PRAMANA
— journal of
physics

© Printed in India

Vol. 43, No. 5,
November 1994
pp. 373–377

Transport coefficients of quasicrystals

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MS received 2 May 1994; revised 29 October 1994

Abstract. The transport coefficients for the nine point groups $5(C_5)$, $\bar{5}(S_{10})$, $\overline{10}(C_{5h})$, $\overline{10}$ $m2(D_{5h})$, $52(D_5)$, $5m(C_{5v})$, $\bar{5}\,2m(D_{5d})$, $235(I)$, $2/m\,\bar{3}\,\bar{5}(I_h)$—which represent the symmetry groups of the quasicrystals in two and three dimensions—have been evaluated and tabulated in this work, employing group-theoretical methods.

Keywords. Galvanomagnetic and thermomagnetic effects; quasicrystals; transport phenomena; non-vanishing and independent tensor coefficients.

PACS No. **78·20**

1. Introduction

The discovery of stable icosahedral phases like the Al–Li–Cu, Al–Cu–Ru by Tsai *et al* [1] and the later determination of their structural long-range order by Guryan *et al* [2], have provided one of the best systems for investigation of unusual electronic properties in icosahedral quasicrystals. With the recent discovery of some thermodynamically stable quasicrystals [3], experimental studies on the physical properties such as resistivity, magnetoresistance, Hall effect, specific heat, etc., of quasicrystalline materials have begun [4]. The work reported by Sokoloff [5] and Kitaev and Pisma [6] revealed that the electronic properties of perfect icosahedral quasicrystals are different from those of the perfect crystals. A more recent study on the Al–Cu–Mg and Ga–Mg–Zn icosahedral alloys by Wagner *et al* [7] showed distinct features in their electronic properties. However, a comprehensive account of the tensor coefficients pertaining to the transport properties of the symmetry groups of the quasicrystals has not been reported, to the best of the knowledge of the authors. Hence an attempt is made in this note to obtain the non-vanishing and independent scheme of tensor coefficients pertaining to some identified transport properties in respect of the seven pentagonal and two icosahedral point groups: $5(C_5)$, $\bar{5}(S_{10})$, $\overline{10}(C_{5h})$, $\overline{10}$ $m2(D_{5h})$, $52(D_5)$, $5\ m(C_{5v})$, $\bar{5}\ 2m(D_{5d})$; $235(I)$, $2/m\ \bar{3}\ \bar{5}(I_h)$—which are quasicrystals' symmetry groups in two and three dimensions—employing the group-theoretical methods.

Since a good amount of experimental work is being carried out on the structure determination and physical properties of a new class of quasicrystalline materials, the authors believe that the tensor coefficients obtained here may serve as valuable check on the experimental determination of transport coefficients, measured in respect of various new materials that exhibit the symmetry of one of the aforesaid point groups. In table 1, a brief classification of the transport properties is made and the

Table 1. Classification of transport properties and character of the reducible representation corresponding to the physical property.

Physical property representing the relation between	Compound character χ_ρ^Γ for the physical property	Maximum number of independent coefficients needed	Transport phenomenon exhibited
Vector and a vector ($\rho_{ik}^0 = \rho_{ki}^0$)	$4C^2 \pm 2C$	6	Electrical resistivity; Thermal conductivity
Second rank anti-symmetric tensor and axial vector (same as axial vector and axial vector) ($\rho_{ikl} = -\rho_{kil}$)	$4C^2 \pm 4C + 1$	9	First order Hall effect, first order Leduc–Righi effect
Second rank symmetric tensor and second rank symmetric tensor (ρ_{iklm}) Notation: In contracted notation this tensor is represented by a fourth rank tensor ρ_{mn}	$(4C^2 \pm 2C)^2$	36	First order magneto-resistance, First order magneto-thermal conductivity piezo-resistance
Axial vector and totally symmetric third rank tensor ($\rho_{iklmn} = -\rho_{kilmn}$ for all permutations of the indices l, m, n). Notation: In contracted notation this tensor is represented with three components p_{qrs} following the notation developed in [11]	$((1 \pm 2C)$ $(\pm 8C^3 + 4C^2 \mp 2C)$	30	Second order Hall effect, Second order Leduc Righi effect

In table 1, C stands for the cosine of the angle of rotation ϕ in the symmetry operation. The + or − sign in the compound character χ_ρ^Γ, have to be taken according to whether the symmetry operation under consideration is a proper rotation or an improper rotation.

notation adopted for denoting the property tensors of various ranks corresponding to the considered transport property is explained. In table 2, the non-vanishing tensor components evaluated for the nine point groups are tabulated in a compact form as was done by Kumaraswamy and Krishnamurthy [8].

