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A Monte-Carlo Calculation for a Size Effect Problem

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Abstract. The Monte-Carlo Method is used for calculating a size effect problem in electrical conductivity in which, besides impurity and surface scattering, small angle electron-phonon scattering is also present. The calculated mean free path shows a dependence on the diameter of the wire in agreement with recent experimental results by OLSEN. The method of calculation and the results are discussed in detail.

I. Introduction

It is well known that one important difficulty in solving the Boltzmann transport equation for electrical conduction at low temperatures lies in the fact that a single electron-phonon collision is quite insufficient to re-establish the electron equilibrium distribution (ZIMAN[1]). Moreover, if there are also other scattering mechanisms present as impurity scattering or boundary scattering, then the problem of calculating a resistance becomes very complicated. So far only special cases have been solved such as BLOCH'S[2]) classical calculation of the high and the low temperature electrical resistance and the treatment of the size effect problem by FUCHS[3]). In the latter case a free electron model is used and the scattering at the wall, which is assumed to be partly diffuse and partly specular, is described by means of boundary conditions for the electron distribution function.

Recently OLSEN[4]) observed a deviation from Matthiessen's rule in measuring the size dependence of the resistance of indium wires. This deviation cannot be explained by any simple extension of Fuchs' calculation still assuming independent relaxation times for the different scattering processes. In the accompanying paper, BLATT and SATZ[5]) present a calculation where account is taken of the fact that the surface scattering and the phonon and impurity scattering cannot be really treated as independent. They also consider the effect of Umklapp scattering**).

We have approached the problem from a purely kinetical standpoint, and have made a Monte-Carlo calculation for this case. Although one only gets numerical expressions for the result, the great advantage of this method is that one can take the different scattering processes exactly into account, especially the small angle electron-phonon interaction at

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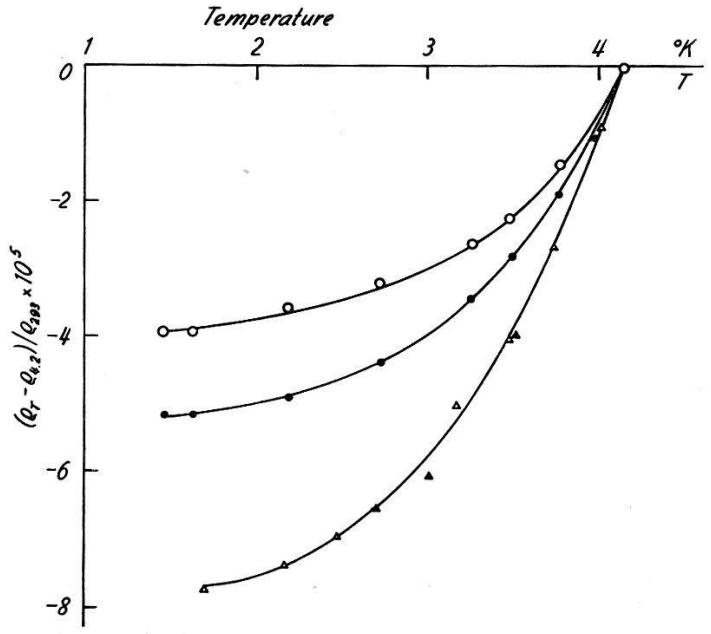
low temperatures. In limiting cases such as impurity scattering only, this method must give the same results as Fuchs' theory. As far as we know the Monte-Carlo Method has not been applied to an electrical conduction problem so far and this is just one example to show its usefulness for this sort of problem.

In the following sections we first describe the physical picture used for the conduction processes and then show details of the computer programme. Finally, the results are presented and discussed.

II. Description of the Method

OLSEN[4]) measured the electrical resistance of indium wires of different diameters from 0·06 mm to 2 mm and between 1° and 4° K. These results are shown in Figure 1 where it will be seen that the change in resistivity



○ In 2 2.0 mm ∅ ● In 8 0.2 mm ∅ △ In 7 0.06 mm ∅

Fig. 1 Resistivity change in indium. Olsen's experimental results

with temperature is greater, the thinner the wires. A similar effect may be found if older size effect measurements by ANDREW[6]) on tin are studied. As already mentioned, these results cannot be explained by a simple application of Fuchs' theory.

