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Electrical resistivity characteristics of the decagonal quasicrystalline alloy $Al_{78}Mn_{22}$

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Abstract. The variation of electrical resistivity ρ with temperature T for decagonal phase of the $Al_{72}Mn_{22}$ has been measured in the temperature range 300–680 K. The ρ–T variation exhibits two main characteristics. One relates to the negative slope in sharp contrast to the corresponding crystalline phase. Evidence and arguments have been advanced to show that the effective transport mechanism in the temperature region studied is thermally activated hopping. The other observed characteristic relates to the possible fine structure in the ρ–T curve, which may be expected to reflect the expected fine structure in the density of states of the quasicrystalline phase.

1. Introduction

Ever since its discovery in rapidly quenched $Al_{86}Mn_{14}$ alloy, [1] the icosahedral phase has been widely studied. As a result, a large number of binary and ternary systems showing icosahedral symmetry have been discovered in the past three to four years. Besides the icosahedral phase, some other phases like decagonal, octagonal and dodecagonal have also been discovered [2–4]. All these phases are termed 'quasicrystals'.

Whereas the icosahedral phase lacks periodicity in all the three dimensions, decagonal, octagonal and dodecagonal phases possess translational periodicity in one dimension. To describe the electronic properties of quasicrystals, theoretical models based mostly on the one-dimensional Fibonacci sequence, as well as two-dimensional Penrose tiling, have been proposed by several workers [5–10]. Some of the salient features emerging out of these models, are as follows:

(i) The electronic states in a quasilattice are quite different to those in a periodic lattice. Most of the states are critical and self-similar [9, 10], i.e. they are neither extended nor localised. A salient feature of these critical states is their power-law decay [9–11, 12].

(ii) In the density of states (DOS) curves it is found that there exists a large number of fine gaps in the energy spectrum. The group of fine gaps is further divided into subgroups which are separated by large gaps. The density of gaps increases as the energy and the system size increases. The self-similarity also exists in the positions of the gaps (13).

Unlike structural investigations, comparatively few experimental studies have been carried out on the electronic characterisation of quasicrystalline materials. Recently,

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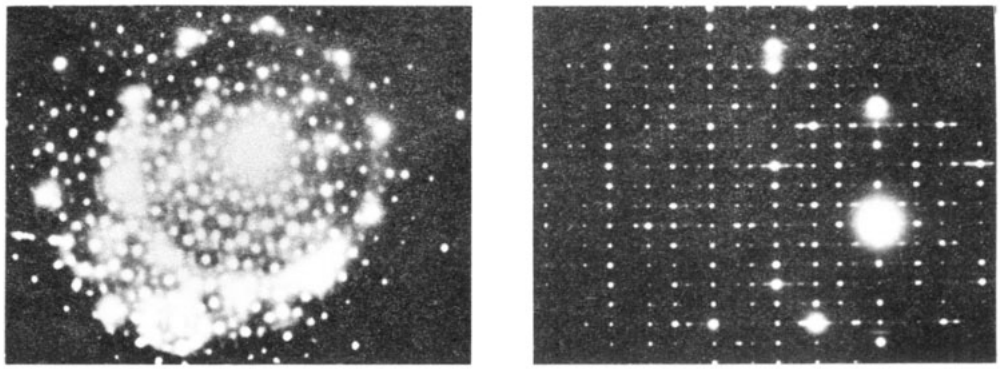

(a) (b)

Figure 1. Electron diffraction patterns of the Al–Mn decagonal phase with electron beam (*a*) along the ten-fold axis, and (*b*) along the two-fold axis perpendicular to the ten-fold axis.

we have investigated the variation of electrical resistivity with temperature in the icosahedral alloy phase of $Al_{86}Mn_{14}$ [14]. It may be mentioned that electrical resistivity measurements of the decagonal phase in $Al_{78}Mn_{22}$ in the temperature range 5–250 K have been carried out [15]. However, no resistivity measurement of this alloy has so far been reported over the temperature range (300–670 K) employed in the present investigation.

In this communication we report the variation of electrical resistivity ρ with temperature T of the pure decagonal phase of $Al_{78}Mn_{22}$. Attempts have been made to explain the ρ–T characteristics in terms of the thermally activated hopping of electrons through the critical states in the expected DOS of the quasicrystalline phase. The present results in regard to the ρ–T characteristics and their possible origin are the first of their type.