2. Transport phenomena, evaluation of tensor coefficients and results

It is well-known that the effect of magnetic field on the electrical and thermoelectrical properties in the absence of a temperature gradient is called galvanomagnetic effect. Physical properties such as electrical resistivity, first order Hall effect, first order magneto-resistance, and second order Hall effect are known as the galvanomagnetic effects. The components of the tensors ρ_{ik}^0, ρ_{ikl}, ρ_{iklm} and ρ_{iklmn} representing respectively the aforesaid four galvanomagnetic effects are called galvanomagnetic coefficients. Similarly the effect of magnetic field on the thermoelectric and thermal properties in

Table 2. Non-vanishing tensor coefficients ρ^0_{ik}, ρ_{ikl}, ρ_{mn}, p_{qrs}.

Pentagonal/ icosahedral point group	Number of independent coefficients needed				Non-vanishing coefficients			
	ρ^0_{ik}	ρ_{ikl}	ρ_{mn}	p_{qrs}	ρ^0_{ik}	ρ_{ikl}	ρ_{mn}	p_{qrs}
$5, \bar{5}, \overline{10}$	2	3	8	6	$\rho^0_{11} = \rho^0_{22}$, ρ^0_{33}	ρ_{123}, $\rho_{131} =$ ρ_{232}, $\rho_{132} =$ $-\rho_{231}$	$\rho_{11} = \rho_{22}, \rho_{12} = \rho_{21}$, $\rho_{13} = \rho_{23}, \rho_{16} = -\rho_{26} =$ $-\rho_{61} = \rho_{62}, \rho_{31} = \rho_{32}$, $\rho_{33}, \rho_{44} = \rho_{55}, \rho_{45} =$ $-\rho_{54}, 2\rho_{66} = \rho_{11} - \rho_{12}$	$p_{111} = 3p_{112} =$ $3p_{216} = p_{222}$, $p_{113} = p_{223}$, $3p_{116} = p_{122} =$ $-p_{211} = -3p_{212}$, $p_{123} = -p_{213}$, $p_{315} = p_{324}$, p_{333}
$52, 5m,$ $\overline{10}\,m2,$ $\bar{5}\,2m$	2	2	6	4	$\rho^0_{11} = \rho^0_{22}$, ρ^0_{33}	ρ_{123}, $\rho_{132} =$ $-\rho_{231}$	$\rho_{11} = \rho_{22}, \rho_{12} = \rho_{21}$, $\rho_{13} = \rho_{23}, \rho_{31} = \rho_{32}$, $\rho_{33}, \rho_{44} = \rho_{55}$, $2\rho_{66} = \rho_{11} - \rho_{12}$	$p_{111} = 3p_{112} =$ $3p_{216} = p_{222}$, $p_{113} = p_{223}$, $p_{315} = p_{324}$, p_{333}
$235,$ $2/m\,\bar{3}\,\bar{5}$	1	1	2	1	$\rho^0_{11} = \rho^0_{22} =$ ρ^0_{33}	$\rho_{123} =$ $-\rho_{132} =$ ρ_{231}	$\rho_{11} = \rho_{22} = \rho_{33}$, $\rho_{12} = \rho_{13} = \rho_{21} = \rho_{23} =$ $\rho_{31} = \rho_{32}, 2\rho_{44} =$ $2\rho_{55} = 2\rho_{66} = \rho_{11} - \rho_{12}$	$p_{111} = 3p_{112} =$ $3p_{113} = 3p_{216} =$ $p_{222} = 3p_{223} =$ $3p_{315} = 3p_{324} =$ p_{333}

the absence of an electric current is called thermomagnetic effect. Thermal conductivity, first order Leduc–Righi effect, first order magnetothermal conductivity, second order Leduc–Righi effect are some known thermomagnetic effects. These effects are represented respectively by the tensors K_{ik}, K_{ikl}, K_{iklm}, K_{iklmn} and the components of these tensors are known as thermomagnetic coefficients. Since the ρ and K coefficients of corresponding order are tensors of the same rank and kind, they have identical schemes of non-vanishing and independent coefficients. The galvanomagnetic effects and the thermomagnetic effects are together known as the transport phenomena [9, 11].

