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1996 J. Phys.: Condens. Matter 8 L725

(http://iopscience.iop.org/0953-8984/8/49/002)

J. Phys.: Condens. Matter **8** (1996) L725–L730. Printed in the UK

LETTER TO THE EDITOR

The metal–insulator transition in quasicrystals

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Received 25 June 1996

Abstract. We have found that the metal–insulator transition can occur in Al–Pd–Re alloys on choosing the annealing conditions appropriately, and McMillan's scaling theory of the metal–insulator transition in amorphous materials can be applied to quasicrystals equally well. That is, the low-temperature conductivity on the metallic side of the metal–insulator transition varies as $\sigma(T) = \sigma_0(1 + \sqrt{T/\Delta})$, and the determined value of the correlation gap Δ, spanning about five orders of magnitude, is proportional to the inverse of the square of the zero-temperature resistivity ρ_0.

Great effort has been devoted to understanding the temperature dependence of the conductivity of quasicrystals (QCs) because of their peculiar properties exhibited at low and high temperatures. Although there is still no theory to be able to explain satisfactorily the temperature dependence of the conductivity at high temperatures ($T > 100$ K), the low-temperature conductivity of quasicrystals such as Al–Cu–(Fe, Ru, Os) [1, 2] and Al–Pd–Mn [3] can be interpreted well by quantum interference effects [4] including the effects of weak localization and electron–electron interactions. However, it is found recently that even quantum interference effects fail to explain the Al–Pd–Re QCs with conductivity $\sigma(4.2\ \text{K})$ as low as 0.4 Ω^{-1} cm^{-1} [5]. This suggests that the electrons in Al–Pd–Re QCs are more strongly localized than those in Al–Cu–(Fe, Ru, Os) and Al–Pd–Mn QCs.

In fact, some reports have shown that the zero-temperature conductivity σ_0 of some Al–Pd–Re alloys is almost equal to zero, indicating that these alloys are already insulators [6] and therefore their conductivity at low temperatures can be described by the variable-range hopping mechanism [7]. This leads us to ask the question: can the scaling theory of the metal–insulator (M–I) transition in amorphous materials be applied to quasicrystals, too?

In 1981 McMillan developed a scaling theory of the M–I transition in amorphous materials by taking into account of localization and correlation with screening on an equal footing and predicted the density of states at $T = 0$ on the metallic side of the M–I transition as [8]

$$N(E) = N(0)(1 + \sqrt{E/\Delta}) \tag{1}$$

where $N(0)$ is the density of states at the Fermi level and Δ is the electron correlation gap. At the M–I transition, Δ and $N(0)$ go to zero simultaneously and the gap begins to open up. Equation (1) has been confirmed by electron tunnelling experiments on amorphous

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0953-8984/96/490725+06$19.50

NbSi [9] and GeAu [10] and granular Al film [11]. The conductivity at finite temperature is predicted as

$$\sigma(T) = \sigma_0(1 + \sqrt{T/\Delta}) = \sigma_0 + m\sqrt{T}. \tag{2}$$

The $\sqrt{T}$ dependence of the conductivity is found in amorphous thin films such as FeSb [12], CrCe [13] and PtSi [14] and amorphous and disordered metals [15]. The values of Δ determined from both the conductivity and electron tunnelling data [14] span eight orders of magnitude. Δ is seen to vary as $\Delta \propto \sigma_0^2 = 1/\rho_0^2$. This differs from $\Delta \propto 1/\rho_0^3$ obtained from

$$\sigma(T) = \sigma_0 + (e^2/4\pi^2\hbar)(1.3/\sqrt{2})(\tfrac{4}{3} - \tfrac{3}{2}\tilde{F})\sqrt{T/\hbar D} \tag{3}$$

with a correction due to Coulomb interaction derived by Altshuler and Aronov based on a weak-coupling approximation [16]. $\tilde{F}$ and D in equation (3) are the screening parameter and electronic diffusion constant, respectively.