OLSEN has explained the results qualitatively as follows: The smaller the diameter of the wire the sooner even electrons initially moving parallel to the axis of the wire will reach the boundary by means of small angle electron-phonon processes which would be insufficient to terminate an effective free path in the bulk material. At the wall, however, the electron suffers a diffuse collision helping to establish the equilibrium distribution again. These processes are responsible for the temperature dependence of

the different specimens: The temperature dependence is more pronounced, the thinner the wire, which is actually also observed.

We believe that this explanation is right in principle and we work with the following physical picture: The isotropic impurity scattering is represented by a fixed mean free path l_i, its actual value is taken from the experiments. The electron-phonon interaction is idealized as follows: A small mean free path l_{ph}^0 is assumed which is the result of a single electron-phonon process and the value of which is estimated by taking the experimentally well founded T^5-law[7]) for the bulk resistance and by dividing the mean free path obtained in this way by a number N_0 defined in the next section. As there are many processes of this sort necessary to randomize the electron momentum, a distribution function is taken to specify the number of such events, which determine an effective electron-phonon process. The scattering at the wall is assumed to be purely diffuse, in accordance with generally current opinions (ZIMAN[1])).

Now, in the Monte-Carlo Method, an electron is observed during its path in the metal. A small distance l_0 (l_0 much smaller than any distance appearing in the problem) is introduced. After having passed this distance, the computer decides whether the electron is scattered or not, and if scattered, which sort of process happens and which new direction the electron takes. After having passed a distance l_0 the total mean free path l is calculated, i.e. the total length travelled, divided by the total number of collisions (impurity, wall and effective electron-phonon collisions). Perhaps it is worth mentioning that we have assumed a free electron model here and that the Pauli principle is not violated, since the electron always has the fixed Fermi velocity. Furthermore, Umklapp-processes are neglected.

III. The Programme and the Calculation

The calculations were carried out on the ERMETH-Computer (Elektronische Rechenmaschine der Eidgenössischen Technischen Hochschule) at the Institute of Applied Mathematics of the ETH. The structure of the programme is shown in Figure 2. The following parameters were used:

1) l_i = mean free path for impurity scattering
2) l_{ph}^0 = mean free path for a single electron-phonon process
3) ω_{ph} = maximum angle at which an electron can be scattered by a phonon
4) N_0 = average value of the number of electron-phonon collisions N necessary to randomize the electron momentum. $N_0 \approx (k/q)^2$ where k = electron wave vector, q = phonon wave vector
5) ΔN = variation width of N_0. Inside the region $2\,\Delta N$ every value N is taken as equally probable
6) d = diameter of the wire
7) L_{tot} = total length passed by an electron during the calculation
8) k = number which specifies the small length l_0 introduced in section II
9) r_0 = random number which starts the calculation of the random numbers r

