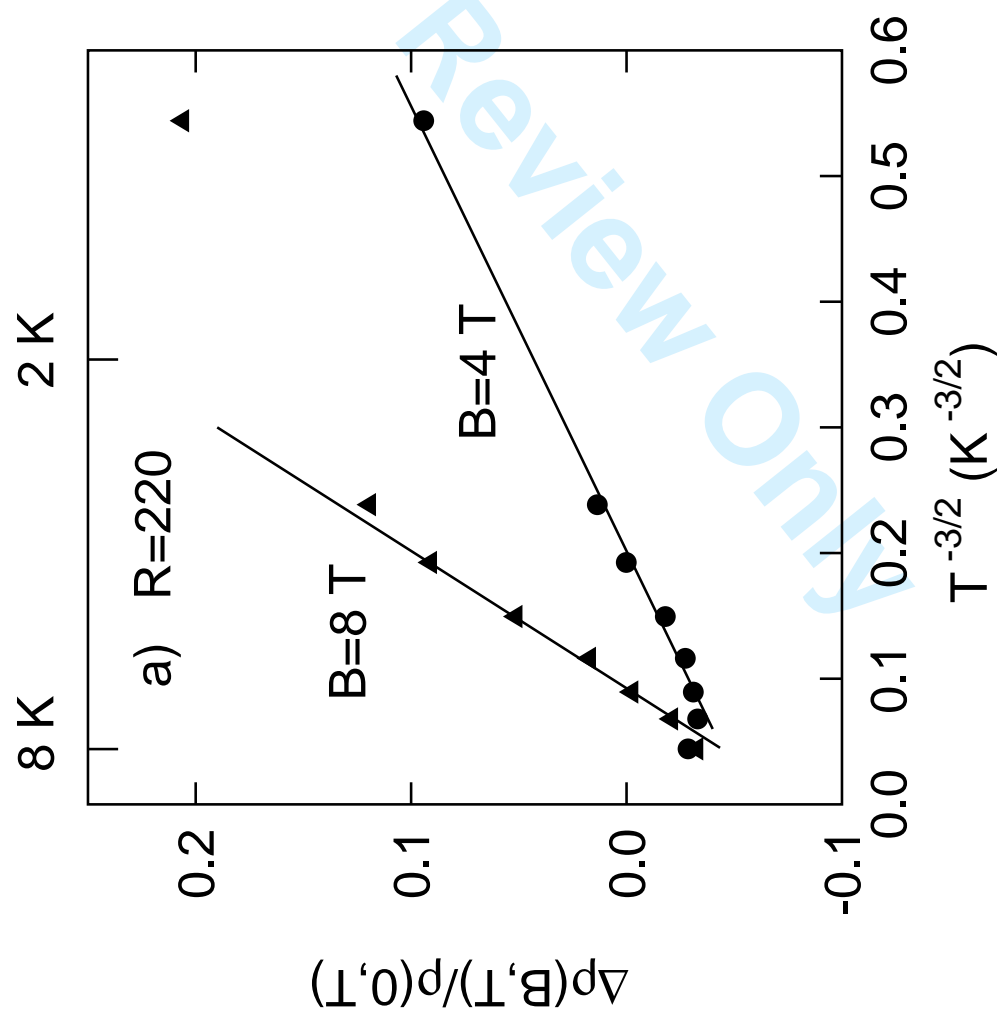
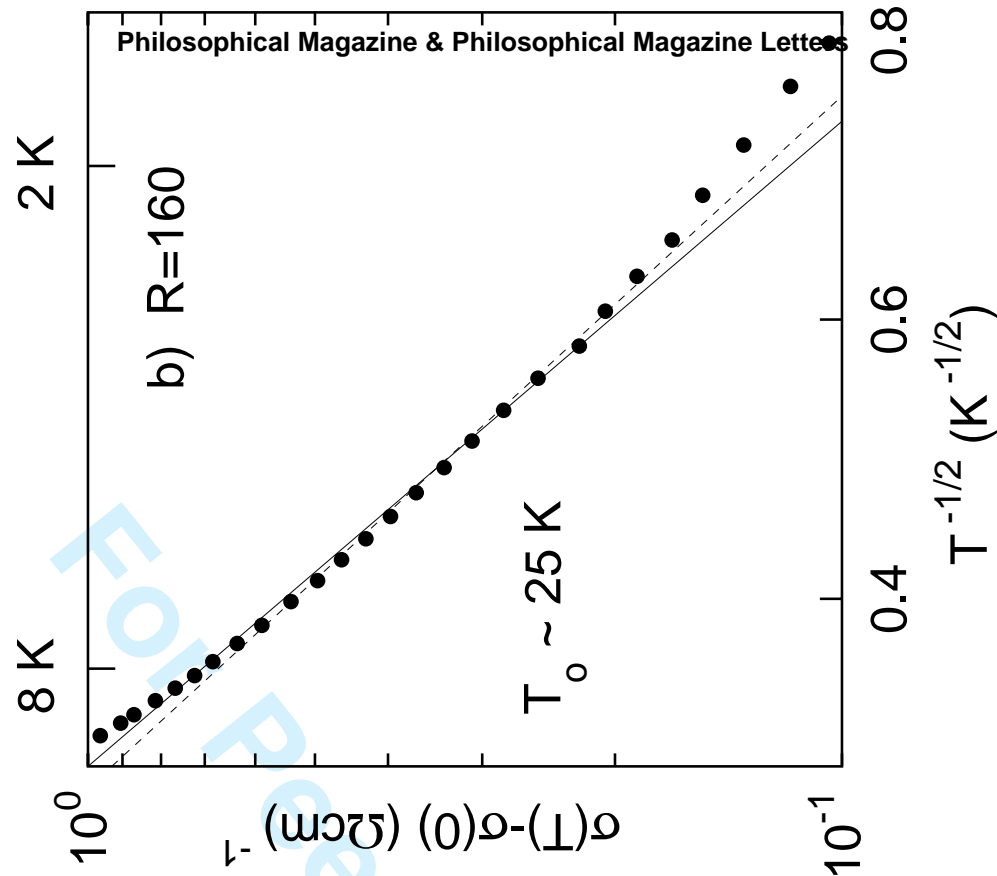
Legends