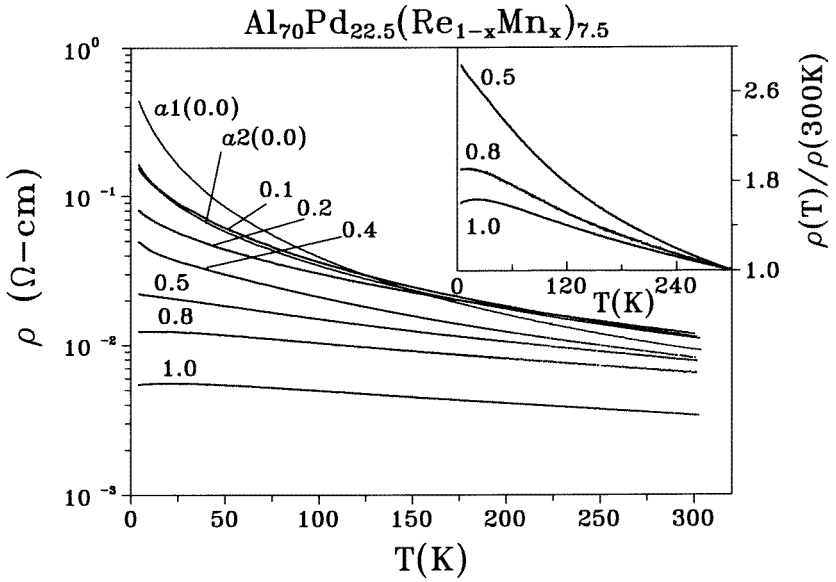

Figure 1. Temperature dependences of the resistivity in the icosahedral $Al_{70}Pd_{22.5}(Re_{1-x}Mn_x)_{7.5}$ ($0.0 \leqslant x \leqslant 1.0$) QCs. '$a2(0.0)$' and '$a1(0.0)$' are samples with $x = 0.0$ ($Al_{70}Pd_{22.5}Re_{7.5}$) annealed at 940 °C for 24 h without additional annealing and with an additional annealing at 600 °C for 2 h, respectively. Inset, normalized resistivity $\rho(T)/\rho(300\ \mathrm{K})$ versus temperature for $x = 1.0$, 0.8 and 0.5.

To see whether McMillan's scaling theory of the M–I transition can be applied to QCs, in this letter we study the temperature dependence of $Al_{70}Pd_{22.5}(Re_{1-x}Mn_x)_{7.5}$ QCs and Al–Pd–Re QCs prepared with different annealing conditions. From previous studies [5, 6], we believe that the compositions of these QCs are near the M–I transition and we can push the samples towards the M–I transition by annealing Al–Pd–Re QCs appropriately.

The resistivity ρ plotted against temperature for $Al_{70}Pd_{22.5}(Re_{1-x}Mn_x)_{7.5}$ QCs is shown in figure 1. It is seen that for the samples with $x = 1.0$ and 0.8, ρ increases as the temperature is lowered, reaches a maximum around $T = 24$ K and 10 K, respectively, and then starts to decrease with decreasing temperature. For other samples, ρ increases

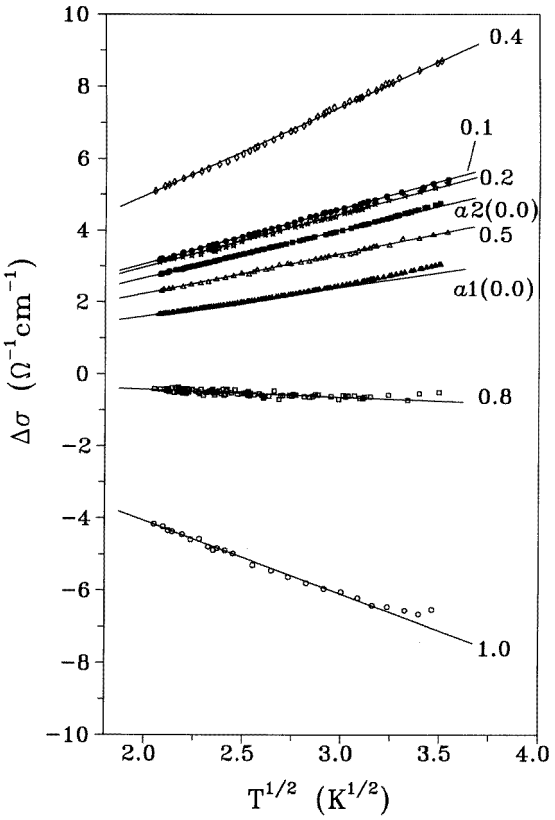

Figure 2. The conductivity data $\Delta\sigma(T) = \sigma(T) - \sigma_0$ plotted against $T^{1/2}$ for $Al_{70}Pd_{22.5}(Re_{1-x}Mn_x)_{7.5}$ QCs.