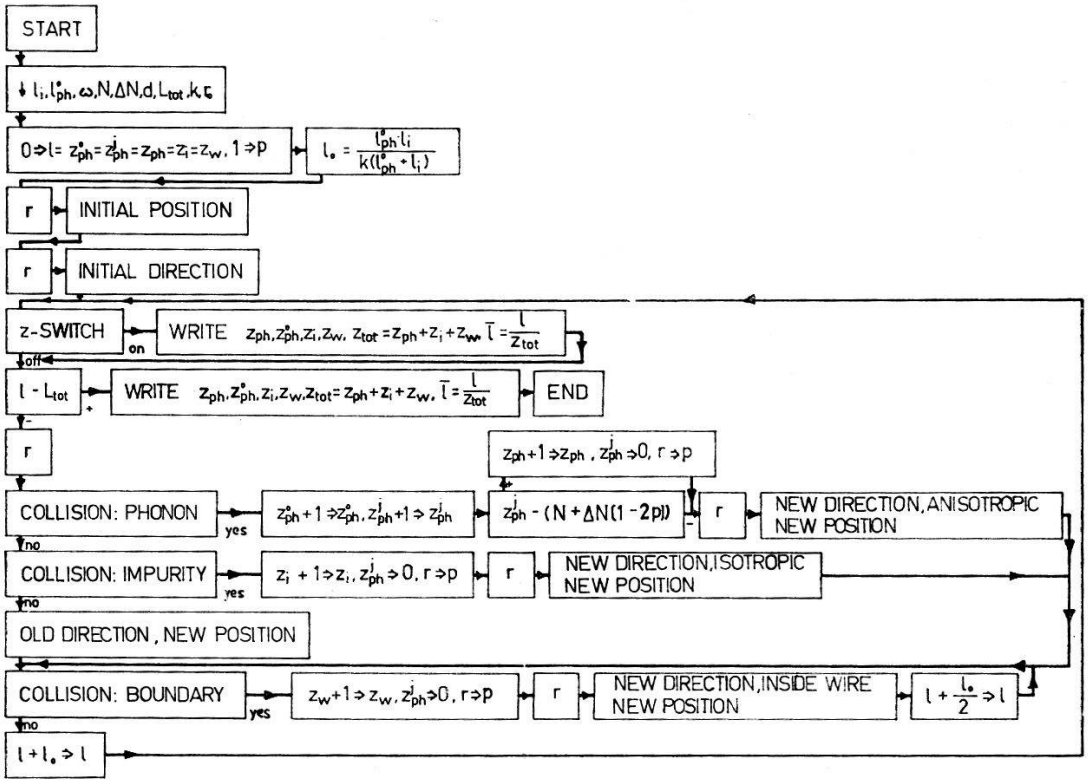


Fig. 2 Structure of the computer programme

Values for all these parameters actually used and the corresponding mean free path l, calculated with the Monte-Carlo method are given in Table I.

Table I

T (°K)	l_i (mm)	l_{ph} (mm)	ω_{ph}	N_0	ΔN	d (mm)	L_{tot} (mm)	k	r_0	l (mm)
0	0·5	10^{150}	0	10^{150}	0	0·05	300	100	12	0·046
1	0·5	5	0·1	100	100	0·05	300	50	5	0·0462
2	0·5	0·625	0·2	25	25	0·05	300	25	25	0·0459
3	0·5	0·185	0·3	11	11	0·05	300	27	12	0·0428
4	0·5	0·08	0·4	6	6	0·05	300	7	13	0·0418
10	0·5	0·005	1	1	1	0·05	300	50	7	0·0063
0	0·5	10^{150}	0	10^{150}	0	0·1	300	100	17	0·0841
1	0·5	5	0·1	100	100	0·1	300	25	6	0·0838
2	0·5	0·625	0·2	25	25	0·1	300	28	4	0·0834
3	0·5	0.185	0·3	11	11	0·1	300	15	8	0·0803
4	0·5	0·08	0·4	6	6	0·1	300	14	7	0·0725
0	0·5	10^{150}	0	10^{150}	0	2·0	300	100	18	0·426
1	0·5	5	0·1	100	100	2·0	300	2	9	0·416
2	0·5	0·625	0·2	25	25	2·0	300	5	4	0·364
3	0·5	0·185	0·3	11	11	2·0	300	7	8	0·326
4	0·5	0·08	0·4	6	6	2·0	300	7	9	0·253
10	0·5	0·005	1	1	1	2·0	300	10	13	0·0069

The actual procedure for the calculation is now the following: The electron starts at a point inside the wire, determined by random numbers. It goes along a direction, also chosen randomly, for a length l_0. Then the computer, always calculating the coordinates of the electron, decides what happens at this point. If no collision occurs, the electron passes another length l_0 in the same direction. If, however, there is an impurity collision, the random numbers determine the new direction of the electron path (every direction of the whole solid angle is taken to be equally probable). If a phonon collision takes place, the new direction can only deviate from the old one inside the region ω_{ph}. Finally, at collisions with the wall, every direction which points into the wire is possible. Along the new direction the electron passes a length l_0 and the same procedure starts again. An effective electron-phonon collision happens, if the number of single electron-phonon collisions is equal to N, where N lies somewhere between $N_0 - \Delta N$ and $N_0 + \Delta N$.

For the creation of the random numbers r by means of the computer the well known method of FIBONACCI[8]) was used. Here, two 14-figure random numbers are added, to this new number the last of the first two is again added, etc. By neglecting the first few figures, in fact by taking only an 11-figure number and by putting an 0.... before the figures, a number is created which varies between 0 and 1 with equal weights.

