On the Hall effect in polycrystalline semiconductors

M. V. Garcia-Cuenca, J. L. Morenza, and J. M. Codina
Departamento de Electricidad y Electrónica, Facultad de Física, Universidad de Barcelona, Diagonal 645, 08028 Barcelona, Spain

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Some problems involved in the interpretation of Hall-effect measurements in polycrystalline semiconductors have not been resolved, especially when the contribution of the boundaries is appreciable. Using the Herring theory of transport properties in inhomogeneous semiconductors, we present an alternative interpretation to that previously proposed. This model permits the calculation of the Hall coefficient under general conditions.

Extensive measurements of the Hall effect in polycrystalline semiconductors have been carried out. Nevertheless the interpretation of these measurements is not simple.

Theoretical analysis has been done. One such is the model proposed by Volger.[1] He considered a material consisting of low-resistivity grains [region (1) in Fig. 1, with resistivity ρ_1 and dimension l_1], separated by boundaries [region (2) with resistivity ρ_2 and dimension l_2]. For one such material where $\rho_2 \gg \rho_1$, $l_1 \gg l_2$, and $i_1/i_2 = l_1/l_2$ [i_1, i_2, being the mean current densities in regions (1) and (2), respectively], theory showed that the measured Hall coefficient was

$$\overline{R} = R_1 + \left[\frac{l_2}{l_1}\right]^2 R_2,$$

where R_1 is the Hall coefficient of the grain and R_2 the Hall coefficient of the boundary region. From this result Volger concluded that $\overline{R}$ was approximately R_1.

Bube[2] proposed an equivalent circuit of the basic unit in the Volger model, and modified versions of the Bube model were considered by other workers.[3–5]

Volger's result has been frequently cited when it has been assumed that in a polycrystalline semiconductor the Hall coefficient is a measure of the carrier concentration in the grain, i.e., $\overline{R} = (qn_1)^{-1}$. However, the conductivity models developed by Petritz,[6] Seto,[7] and other authors,[10–13] indicate that the assumptions of the Volger model are not always valid. In fact, if the region (2) is the boundary between grains, the condition $\rho_2 \gg \rho_1$ will be true only for light depletion of the grain; in general ρ_2 can be comparable to ρ_1, depending on the trap states density, the doping level, the grain size, and surface scattering effects. In addition, the consideration of two different current densities seems to us only justified in the quite simplified model of Volger. In spite of this, no theoretical work on the Hall effect not based on the Volger model, has been reported. The depletion of the grain was considered by Seto; he assumed $\overline{R} = R_1$, but, since the carrier concentration is not uniform, he calculated n_1 from the one-dimensional average of the carrier concentration in the grain

$$n_1 = \frac{1}{l_1}\int_0^{l_1} n(x)\,dx. \tag{1}$$

Many authors have followed Seto in the application of this expression.

From the earlier discussison it is clear that previous theoretical treatments of the problem do not consider the boundary contribution to the measured Hall coefficient in a general situation. Furthermore, we fail to know any theoretical justification for Eq. (1).

In this letter, we propose an alternative interpretation that permits the calculation of $\overline{R}$ under general conditions, and we calculate $\overline{R}$ in a particular situation.

In the Volger model two different current densities flow in the basic unit. It seems however more reasonable to consider that the same current density flows in the grain and in the boundary, because of a general random arrangement of grains (Fig. 2). In this case, since each current line goes through neutral, depletion, and boundary regions, we assume that the current lines are almost uniform. Upon making this assumption we may apply the results obtained by Herring[14] for inhomogeneous semiconductors with small fluctuations in electrical properties. Actually the application to polycrystalline semiconductors was suggested in Herring's paper.

