TABLE VI. Dipole sums $\mathcal{C}(\mathbf{y},k,k')$ for the zincblende structure where $\mathcal{C}(\mathbf{y},k,k')=C(\mathbf{y},k,k')/[e_k e_{k'}/v]=4\pi\mathbf{y}\mathbf{y}/|\mathbf{y}|^2-vQ(\mathbf{y},k,k')$.

Along Δ $(y,0,0)$, $\mathcal{C}(\mathbf{y},k,k')$ has the forms:

$$k=k',\ \begin{pmatrix} 2A & 0 & 0 \\ 0 & -A & 0 \\ 0 & 0 & -A \end{pmatrix};\quad k\neq k',\ \begin{pmatrix} 2B & 0 & 0 \\ 0 & -B & -iC \\ 0 & -iC & -B \end{pmatrix}$$

2 *ya*	*A*	*B*	*C*
0.0 (Γ)	4.189	4.189	0.0
0.2	4.006	3.979	3.123
0.4	3.517	3.374	6.022
0.6	2.893	2.444	8.424
0.8	2.370	1.281	10.046
1.0 (*X*)	2.166	0.0	10.624

Along Λ (y,y,y), $\mathcal{C}(\mathbf{y},k,k')$ has the forms:

$$k=k',\ \begin{pmatrix} 0 & A & A \\ A & 0 & A \\ A & A & 0 \end{pmatrix};\quad k\neq k',\ \begin{pmatrix} 0 & B+iC & B+iC \\ B+iC & 0 & B+iC \\ B+iC & B+iC & 0 \end{pmatrix}$$

2 *ya*	*A*	*B*	*C*
0.0 (Γ)	4.189	4.189	0.0
0.1	4.131	4.266	−1.547
0.2	3.986	4.471	−2.920
0.3	3.812	4.706	−4.011
0.4	3.668	4.928	−4.657
0.5 (*L*)	3.615	4.948	−4.948

Along Σ $(y,y,0)$, $\mathcal{C}(\mathbf{y},k,k')$ has the forms:

$$k=k',\ \begin{pmatrix} A & B & 0 \\ B & A & 0 \\ 0 & 0 & -2A \end{pmatrix};\quad k\neq k',\ \begin{pmatrix} C & D & iE \\ D & C & iE \\ iE & iE & -2C \end{pmatrix}$$

2 *ya*	*A*	*B*	*C*	*D*	*E*
0.0 (Γ)	2.095	6.283	2.095	6.283	0.0
0.1	2.048				
0.25	1.780	5.874	1.770	6.769	−3.668
0.4	1.224				
0.5	0.669	4.262	1.018	8.117	−5.694
0.6	−0.015				
0.75 (*K*)	−1.132	1.546	0.173	9.683	−4.524

Along Σ $(1/2a,y,y)$, $\mathcal{C}(\mathbf{y},k,k')$ has the forms:

$$k=k',\ \begin{pmatrix} -2A & 0 & 0 \\ 0 & A & B \\ 0 & B & A \end{pmatrix};\quad k\neq k',\ \begin{pmatrix} 2iC & -E & -E \\ -E & -iC & -iD \\ -E & -iD & -iC \end{pmatrix}$$

2 *ya*	*A*	*B*	*C*	*D*	*E*
0.25 (*K′*)	−1.132	1.546	0.173	9.683	−4.524
0.125	−1.878	0.430	0.078	10.389	−2.544
0.0 (*X*)	−2.167	0.0	0.0	10.624	0.0

Along Z $(1/2a,y,0)$, $\mathcal{C}(\mathbf{y},k,k')$ has the forms:

$$k=k',\ \begin{pmatrix} A & 0 & 0 \\ 0 & -A-B & 0 \\ 0 & 0 & B \end{pmatrix};\quad k\neq k',\ \begin{pmatrix} 0 & C & 0 \\ C & 0 & -iD \\ 0 & -iD & 0 \end{pmatrix}$$

2 *ya*	*A*	*B*	*C*	*D*
0.0 (*X*)	4.333	−2.166	0.0	10.624
0.25	3.224	−1.355	4.808	10.138
0.5 (*W*)	0.788	0.788	8.364	8.364

We find that our numbers are accurate to about ±0.002 near $\mathbf{y}=0$. The accuracy improves by a factor of ten as we approach the zone boundary.