monotonically with decreasing temperature. Figure 2 shows the plot of $\Delta\sigma(T)$ as a function of $\sqrt{T}$ for the series of $Al_{70}Pd_{22.5}(Re_{1-x}Mn_x)_{7.5}$ QCs. The curves of $\Delta\sigma(T)$ against $\sqrt{T}$ for other Al–Pd–Re QCs having similar characteristics are not shown here. The straight lines indicated in figure 2 are obtained by least-squares fitting of the data to equation (2). Then the value of Δ can be calculated from the slope m of the straight line. For the samples with $x = 0.8$ and 1.0, the value of slope m is negative, indicating that the low-temperature conductivity of these samples is better described by equation (3) because this equation allows the value of m to be negative if the value of the screening parameter $\tilde{F} > \frac{8}{9}$. Samples with a negative value of m will be analysed and discussed elsewhere, not here. The temperature range 4.2–16 K, which we used to analyse the data, seems higher. Fortunately, Pierce *et al* found that except for the Al–Pd–Re QCs with very low $\sigma(4.2\ \text{K})$ ($\sim$0.67 Ω cm), $\sigma(T)$ at low temperatures (0.45 K $< T <$ 4.2 K) varies as T^{β} with $\beta \simeq 0.5$–0.6 [6]. Thus our values of Δ determined from the higher-temperature range may not deviate much from those determined from the lower-temperature range ($T <$ 4.2 K). Table 1 lists the compositions of samples, the sample annealing conditions, the values of ρ_0, the slope of the straight line m, and the value of Δ. $\rho_0 = 1/\sigma_0$ is obtained by extrapolation of the straight-line portion of the plot of $\sigma(T)$ against $\sqrt{T}$ down to zero temperature. These curves are not shown here.

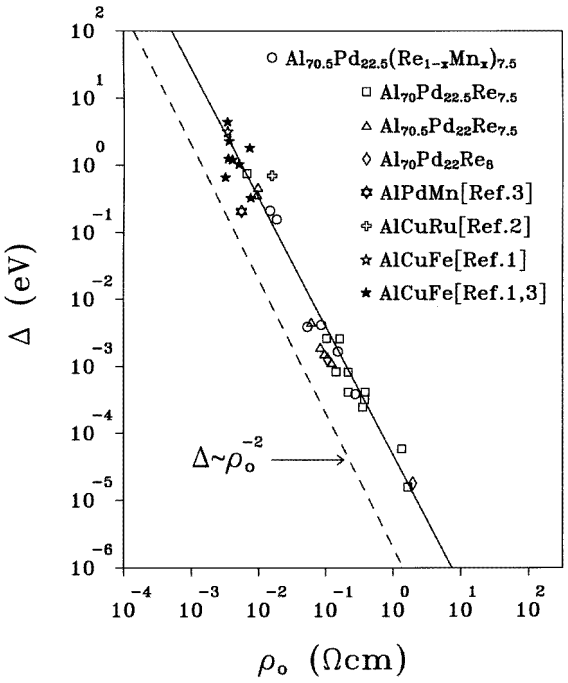

Figure 3. Double-logarithmic plot of the correlation gap Δ (eV) versus the resistivity ρ_0 (Ω cm). The dashed line is obtained from [9] and [11] for comparison with other systems (amorphous NbSi and granular Al film).

The most remarkable results shown in table 1 are that annealing the Al–Pd–Re QCs with different conditions not only can vary the value of ρ_0 significantly, as expected, but also can change the value of Δ greatly, and a higher value of ρ_0 in general has a lower value of the correlation gap Δ.