2. Experimental methods, results and discussion

Pure (99.99%) aluminium and manganese in atomic ratio $Al_{78}Mn_{22}$ were melted in a silica crucible by induction melting under an argon atmosphere. A portion of the alloy was remelted and rapidly solidified by the melt-spinning technique (3000 rpm, 13.5 cm diameter copper wheel). As a result ribbons 1 mm wide, 30–40 μm thick and several centimetres long were formed. The ribbons was characterised by x-ray powder diffractometry (Philips PW 1710) and electron microscopy (Philips EM CM-12). The resistivity measurements were carried out on samples nearly 1 cm long by the conventional four-probe DC resistivity method using a Keithley 181 nanovoltmeter and a Keithley 220 constant-current source under a vacuum of 10^{-5} Torr. The heating rate was kept below 2 K min^{-1}. The contact leads employed were made of platinum.

The XRD profile clearly reveals that the sample contains a single phase decagonal quasicrystal $Al_{78}Mn_{22}$. In the electron microscopic characterisation of the materials, the presence of some amount of icosahedral phase, besides the dominant decagonal phase was also noticed. The decagonal phase was monitored through electron diffraction patterns corresponding to two orientations. One of these corresponded to the ten-fold spot arrangement (electron beam along the decagonal axis) and the other one to the one-dimensional periodic spot arrangement (electron beam perpendicular to the decagonal axis). These patterns are shown in figure 1. In the two-fold diffraction patterns a nearly

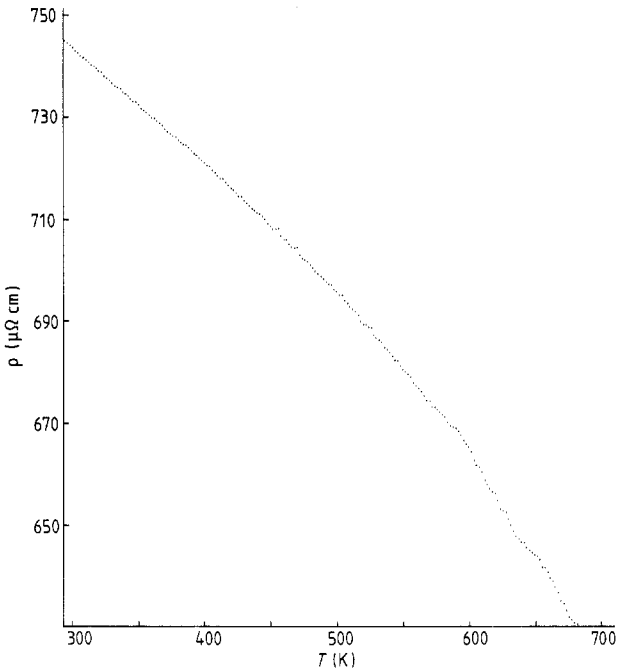

Figure 2. The resistivity–temperature (ρ–T) variation for the quasicrystalline alloy $Al_{78}Mn_{22}$.

continuous streak along the quasiperiodic direction was observed. This indicates the presence of a significant degree of disorder only along the quasiperiodic direction.

The room temperature resistivity was found to be approximately 745 $\mu\Omega$ cm which is in agreement with the other reported values [12, 15]. The ρ–T curve of the as-quenched $Al_{78}Mn_{22}$ decagonal quasicrystal shown in figure 2, clearly reveals that the resistivity decreases with increasing temperature; however, the variation is different in different temperature regions. The above behaviour was found to be invariably present in all the runs performed on different samples, during both heating and cooling.

Nearly all the calculations of the density of states reveal a fine structure of gaps governed by a branching rule and most of the states are critical [16]. The magnitude of gaps has been reported to be of the order of 1–10 meV [17]. It is generally believed that the electrical transport in quasicrystalline materials can not be understood through conventional mechanisms [12]. We considered several possible models and plotted ln ρ versus $1/T$ (figure 3) and ln ρ versus ln T (figure 4). The non-linear behaviour of ln ρ versus $1/T$ suggests that the conduction is not taking place through localised states. The optimum fit between the observed and the explored models was obtained for ln ρ versus ln T. This suggests a power law dependence [11, 12] of the type $\rho \propto T^a$ with $a = -0.11$, -0.22 and -0.48. These three values of a were obtained for the temperature regions 290–440 K, 440–610 K and 610–670 K, respectively. It may be mentioned that the power law dependence of ρ on T is in keeping with other similar observations in quasicrystalline materials [12]. The above observed behaviour can be explained based on the following reasonings.