PHYSICAL REVIEW VOLUME 130, NUMBER 1 1 APRIL 1963

Conductivity of Polycrystals

Z. HASHIN
The Towne School of Civil and Mechanical Engineering, University of Pennsylvania, Philadelphia, Pennsylvania
AND
S. SHTRIKMAN*
The Franklin Institute Laboratories, Philadelphia, Pennsylvania

(Received 17 September 1962; revised manuscript received 26 December 1962)

The problem of the prediction of the effective electric or thermal conductivity of a polycrystal in terms of the conductivities of the constituting single crystals is treated by a variational method. It is assumed that the crystals are all of the same kind and randomly oriented. Consequently, the polycrystal is assumed to be homogeneous and isotropic in the large. However, no assumptions about the shape of the crystals have to be introduced.

Lower and upper bounds for the effective conductivity are derived on the basis of a new variational formulation of the conductivity problem in anisotropic and nonhomogeneous media. For reasons of mathematical analogy the results are also valid for the effective dielectric constant and magnetic permeability of polycrystals. The bounds obtained are close when the anisotropy of the single crystals is not too large.

I. INTRODUCTION

THE present paper is concerned with the problem of the determination of the gross isotropic conductivity σ of a polycrystal in terms of the principal conductivities $\sigma_1<\sigma_2<\sigma_3$, of the constituting anisotropic crystals.[1] This problem may be considered as one of the determination of effective properties of a heterogeneous

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* On leave of absence from the Weizmann Institute of Science, Rehovoth, Israel.

[1] For reference to previous work on this subject, see J. K. Alstad, R. V. Colvin, and S. Legvold, Phys. Rev. **123**, 418 (1961). Volume and page in reference 2 should read **A138**, 348 (1932).

material, since a polycrystal can be regarded as a material that consists of an infinite number of anisotropic phases.

A widely studied problem in heterogeneous material behavior is that of the conductivity of two-phase materials.[2] This has been treated by the authors by a variational method which has proved to be quite powerful.[3] The present problem will be analyzed by an extension of this method. For this purpose, the previous variational theorems, which have been formulated[3] for isotropic materials only, have to be extended to cover anisotropic materials as well. This will be done in Part II. In Part III, upper and lower bounds for σ, in terms of σ_1, σ_2, and σ_3, will be derived using the variational principles given in II. The results will be discussed in Part IV.

II. VARIATIONAL PRINCIPLES

Let **J** and **E** denote[4] the current density and electric field intensity vectors, respectively, obeying

$$\mathrm{div}\mathbf{J}=0 \tag{2.1a}$$

and

$$\mathrm{curl}\mathbf{E}=0, \tag{2.1b}$$

where the last equation may also be written as

$$\mathbf{E}=-\mathrm{grad}\psi. \tag{2.1c}$$

Consider a homogeneous body of volume V and surface S, of isotropic material of conductivity σ_0. Let the current density and electric field vectors in this body, for prescribed surface potential

$$\psi=\psi^0(S), \tag{2.2}$$

be denoted by $\mathbf{J}^0$ and $\mathbf{E}^0$, respectively. These vectors must satisfy relations (2.1a) and (2.1b) and also Ohm's law,

$$\mathbf{J}^0=\sigma_0\mathbf{E}^0. \tag{2.3}$$

Equation (2.3) may also be written in indicial notation as follows:

$$J_i^0=\sigma_0\delta_{ij}E_j^0. \tag{2.4}$$

Here the range of the subscripts is 1, 2, 3; a repeated subscript denotes summation and δ_{ij} is the Kronecker delta.