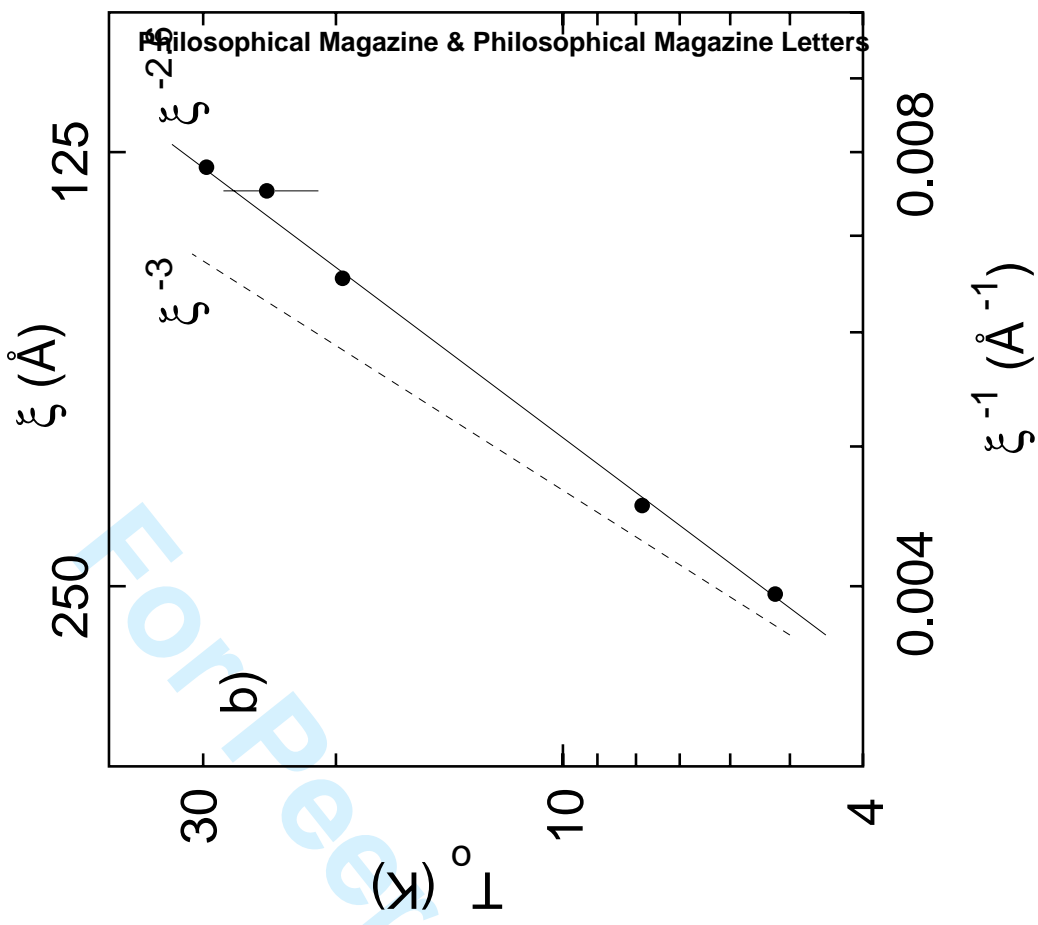
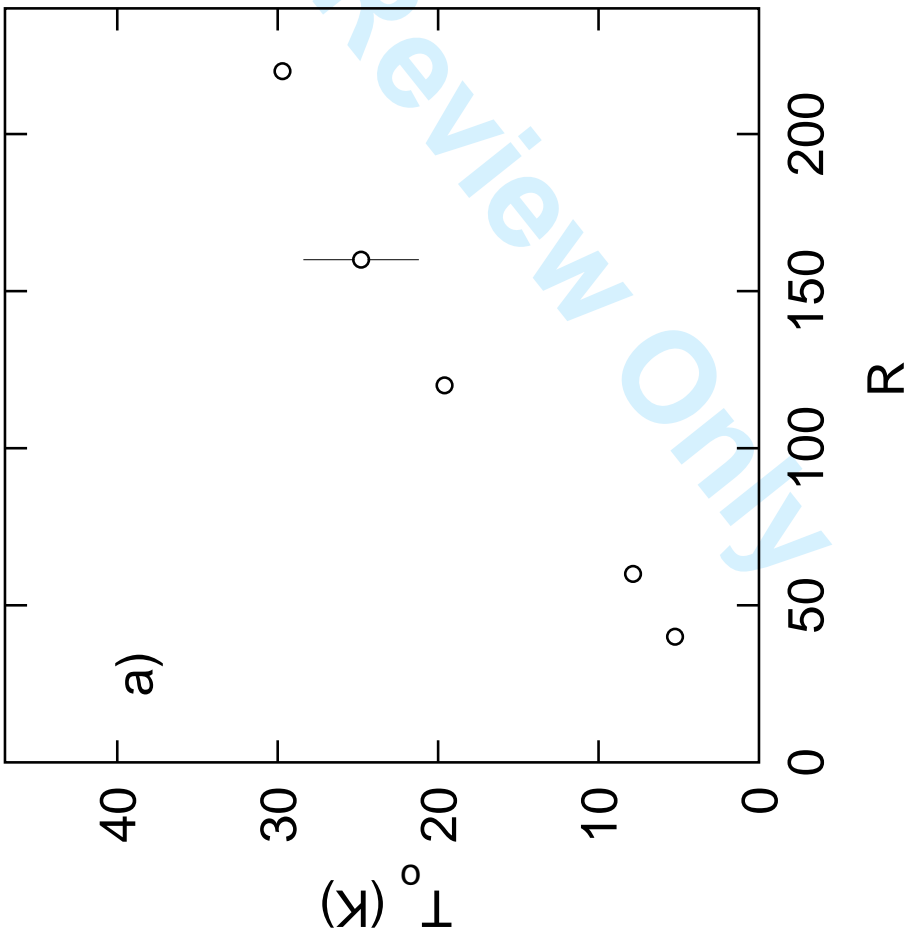
Fig. 1. Analyses to determine T_0 and ξ . Panel a); magnetoresistance in the B^2 region as a function of temperature at two constant magnetic fields. The $T^{-3/2}$ relation shows that VRH is of Efros Shklovskii type, Eq. (2b). Panel b) $\log[\sigma(T) - \sigma(0)]$ vs $T^{-1/2}$. T_0 is the only adjustable parameter. The range of $\sigma(T)$ fitted is smaller by a factor of three than found [8] for other AlPdRe samples, and T_0 is more uncertain. The full line gives $T_0=24.8$ K, the dashed line $T_0=21.2$ K.