A logarithmic plot of Δ against ρ_0 is shown in figure 3. The solid line is obtained by least-squares fitting of the data to the equation $\ln \Delta = A - \alpha \ln \rho_0$ (i.e. $\Delta = A' \rho_0^{-\alpha}$). The value of α is determined to be 1.92 ± 0.08. For comparison, the dashed line obtained from amorphous materials and granular Al film [9, 11] is also shown in figure 3. This figure clearly reveals that the relation $\Delta \propto \rho_0^{-2}$ holds for both amorphous materials and QCs. That is, McMillian's theory of the M–I transition can be applied to QCs equally well. It is seen in figure 3 that the solid line does not fall on the dashed line; instead, it shifts, remaining nearly parallel, towards higher resistivity. This indicates that the dependence of Δ on ρ_0 is not universal. Similar results are also observed in amorphous materials [17]. However for these studied QCs $\Delta\sigma(T) = \sigma_0\sqrt{T/\Delta} = (1/\sqrt{A'})\sqrt{T} \approx 1.3\sqrt{T}$. Thus, $\Delta\sigma(T)$ at low temperatures is almost independent of σ_0 and material.

The above results also signal that, due to both localization and electron–electron interactions, the M–I transition can occur in Al–Pd–Re QCs on choosing the annealing conditions appropriately. In fact, the sample Al–Pd–Re marked $c3$ (listed in table 1), which has the highest resistivity (~ 0.71 Ω cm) at 4.2 K, may be already an insulator because, by extrapolating the $\sqrt{T}$ dependence of $\sigma(T)$ down to zero temperature, we will obtain a negative value of σ_0. This implies that at low temperatures ($T < 4.2$ K) $\sigma(T)$ may depend on another functional form of T rather than $\sqrt{T}$.

Table 1. The compositions of samples, the sample annealing conditions, the values of ρ_0, the values of m in $\sigma(T) = \sigma_0 + m\sqrt{T}$, and the values of Δ for Al–Pd–Re–Mn and Al–Pd–Re quasicrystals. * denotes the resistivity at 4.2 K.

Sample	Annealing temperature (time)	ρ_0 (Ω cm)	m (Ω cm $K^{1/2})^{-1}$	Δ (μeV)
$Al_{70}Pd_{22.5}(Re_{1-x}Mn_x)_{7.5}$				
$x = 0.1$	950 °C (24 h)	0.3433	1.54	310
$x = 0.2$	945 °C (24 h)	0.1079	1.49	3 330
$x = 0.4$	880 °C (24 h)	0.0670	2.49	3 103
$x = 0.5$	840 °C (24 h)	0.0235	1.12	124 699
$Al_{70}Pd_{22.5}Re_{7.5}$				
*a*1	940 °C (24 h)	1.6849	0.81	47
	+ 600 °C (2 h)			
*a*2	940 °C (24 h)	0.2691	1.34	665
*a*3	940 °C (24 h)	0.4426	1.49	198
*a*4	940 °C (24 h)	0.2695	1.89	330
*a*5	940 °C (24 h)	0.1287	1.57	2 104
*a*6	940 °C (24 h)	0.2016	1.01	2 066
*a*7	950 °C (24 h)	2.0665	1.27	13
*a*8	960 °C (24 h)	0.4717	1.22	259
*a*9	980 °C (24 h)	0.1769	2.03	671
*a*10	920 °C (24 h)	0.4852	1.05	331
*a*11	980 °C (24 h)	0.0083	1.44	604 261
$Al_{70.5}Pd_{22}Re_{7.5}$				
*b*1	940 °C (24 h)	0.0118	1.45	292 311
*b*2	950 °C (24 h)	0.1041	2.27	1 546
*b*3	950 °C (24 h)	0.0766	2.00	3 668
*b*4	980 °C (24 h)	0.0123	1.23	373 909
*b*5	920 °C (24 h)	0.1525	2.00	923
*b*6	900 °C (24 h)	0.1203	2.19	1 243
$Al_{70}Pd_{22}Re_8$				
*c*1	940 °C (24 h)	0.1340	2.17	1 022
*c*2	940 °C (24 h)	2.4420	1.01	14
*c*3	940 °C (24 h)	0.71*	—	—
	+ 600 °C (2 h)			

Lower temperature ($T < 4.2$ K) is necessary to study the characteristics of the variation of conductivity with temperature in Al–Pd–Re QCs near and at the M–I transition and to check the accuracy of the results obtained here.

We are indebted to the National Science Council of the Republic of China for the financial support of this work.

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