Let the body now be changed to a material of anisotropic and space variable conductivity σ_{ij} without, however, changing the surface potential $\psi^0(S)$.

Let the current polarization vector **C** be defined by

$$\mathbf{C}=\mathbf{J}-\sigma_0\mathbf{E}. \tag{2.5}$$

Define also

$$\psi'=\psi-\psi^0, \tag{2.6}$$

$$\mathbf{E}'=\mathbf{E}-\mathbf{E}^0, \tag{2.7}$$

and the second rank tensor k_{ij} by

$$k_{ir}(\sigma_{rj}-\sigma_0\delta_{rj})=\delta_{ij}. \tag{2.8}$$

Then the volume integral is

$$U_C=U_0-\int_{(V)}(k_{ij}C_iC_j-2C_iE_i^0-C_iE_i')dV, \tag{2.9a}$$

where

$$U_0=\int_{(V)}\sigma_0E_i^0E_i^0dV, \tag{2.9b}$$

subject to the subsidiary condition

$$\sigma_0\,\mathrm{div}\mathbf{E}'+\mathrm{div}\mathbf{C}=0, \tag{2.10}$$

and the boundary condition

$$\psi'(S)=0, \tag{2.11}$$

is stationary[5] for

$$C_i=(\sigma_{ij}-\sigma_0\delta_{ij})E_j. \tag{2.12}$$

It should be noted that because of (2.5), (2.12) is equivalent to

$$J_i=\sigma_{ij}E_j,$$

which is the relation between the current density and electric field intensity vectors for the anisotropic and nonhomogeneous medium, and is thus a result of the variational principle. Thus, the variational principle is equivalent to a formulation of the conduction boundary value problem, with prescribed surface potential, for such media.

The stationary value U_C^s of U_C is an absolute maximum when

$$\sigma_0<\bar{\sigma}_1, \tag{2.13a}$$

and an absolute minimum when

$$\sigma_0>\bar{\sigma}_3. \tag{2.13b}$$

Here $\bar{\sigma}_1$ and $\bar{\sigma}_3$ are the smallest and the largest principal values, respectively, of the σ_{ij}. It follows that when (2.13a) holds, then, in general,

$$U_C<U_C^s, \tag{2.13c}$$

and when (2.13b) holds,

$$U_C>U_C^s. \tag{2.13d}$$

To prove these theorems the variation ΔU_C of U_C with respect to a variation $\delta\mathbf{C}$ of **C** is computed. The variation of U_C is composed of only first- and second-order terms in **C**, which will be treated separately in the following, i.e.,

$$\Delta U_C=\delta U_C+\delta^2U_C. \tag{2.14}$$

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[2] See, for example, G. A. Reynolds and G. M. Hough, Proc. Phys. Soc. (London) **B70**, 769 (1957).

[3] Z. Hashin and S. Shtrikman, J. Franklin Inst. **271**, 423 (1961).

[4] In the following, vector notation will be used wherever possible. In other cases, indicial notation will be used.

[5] Here U_C is computed using any **C** and **E**′ satisfying (2.10) and (2.11) but not (2.12).

From (2.9) one finds

$$\delta U_C=\int_{(V)}\left[2(-k_{ij}C_j+E_i^0+E_i')\delta C_i -E_i'\delta C_i+\delta E_i'C_i\right]dV. \quad (2.15)$$

The expression in the parentheses multiplying δC_i vanishes when (2.12) holds, as can be seen from substitution of (2.7) and (2.8) into (2.15). Expression (2.15). then reduces to

$$\delta U_C=\int_{(V)}(-E_i'\delta C_i+\delta E_i'C_i)dV. \quad (2.16)$$

Putting

$$\mathbf{T}=\sigma_0\mathbf{E}'+\mathbf{C}, \quad (2.17)$$

and substituting for **C** and δ**C** into (2.16) from (2.17), the following result is obtained:

$$\delta U_C=\int_{(V)}(-E_i'\delta T_i+T_i\delta E_i')dV. \quad (2.18)$$

Taking account of (2.10) in (2.17) it is found that

$$\operatorname{div}\mathbf{T}=0. \quad (2.19)$$

Using the divergence theorem and (2.19), (2.18) reduces to

$$\delta U_C=\int_{(S)}(\psi'\delta\mathbf{T}-\mathbf{T}\delta\psi')d\mathbf{S}, \quad (2.20)$$

which vanishes because of (2.11). This proves the extremum condition.