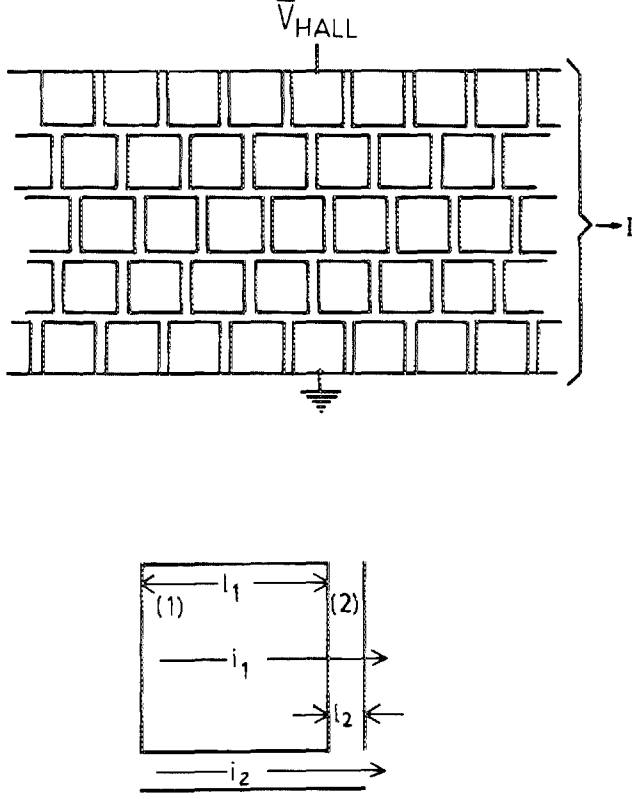

FIG. 1. Model for a polycrystalline semiconductor and basic unit from Ref. 1.

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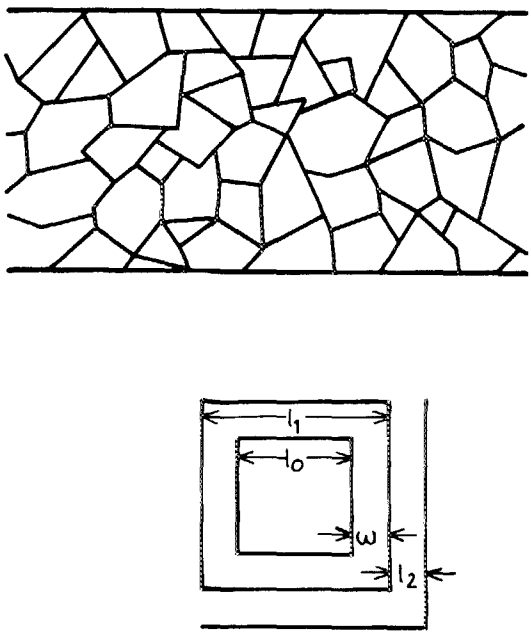

FIG. 2. Grain random arrangement and basic unit with neutral, depletion, and boundary regions.

The Herring formula for isotropic fluctuations is

$$\overline{R} = \frac{\langle \sigma^2 R \rangle}{\langle \sigma \rangle^2}, \tag{2}$$

where angular brackets denote spatial averages and $\sigma = \rho^{-1}$.

In order to calculate the averages for a polycrystalline semiconductor, we propose the following hypotheses: (a) Because of the grain depletion, the carrier concentration is function of coordinates according to Seto's model. This function depends on the partial or whole depletion of the grain, and on the material degeneration.[12,13] (b) The mobility has approximately the same value μ_1 in the whole grain and has a value μ_2 in the boundary region. μ_1 is related to the mobility of the monocrystalline material and μ_2 is related to the transport mechanism across the boundary, that is $\mu_2 = (\sigma/qn)$ boundary.

As an example, we consider the application of the small fluctuation theory to not degenerated polycrystalline semiconductors, with columnar grains. The effect of the surface is not considered. $\overline{R}$ is calculated in two situations:

(1) Partial depletion of the grain. We take as the basic unit the usual square geometry with average dimensions. There are three different regions (Fig. 2): The neutral region with carrier concentration n_0, the depletion region with carrier concentration $n_0 \exp(-\phi/kT)$, where $\phi = \phi_B(\omega - x)^2/\omega^2$ is the energy barrier (being ω the width of the depletion region and x the distance to the boundary),[9] and the boundary region with carrier concentration $n_0 \exp(-\phi_B/kT)$, where $\phi_B = \phi(x = 0)$ is the energy barrier height. Therefore the average conductivity is given by

$$\langle \sigma \rangle = \frac{l_0^2 q n_0 \mu_1}{(l_1 + l_2)^2}\left[1 + 2\left(\frac{\omega}{l_0} + \frac{\omega^2}{l_0^2}\right)\left(\frac{\pi kT}{\phi_B}\right)^{1/2} \operatorname{erf}\left(\frac{\phi_B}{kT}\right) + \left(1 + \frac{2\omega}{l_0} + \frac{l_2}{2l_0}\right)\frac{2l_2\mu_2}{l_0\mu_1}\exp\left(-\frac{\phi_B}{kT}\right)\right], \tag{3}$$

where l_0 is the neutral region dimension. The terms in brackets correspond to the neutral, the depletion, and the boundary regions, respectively.

Evidently, $\langle \sigma^2 R \rangle$ is obtained from the expression for $\langle \sigma \rangle$ by substituting μ_1 and μ_2 for μ_1^2 and μ_2^2. $\langle \sigma \rangle$ becomes $q\langle n \rangle$ with $\mu_1 = \mu_2 = 1$.

For reasonable values of parameters (for example, $l_2 = 2\ nm$, $l_1 > 10\ nm$, $\mu_2/\mu_1 < 1$ and $\phi_B > 3\ kT$), the third term is not appreciable. This result is valid also with $\mu_1/\mu_2 = 1$, therefore, the average conductivity can be expressed as

$$\langle \sigma \rangle = q\mu_1\langle n \rangle \tag{4}$$

and

$$\langle \sigma^2 R \rangle = q\mu_1^2\langle n \rangle, \tag{5}$$

where Hall factor is taken $r = 1$ and $\langle n \rangle$ is the average carrier concentration in the grain. From Eqs. (2), (4), and (5) we find

$$\overline{R} = (q\langle n \rangle)^{-1}. \tag{6}$$

The conclusion from this calculation is that, when the contribution of boundaries can be expected to be insignificant, Herring's theory gives a similar expression to that usually applied (numerical values of $\langle n \rangle$ and n_1 are very close). This result supports the theory proposed here.

(2) Whole depletion of the grain and $l_D > l_1$ (l_D being the Debye length). In this situation, because of the little band bending, the carrier concentration n is approximately uniform.[12] Then the average conductivity is given by

$$\langle \sigma \rangle = \frac{l_1^2 q n \mu_1}{(l_1 + l_2)^2}\left[1 + \frac{\mu_2}{\mu_1}\left(\frac{2l_2}{l_1} + \frac{l_2^2}{l_1^2}\right)\right], \tag{7}$$

and from Eq. (2)

$$\overline{R} = \frac{1}{qn}\left(1 + \frac{l_2}{l_1}\right)^2 \frac{1 + \frac{\mu_2^2}{\mu_1^2}\left(\frac{2l_2}{l_1} + \frac{l_2^2}{l_1^2}\right)}{\left[1 + \frac{\mu_2}{\mu_1}\left(\frac{2l_2}{l_1} + \frac{l_2^2}{l_1^2}\right)\right]^2}. \tag{8}$$

This case has been proposed as an example for which the contribution of the boundaries is expected to be significant. Evidently, the problem cannot be solved in terms of the Volger model and the derived result that $\overline{R} = R_1$ is not applicable to this situation.

According to Eq. (8), the Hall coefficient measures a reduced carrier concentration because of the inhomogeneity in mobility. The corrective factor can be very important especially for small grain sizes.

In conclusion, we have proposed a model for applying Herring's theory to polycrystalline semiconductors. For the case where $\rho_2 \gg \rho_1$ and $l_1 \gg l_2$, the result $\overline{R} = R_1$, about which there is a general agreement, is obtained from the model. Furthermore, theory gives a theoretical justification for calculating R_1 from the spatial average of the carrier concentration. For the cases where the above conditions are not valid, theory permits a calculation of $\overline{R}$ taking into account the contribution of the boundaries. This contribution will be important for small size and hard depletion of the grains. Two examples have been considered in support of these conclusions.

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