Since the ERMETH-Computer is too slow for this sort of problem as a Monte-Carlo calculation if the correct physical value of ω_{ph} is used in it, a number of simplifications had to be introduced: 1) The values listed in Table I for ω_{ph} and N_0 are not the theoretically estimated ones ω'_{ph}, N'_0, but corrected in the sense that the amount of calculation is diminished considerably: $\omega_{ph} = 10\,\omega'_{ph}$, $N_0 = 1/100\,N'_0$. 2) The typical length l_0 was always chosen 10 times smaller than the smallest distance appearing in the problem. A detailed analysis of this showed that l_0 was still too big to give exact agreement in cases where the problem is solvable theoretically (see next section). 3) For reducing the statistical error further the calculated mean free path was plotted as a function of the total number

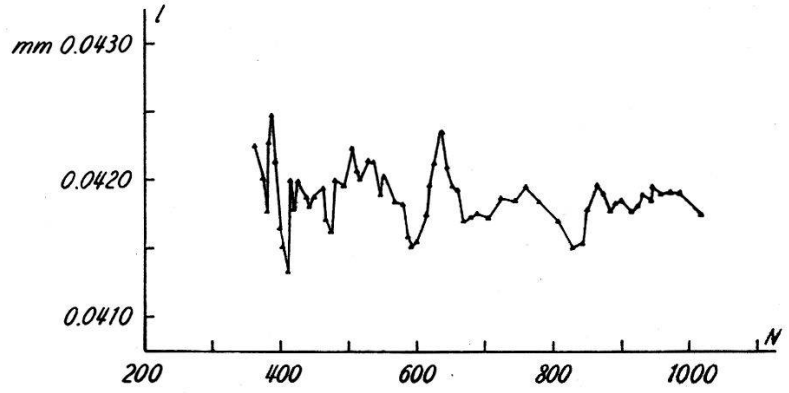


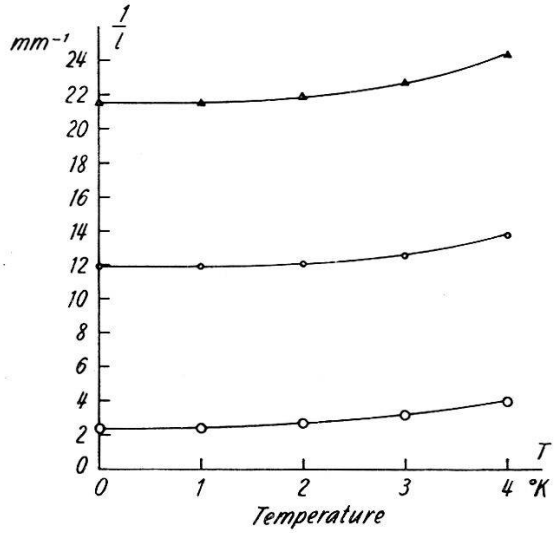
Fig. 3 The mean free path as a function of the total number of collisions

of collisions as shown in Figure 3. In this way the actual fluctuation is seen and an approximative statistical error can be determined.

Finally it is assumed that the computer could withstand psychokynetical influences of the authors (for detailed arguments see RHINE[9]).

IV. Results and Discussion

The following programme was calculated: 3 different specimens of 0·05, 0·1 and 2 mm diameter and at temperatures of 0, 1, 2, 3, 4 and 10° K. The parameters used are given in Table I. The results are plotted in Figure 4 which shows the temperature dependence and the actual value



○ 2.0 mm ∅ ○ 0.1 mm ∅ ▲ 00.5 mm ∅

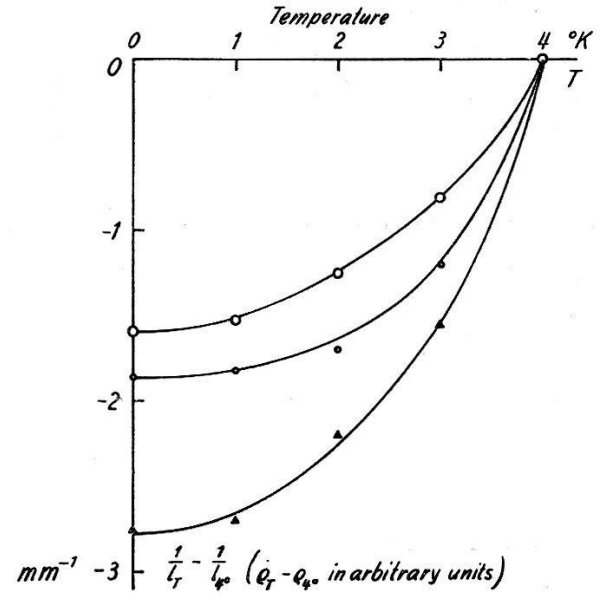
Fig. 4 Temperature dependence and actual value of the resistance, calculated by the Monte-Carlo Method

of the resistance. The violation of Matthiessen's rule is made clear in Figure 5 in a representation similar to Figure 1. One recognizes a striking agreement between the two figures, which shows that our model used for calculating this effect is essentially correct.