Consider now the second-order term $\delta^2 U_C$ in ΔU_C,

$$\delta^2 U_C=\int_{(V)}(-k_{ij}\delta C_i\delta C_j+\delta C_i\delta E_i')dV. \quad (2.21)$$

Using (2.17), (2.21) assumes the form

$$\delta^2 U_C=\int_{(V)}(-k_{ij}\delta C_i\delta C_j-\sigma_0\delta E_i'\delta E_i')dV. \quad (2.22)$$

Here use was made of the relation

$$\int_{(V)}\delta\mathbf{T}\cdot\delta\mathbf{E}'dV=0, \quad (2.23)$$

the proof of which is analogous to that of the vanishing of (2.18).

Since σ_0 is positive, it follows from (2.22) that

$$\delta^2 U_C<0 \quad \text{for} \quad k_{ij} \text{ positive definite.} \quad (2.24)$$

Transforming the k_{ij} to diagonal form, using (2.8), and remembering that $\delta U_C=0$, (2.13a) is obtained as maximum condition.

To prove the minimum condition (2.13b), the following result, which can be proved, using (2.17) and (2.23), will be needed:

$$\int_{(V)}(\delta\mathbf{C}\cdot\delta\mathbf{C})dV=\int_{(V)}(\sigma_0^2\delta\mathbf{E}'\cdot\delta\mathbf{E}'+\delta\mathbf{T}\cdot\delta\mathbf{T})dV. \quad (2.25)$$

Using (2.25) in (2.22) it is found that

$$\delta^2 U_C=\int_{(V)}\left[-(k_{ij}+\sigma_0^{-1}\delta_{ij})\delta C_i\delta C_j +\sigma_0^{-1}\delta T_i\delta T_i\right]dV, \quad (2.26)$$

so that

$$\delta^2 U_C>0 \quad \text{for} \quad -(k_{ij}+\sigma_0^{-1}\delta_{ij}) \text{ positive definite.} \quad (2.27)$$

Transforming k_{ij} to its diagonal form, using (2.8) and remembering that $\delta U_C=0$, (2.14b) is obtained as minimum condition.

The variational principles formulated above apply in the case when the surface potential is prescribed. Two analogous principles hold for a prescribed normal component $J_n(S)$ of **J** on the surface of the body.

To formulate these, define the electric field polarization **F** by

$$\mathbf{F}=\mathbf{E}-\rho_0\mathbf{J}, \quad (2.28)$$

where

$$\rho_0=1/\sigma_0. \quad (2.29)$$

Also define

$$\mathbf{J}'=\mathbf{J}-\mathbf{J}^0, \quad (2.30)$$

$$f_{ik}(\rho_{kj}-\rho_0\delta_{kj})=\delta_{ij}, \quad (2.31)$$

$$\rho_{ik}\sigma_{kj}=\delta_{ij}. \quad (2.32)$$

Then the integral

$$U_F=\int_{(V)}(\rho_0J_i^0J_i^0-f_{ij}F_iF_j+2F_iJ_i^0+F_iJ_i')dV, \quad (2.33)$$

subject to the subsidiary condition

$$\rho_0\operatorname{curl}\mathbf{J}+\operatorname{curl}\mathbf{F}=0 \quad (2.34)$$

and the boundary condition

$$J_n'(S)=0, \quad (2.35)$$

is stationary for

$$F_i=(\rho_{ij}-\rho_0\delta_{ij})J_j. \quad (2.36)$$

Because of (2.28), (2.36) is equivalent to

$$E_i=\rho_{ij}J_j,$$

which is the relation between electric field intensity and current density for the nonhomogeneous and anisotropic medium. (Compare with analogous result for the previous variational formulation, above).