Fig. 2. In both panels one moves into the insulator in the direction of the abscissa. Panel a); T_0 vs R . No assumption has been made about the location of the MIT where $T_0 \rightarrow 0$. Panel b); T_0 vs ξ^{-1} . [The R values of the samples are the same from left to right as in panel a)]. The dashed and full lines indicate different functions of ξ . Data are seen to obey $T_0 \sim \xi^{-2.6}$. This result and Eq (3) suggest an additional contribution to T_0 from a decrease of the density of states into the insulator.

Fig. 3. T_0 (open circles, left hand scale) and ξ (closed circles, right hand scale), vs $[1-n/n_c]$, measuring the distance to the MIT. The MIT is assumed to occur at $R_c=20$. n and n_c are estimated from Eq(4). The straight lines show $T_0 \sim [1-n/n_c]^{1.2}$ and $\xi \sim [1-n/n_c]^{-0.46}$.

1
2
3
4
5
6
7
8
9
10
11
12
13
14
15
16
17
18
19
20
21
22
23
24
25
26
27
28
29
30
31
32
33
34
35
36
37
38
39
40
41
42
43
44
45
46
47
48
49
50
51
52
53
54
55
56
57
58
59
60





1
2
3
4
5
6
7
8
9
10
11
12
13
14
15
16
17
18
19
20
21
22
23
24
25
26
27
28
29
30
31
32
33
34
35
36
37
38
39
40
41
42
43
44
45
46
47
48
49
50
51
52
53
54
55
56
57
58
59
60

1
2
3
4
5
6
7
8
9
10
11
12
13
14
15
16
17
18
19
20
21
22
23
24
25
26
27
28
29
30
31
32
33
34
35
36
37
38
39
40
41
42
43
44
45
46
47
48
49
50
51
52
53
54
55
56
57
58
59
60