The values of the mean free path at $T = 0°\,\mathrm{K}$ should agree with the values calculated by the theory of FUCHS[3]), as evaluated by DINGLE[10]) for the case of diffuse scattering and cylindrical wires. Table II gives the theoretical values of Dingle and our values from the Monte-Carlo calculation.

The small discrepancy between these two sorts of values (in the worst case only 6%) is, as a special analysis showed, due to the fact that the length l_0 was not chosen small enough. In Figure 6 the dependence of the computed mean free path on l_0 is plotted and one can see that Dingle's value is reached asymptotically for $l_0 \to 0$.

Our values for $T = 0°\,\mathrm{K}$ and for different sizes fulfil the Nordheim relation[11]) $1/l = 1/l_i + 1/d$ as shown in Figure 7 by the straight line which cuts the ordinate roughly at the expected value $l = 0{\cdot}5$ mm.



○ 2.0 mm ⌀ ∘ 0.1 mm ⌀ ▲ 0.05 mm ⌀

Fig. 5 Violation of Matthiessen's rule, calculated by the Monte-Carlo Method

Table II

d (mm)	l (Dingle) (mm)	l (Monte Carlo) (mm)
0·05	0·0437	0·0464
0·1	0·079	0·0841
2·0	0·394	0·426

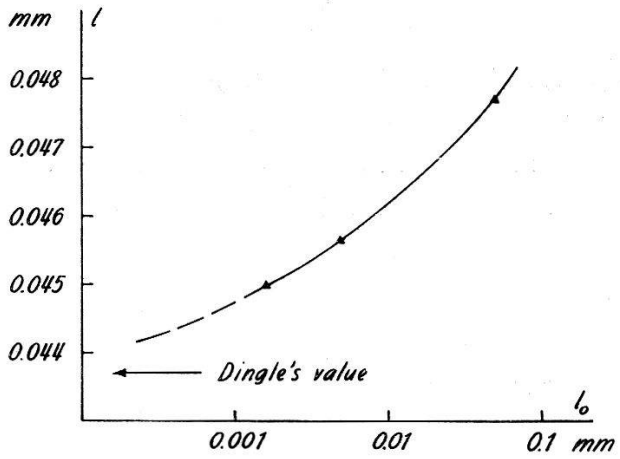


Fig. 6 The dependence of the mean free path on l_0

By using the Monte-Carlo Method we have been able to determine the electrical resistance of such a complicated case as a thin wire in the presence of a variety of scattering mechanisms. Although some simplifications had to be introduced, we believe that the neglected parameters would not have a great influence because they average out partly as for

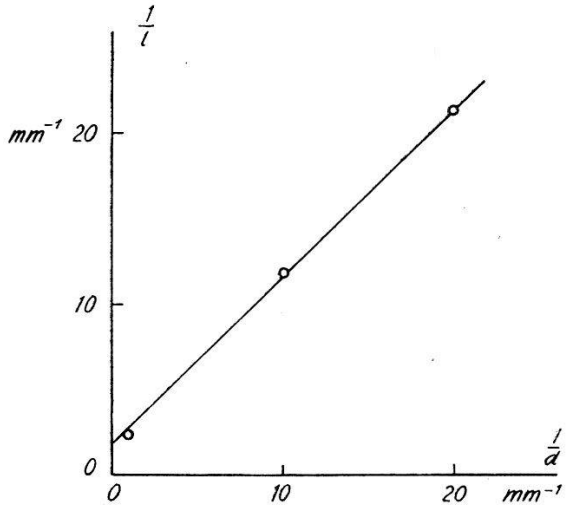


Fig. 7 Nordheim relation

example the detailed band structure or the actual electron-phonon interaction with all refinements involved or Umklapp-processes etc.

Generalisations of this method to similar problems, as for instance a similar size effect in thermal conductivity or the magnetoresistive size effect (which shows a deviation of Kohler's rule[4])) etc. are obvious, although the time of calculation with a computer of the ERMETH-type may become enormous.

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