Also

$$U_F \text{ is an absolute maximum for } \rho_0<\bar{\rho}_1, \quad (2.37a)$$

$$U_F \text{ is an absolute minimum for } \rho_0>\bar{\rho}_3, \quad (2.37b)$$

where inequalities analogous to (2.13c) and (2.13d) follow. The proof of the last two principles is analogous to that of the first two.

Lastly, it should be noted that the stationary value of U_C is equal to the total power dissipated in V.

To show this, (2.12) is introduced into (2.9), taking into account (2.5), (2.7), and (2.8), to obtain

$$U_C{}^s=\int_{(V)}(\mathbf{E}^0\cdot\mathbf{J}-\mathbf{E}'\cdot\mathbf{J}^0)dV. \tag{2.38}$$

The relation

$$\int_{(V)}\mathbf{E}'\cdot\mathbf{J}^0dV=\int_{(V)}\mathbf{E}'\cdot\mathbf{J}dV=0 \tag{2.39}$$

is easily derived [compare proof that (2.18) vanishes]. Introducing (2.7) and (2.39) into (2.38), one obtains

$$U_C{}^s=\int_{(V)}\mathbf{E}\cdot\mathbf{J}dV. \tag{2.40}$$

By an analogous procedure it is found that the same holds for $U_F{}^s$.

III. THE EFFECTIVE CONDUCTIVITY OF A POLYCRYSTAL

Consider a polycrystalline body of volume V and surface S. The polycrystal is assumed to be quasi-homogeneous and quasi-isotropic. This is a valid assumption when the crystal sizes are very small compared to the body and the directions of the crystallographic axes in the different crystals are completely uncorrelated. Also, it is assumed that there are no size effects and that grain boundaries have no surface resistance.

The effective conductivity σ of the polycrystal is now defined as follows. Apply a potential $\psi^0(S)$, which is associated with a homogeneous field $\mathbf{E}^0$, to the surface of the polycrystalline body, and calculate the power U dissipated. Then σ is given by[6]

$$\sigma=U/V\mathbf{E}^{02}. \tag{3.1}$$

To calculate σ accurately one would have to solve (2.1) subject to the boundary conditions on ψ for

$$J_i=\sigma_{ij}E_j, \tag{3.2}$$

where the σ_{ij}, referred to a coordinate system common to all the crystals, change erratically in space. This is certainly not easy to carry out, if at all possible.

A simpler approach, which will be followed here, consists of the establishment of bounds for σ. This can be done by aid of the variational theorems given in Part II. For this purpose, a trial polarization $\mathbf{C}$ has to be introduced into (2.9). The $\mathbf{C}$ chosen here will be a function of the orientation of the crystal, denoted symbolically by Ω, only. As a result of this choice, the integration with respect to V can be replaced, in the first three terms of (2.9) by integration with respect to Ω, i.e.,

$$U_C/V=\int_{(\Omega)}[\sigma_0E_i^0E_i^0-k_{ij}C_i(\Omega)C_j(\Omega)+2C_i(\Omega)E_i^0]d\Omega+\frac{1}{V}\int_{(V)}C_iE_i'dV. \tag{3.3}$$

Here and in the following it is assumed that Ω is normalized so that

$$\int_{(\Omega)}d\Omega=1. \tag{3.4}$$

Using a technique due to Néel[7] to calculate magnetostatic energies in porous media, which has been described in detail elsewhere,[8,9] the last term in (3.3) can be transformed into

$$\frac{1}{V}\int_{(V)}\mathbf{C}\cdot\mathbf{E}'dV=-\frac{1}{3\sigma_0}\int_{(\Omega)}\mathbf{C}^2(\Omega)d\Omega+\frac{1}{3\sigma_0}\left[\int_{(\Omega)}\mathbf{C}(\Omega)d\Omega\right]^2. \tag{3.5}$$