It is now generally believed that the electronic states in the quasicrystalline systems are neither strictly extended nor localised [5–11, 13] but critical. Since the activation energy is of the order of a few kT (about the magnitude of the fine energy gaps), at a finite temperature the inter-band hopping of electrons may be considered to be the

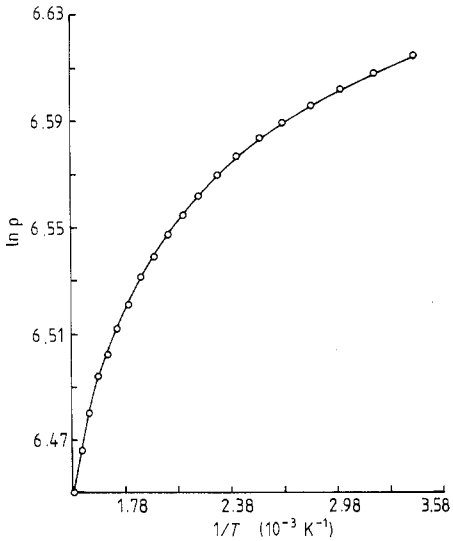

Figure 3. Plot of $\ln \rho$ versus $1/T$ for the quasicrystalline alloy $Al_{78}Mn_{22}$.

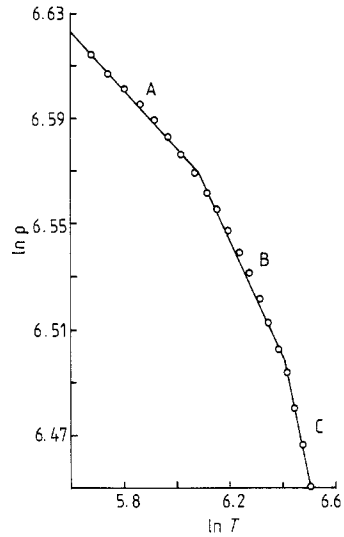

Figure 4. Plot of $\ln \rho$ versus $\ln T$ for the quasicrystalline alloy $Al_{78}Mn_{22}$ showing power-law dependence $\rho \propto T^a$. Curve A, $a = -0.11$; curve B, $a = -0.22$; curve C, $a = -0.48$.

effective mechanism for electrical transport. The electrons from mini-bands embodying critical states below the Fermi level hop to those above it. The variation of resistivity according to this mechanism is expected to follow the relation

$$\rho = \rho_0 \exp(\Delta E/kT) \tag{1}$$

where ΔE is the activation energy. The present $\ln \rho$ versus $1/T$ plot (see figure 3) is not linear as would be expected on the basis of this mechanism. This is explicable since the $\ln \rho$ versus $1/T$ curve as brought out by equation (1) is applicable only to the case of completely localised states. Therefore, we explored the applicability of the other hopping mechanism. It may be mentioned that the hopping probability depends on the nature of decay of the wavefunctions, e.g. for localised states this decay is exponential and therefore the ρ–T variation is given by (1). However, the states in quasicrystalline system are critical and the wavefunctions follow a power law decay [9–12]. This may lead to the ρ–T characteristic to be given by power law, i.e. $\rho \propto T^a$ [12]. This is in conformity with the observed result (see figure 4).

We consider now the occurrence of possible local fine structure in the ρ–T curve (figure 2). It has been established that the integrated density of states (IDOS) for the quasicrystalline system has fine-structure-like features. The electrical conduction involves electrons within the energy range of $\pm kT$ around E_F. The energy range widens up with increasing temperature, and hence the ρ–T curve is also expected to reflect the fine-structure-like features present in the IDOS of quasicrystalline phase.

When the decagonal foils were annealed through the transition temperature they transformed, as expected, to the equilibrium crystalline structure [18]. The ρ–T variation of the annealed (crystallised) samples has been found to exhibit the expected crystalline behaviour, i.e. the resistivity increases linearly with temperature in accordance with the phonon scattering contribution to the temperature coefficient of resistivity [14].

In summary, the present experimental results reveal that

(i) the mechanism of transport for the decagonal phase of $Al_{78}Mn_{22}$ over the temperature range 300–680 K is that of hopping through critical states which results in a power law variation of ρ with T, i.e. $\rho \propto T^a$ [12];

(ii) the possible fine structure in the ρ–T curve appears to reflect the proposed fine structure in the IDOS of quasicrystalline materials. Further work on the electrical transport behaviour of the Al–Mn system, including measurement of thermopower, is in progress and the results will be forthcoming.

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