The permutation (of indices) symmetries and other characteristics (like peseudo, or polar, time-reversal symmetric or otherwise) of the tensors ρ^0_{ik}, ρ_{ikl}, ρ_{iklm} and ρ_{iklmn} together with the character χ^Γ_ρ of the corresponding reducible representation are briefly summarized in table 1. The maximum number n_i of non-vanishing and independent coefficients required by each one of the nine point groups, corresponding to the property tensor under consideration are determined employing the well-known formula

$$n_i = \frac{1}{g}\sum_\rho h_\rho \chi^\Gamma_\rho(R)\chi^{\Gamma_i}_\rho(R) \tag{1}$$

with the usual notation. The n_is obtained using this formula are given in table 2.

In order to determine the non-vanishing, independent coefficients the following transformation equations are used.

$$\begin{aligned}
&\rho^0_{ik} = a_{im}a_{kn}\rho^0_{mn} \quad \text{with} \quad \rho^0_{ik} = \rho^0_{ki}\\
&\rho_{ikl} = a_{im}a_{kn}a_{lp}\rho_{mnp} \quad \text{with} \quad \rho_{ikl} = -\rho_{kil}\\
&\rho_{iklm} = a_{ip}a_{kq}a_{lr}a_{ms}\rho_{pqrs} \quad \text{with} \quad \rho_{iklm} = \rho_{ikml} = \rho_{kilm} = \rho_{kiml}\\
&\rho'_{iklmn} = a_{ip}a_{kq}a_{lr}a_{ms}a_{nt}\rho_{pqrst}\\
&\rho_{iklmn} = -\rho_{kilmn} \quad \text{for all permutations of } l, m, n.
\end{aligned} \tag{2}$$

where a_{im} are the elements of the transformation matrix.

By demanding the invariance of the components under symmetry transformations (2), the desired results are obtained. The coefficients thus obtained in respect of all the nine point groups are listed in table 2 in a compact form as was done [8].

From table 2, it can be seen that the number of non-vanishing and independent tensor coefficients for the ρ^0_{ik}, ρ_{ikl}, ρ_{iklm}, ρ_{iklmn} obtained in respect of the icosahedral point groups are 1, 1, 2 and 1 respectively, fewer than those needed for any one of the 32 crystallographic point groups. It may be noted that the above tensor coefficients (ρ's) are just the same as those needed for an isotropic medium.

In view of the interest now being shown by several experimentalists on the electronic and other physical properties of the quasicrystalline materials (alloys) [4, 10], it is hoped that the results reported here may be useful to material scientists in systematizing transport data on quasicrystals.

Acknowledgement

The authors are thankful to the referee for constructive suggestions for modification.

References

[1] A Tsai, A Inoue and T Masumoto, *Jpn. J. Appl. Phys.* **26**, L1505 (1987)
[2] C A Guryan, A I Goldman, P W Stephens, K Hiraga, A Tsai, A Inoue and T Masumoto, *Phys. Rev. Lett.* **62**, 2409 (1989)
[3] Y Calvayarac, A Quivy, M Bessiee, S Lefebve, M Cornier Quiquandon and D Gratias, *J. Phys.* (*Paris*) **51**, 417 (1990)
[4] T Klein, C Berger, D Mayou and F Cyrot–Lackman, *Phys. Rev. Lett.* **66**, 2907 (1991)
[5] J B Sokoloff, *Phys. Rev. Lett.* **57**, 2223 (1986)
[6] A Yu Kitaev, *Zh Pisma Eksp. Teor. Fiz.* **48**, 270 (1988)
A Yu Kitaev, *JETP Lett.* **298**, 48 (1988)
[7] J L Wagner, B D Biggs and S J Poon, *Phys. Rev. Lett.* **65**, 203 (1990)
[8] K Kumaraswamy and N Krishnamurthy, *Acta Cryst.* **A36**, 760 (1980)
[9] J F Nye, *Physical properties of crystals* (Oxford: Clarendon, 1985)
[10] C Berger and J J Prejcan, *Phys. Rev. Lett.* **64**, 1769 (1990)
[11] S Bhagavantham, *Crystal symmetry and physical properties* (Academic, London, 1966)