In order to approach the actual value of U as closely as possible, with the present choice of the polarization field, (3.3) subject to (3.5) is maximized, with respect to $\mathbf{C}(\Omega)$, when (2.13a) applies, and minimized with respect to $\mathbf{C}(\Omega)$, when (2.13b) applies, yielding

$$C_i(3\sigma_0k_{ij}+\delta_{ij})=3\sigma_0E_j^0+\bar{C}_j. \tag{3.6}$$

Here $\bar{C}_i$ is the average of C_i, i.e.,

$$\bar{C}_i=\int_{(\Omega)}C_i(\Omega)d\Omega. \tag{3.7}$$

Solving for C_i in (3.6) and integrating with respect to Ω, one finds

$$\bar{C}_i=(3\sigma_0E_j^0+\bar{C}_j)Q_{ij}. \tag{3.8}$$

Here

$$Q_{ij}=\int_{(\Omega)}P_{ij}d\Omega, \tag{3.9a}$$

where

$$P_{ir}(3\sigma_0k_{rj}+\delta_{rj})=\delta_{ij}, \tag{3.9b}$$

from which it follows that

$$Q_{ij}=Q\delta_{ij}. \tag{3.10}$$

Equating the traces of (3.9) and (3.10) it is found that

$$Q(\sigma_0)=\tfrac{1}{3}\sum_i\frac{\sigma_i-\sigma_0}{\sigma_i+2\sigma_0}. \tag{3.11}$$

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[6] Note that, as follows from reference 7, this is also equivalent to defining σ as the ratio of the average current density to the average field intensity.

[7] L. Néel, J. Phys. Radium **9**, 184 (1948).

[8] Z. Hashin and S. Shtrikman, J. Mech. Phys. Solids (to be published). For treatment of the problem of elastic behavior of polycrystals, see: J. Mech. Phys. Solids, **10**, 335, 343 (1962).

[9] Z. Hashin and S. Shtrikman, J. Appl. Phys. **33**, 3125 (1962).

The average polarization can now be determined from (3.8), (3.10), and (3.11), and is found to be

$$\bar{C}_i(\sigma_0)=3\sigma_0\frac{Q(\sigma_0)}{1-Q(\sigma_0)}E_i^0. \tag{3.12}$$

It follows from (2.13), (2.40), and (3.1) that σ can be estimated from

$$\begin{aligned}\sigma&>U_c/V\mathbf{E}^{02} \quad \text{for} \quad \sigma_0<\sigma_1,\\ \sigma&<U_c/V\mathbf{E}^{02} \quad \text{for} \quad \sigma_0>\sigma_3.\end{aligned} \tag{3.13}$$

Substituting (3.3) in (3.13), using (3.5), (3.6), and (3.12), and integrating, one finds

$$\begin{aligned}\sigma&>\sigma_0\frac{1+2Q(\sigma_0)}{1-Q(\sigma_0)} \quad \text{for} \quad \sigma_0<\sigma_1,\\ \sigma&<\sigma_0\frac{1+2Q(\sigma_0)}{1-Q(\sigma_0)} \quad \text{for} \quad \sigma_0>\sigma_3.\end{aligned} \tag{3.14}$$

To obtain the best bounds for σ from (3.14), note that the right-hand side of (3.14) is a monotonously increasing function of σ_0. Therefore, the best bounds for σ are obtained by substituting σ_1 and σ_3 for σ_0 obtaining

$$\sigma_3\frac{1+2Q(\sigma_3)}{1-Q(\sigma_3)}>\sigma>\sigma_1\frac{1+2Q(\sigma_1)}{1-Q(\sigma_1)}, \tag{3.15}$$

which can also, by use of (3.11), be written in the form

$$\begin{aligned}&\sigma_3\frac{4\sigma_3^2+8\sigma_3\sigma_2+8\sigma_1\sigma_3+7\sigma_2\sigma_1}{16\sigma_3^2+5\sigma_3\sigma_2+5\sigma_1\sigma_3+\sigma_2\sigma_1}\\ &\qquad>\sigma>\sigma_1\frac{4\sigma_1^2+8\sigma_1\sigma_2+8\sigma_1\sigma_3+7\sigma_2\sigma_3}{16\sigma_1^2+5\sigma_1\sigma_2+5\sigma_1\sigma_3+\sigma_2\sigma_3}.\end{aligned} \tag{3.16}$$

Here $\sigma_3>\sigma_2>\sigma_1$ are the principal conductivities of the crystal considered.

IV. DISCUSSION

The most widely used formulas for the conductivity of polycrystals are the average expressions

$$\sigma=\tfrac{1}{3}(\sigma_1+\sigma_2+\sigma_3), \tag{4.1}$$

and

$$1/\sigma=\tfrac{1}{3}(1/\sigma_1+1/\sigma_2+1/\sigma_3). \tag{4.2}$$

Substituting $\sigma_0=0$ and $\sigma_0=\infty$ in (3.14) one finds[10]

$$\frac{3}{1/\sigma_1+1/\sigma_2+1/\sigma_3}<\sigma<\frac{\sigma_1+\sigma_2+\sigma_3}{3}, \tag{4.3}$$

which shows that (4.1) and (4.2) are actually upper and lower bounds for σ. Since the right-hand side of (3.14) increases monotonously with σ_0, the bounds given by (3.16) are more restrictive and, therefore, superior to those given by (4.3). This also shows that (4.1) and (4.2) cannot be correct.

A question that arises is the following: Is the effective conductivity uniquely determined for the model of the polycrystal described above? In the case of a two-phase material it was shown[9,11] that the effective conductivity is not uniquely determined in terms of volume fractions and phase conductivities. Whether or not a similar situation arises here is not known at present. The present treatment avoids the problem of the existence of a unique solution by establishing bounds for the effective conductivity of the polycrystal. In the derivation of the various formulas given in reference 1, the problem is not mentioned. Unique results are found by introducing additional arbitrary restrictions which are not consistent with the actual conditions in the polycrystal. Thus, for example, (4.1) and (4.2) are derived assuming that **E** and **J**, respectively, are uniform in the material, which certainly is not true. It is, on the other hand, assumed in Bruggeman's[12] approach that the crystals can be considered as spheres in an isotropic environment. This is certainly a good approximation, but not an exact treatment.

It is of interest to compare the present and previously found theoretical results with experimental values. However, here one encounters the difficulty that in most crystals $\sigma_1\simeq\sigma_2\simeq\sigma_3$ for which case all the different formulas give practically indistinguishable results. The case of yttrium is, as shown in Table I, somewhat different.

TABLE I. Calculated and measured resistivities (in 10^{-6} Ω cm) of yttrium, at 300°K, with residual subtracted.

Sample Y-I	Sample Y-II	Sample Y-III	Eq. (4.1)	Eq. (3.16)	Eq. (4.2)	Eq. (3)[a]
60.0	59.5	59.6	59.3	54.5; 55.5	52.8	55.2

[a] See reference 1.

In this example, the resistivity is significantly larger than the upper limit derived here. Further experimental studies will be needed in order to find the cause of this discrepancy.

Lastly, it should be pointed out that the problem of the conductivity of polycrystals which has been studied here is mathematically analogous to the problem of the dielectric constant, heat conductivity, and magnetic permeability of polycrystals.

The results found here thus apply directly to these cases.

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[10] It is interesting to note here, that in the special cases $\sigma_0\rightarrow 0$ and $\sigma_0\rightarrow\infty$, the variational theorems given in Part II also simplify considerably. See also references 8 and 9.

[11] W. F. Brown, Jr., J. Chem. Phys. **23**, 1514 (1955).

[12] D. A. Bruggeman, Ann. Physik **25**, 645 (1936).