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"Current Striction"—A Mechanism of Electrostriction in Many-Valley Semiconductors*

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Previously reported experiments tentatively suggest that electric fields applied to germanium produce deformations which are about 10^4 times as large as those expected from conventional electrostriction mechanisms. We have calculated the magnitude, temperature dependence, and angular dependence of this effect for n-type many-valley semiconductors. Our model does not involve a polarization in real space but, like the current, is mediated by a shift of the electron distribution in reciprocal space. This field-induced shift increases the energy of the electrons within each valley, but the increase is largest in those valleys with smallest effective mass parallel to the field direction. It then becomes energetically favorable for the lattice to deform in such a way that the deformation potential lowers the energy of the high-curvature valleys at the expense of the low-curvature valleys. We calculate a much larger effect in germanium than in silicon, predicting also that the induced strain should be a pure shear in germanium, and a pure volume-preserving linear dilatation in silicon.

1. INTRODUCTION

We here present a theory of a mechanism whereby electric fields applied to germanium can induce elastic deformations of the order of 10^4 times larger than those expected from conventional mechanisms of electrostriction. The effect is an intrinsically irreversible phenomenon, associated with the flow of current in the semiconductor. Consequently the thermodynamic Maxwell relation

$$\partial^2\Sigma/\partial E^2 = \partial\epsilon/\partial t \tag{1.1}$$

is violated, the left-hand member being of the order of 10^4 times the right-hand member[1] (Σ, t, and ϵ are appropriate elements of the strain, stress, and dielectric constant tensors, and E is the applied electric field). To emphasize the nonequilibrium nature of the effect, and to distinguish it from conventional electrostriction, we refer to it as "current striction".

Although current striction should occur in any semiconductor we here carry out the theory explicitly for n-type many-valley semiconductors, such as germanium or silicon (but the calculated values for germanium are of the order of 100 times larger than for silicon). The essential mechanism is as follows. Within each valley the applied field shifts the electron distribution in k space, thereby increasing the energy of the electrons. This increase in energy is greatest if the curvature of ϵ versus k is largest in the direction of the applied field; that is, it is greatest for those valleys with small effective mass parallel to the field direction. It then becomes energetically favorable for the lattice to deform so as to lower the energy of the high-curvature valleys at the expense of the low-curvature valleys. *The lattice deforms so as to energetically favor those valleys with largest effective mass parallel to the field direction.*

Although a general suggestive similarity exists between the current striction effect and the acousto-electric effect[2] it should be noted that the two effects are not reciprocally related, but are quite distinct and independent. The acousto-electric effect is intrinsically a dynamical effect and depends essentially on the spatial inhomogeneity induced by the phonon, whereas the current-striction effect is static and spatially homogeneous.

Some three years ago one of us (A.G.) observed[3] electromechnical oscillations in a small area metallic contact to a germanium crystal. A simple equivalent-circuit analysis suggested the existence of a remarkably large electrostrictive coupling. An attempt was then made to measure, in a direct fashion, this giant electrostrictive effect. The direct measurement is very difficult, but early results[4] seemed to corroborate the sought for value. The theory here to be reported was then developed, but publication was delayed while two of us (P. K.

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‡ Work supported by the U. S. Office of Naval Research.

[1] K. J. Schmidt—Tiedemann, J. Appl. Phys. 32, 2058 (1961).

[2] G. Weinreich, T. M. Sander, Jr., and H. C. White, Phys. Rev. 114, 33 (1959).

[3] A. A. Gundjian, Ph.D. dissertation, Moore School of Electrical Engineering, University of Pennsylvania, 1965 (unpublished).

[4] A. A. Gundjian, Solid State Commun. 3, 279 (1965).

and A. G.) attempted to refine the experiments and obtain definitive data. The result of that experimental effort has raised some doubts as to the previous[3] measurement. The theory therefore stands without quantitative experimental verification at this time.

2. FREE ENERGY OF THE PERTURBED ELECTRON DISTRIBUTION

We consider a set of ellipsoidal valleys, designated by the index i, with effective mass tensors $\mathbf{m}_i^*$, and with energy minima ϵ_{0i}. In the unstrained equilibrium state all the ϵ_{0i} would be equal, but we consider an arbitrarily strained crystal in which the ϵ_{0i} have certain specified values.

In the absence of an electric field the number of electrons in the ith valley (per unit volume) is

$$\tilde{N}_i=2\sum_{\mathbf{k}(i)}\tilde{f}_i(\mathbf{k})\,, \tag{2.1}$$

where

$$\tilde{f}_i(\mathbf{k})=[\exp\beta(\epsilon_i(\mathbf{k})-\tilde{\mu})+1]^{-1}\,, \tag{2.2}$$

$$\epsilon_i(\mathbf{k})=\epsilon_{0i}+\tfrac{1}{2}\hbar^2\mathbf{k}_i\cdot\frac{1}{\mathbf{m}_i^*}\cdot\mathbf{k}_i\equiv\epsilon_{0i}+\epsilon_{1i}\,. \tag{2.3}$$

Here the summation is over all $\mathbf{k}$ vectors within the ith valley and $\mathbf{k}_i$ denotes the value of $\mathbf{k}$ relative to the center of the valley. The factor of 2 in Eq. (2.1) arises from electron spin. Although the numbers $\tilde{N}_i$ do depend upon the ϵ_{0i}, the sum $N=\sum_i\tilde{N}_i$ (or the total density of electrons in the conduction-band valleys) is independent of the ϵ_{0i} to first order. This is shown in Appendix A, where we also show that $\tilde{\mu}$ is shifted from its unstrained equilibrium value μ_0:

$$\tilde{\mu}=\mu_0+\frac{1}{l}\sum_{i=1}^{l}\epsilon_{0i} \tag{2.4}$$

and consequently, that $\tilde{f}_i(\mathbf{k})$ is related to the unstrained equilibrium distribution $f_i^0(\mathbf{k})$ by

$$\tilde{f}_i=f_i^0+\left[\epsilon_{0i}-\frac{1}{l}\sum_{j=1}^{l}\epsilon_{0j}\right]\frac{\partial f_i^0}{\partial\epsilon_i}\equiv f_i^0+(\delta\epsilon_{0i})\frac{\partial f_i^0}{\partial\epsilon_i}\,. \tag{2.5}$$

The application of the electric field $\mathbf{E}$ tends to displace the distribution function in each valley in the field direction ($\hbar\dot{\mathbf{k}}=-e\mathbf{E}$); this tendency is compensated by both intervalley and intravalley scattering. However, since the field-induced transitions are between neighboring $\mathbf{k}$ states (intravalley), the field directly induces no net change in the number of electrons in each valley $\tilde{N}_i$. By an iterative solution of the Boltzmann equation, including both intervalley and intravalley scattering, we show in Appendix B that, to second order in $\mathbf{E}$,

$$f_i=\tilde{f}_i+e\tau\mathbf{E}\cdot v_i\frac{\partial\tilde{f}_i}{\partial\epsilon_i}+e^2\tau^2\mathbf{E}\cdot\frac{1}{\mathbf{m}_i^*}\cdot\mathbf{E}\frac{\partial\tilde{f}_i}{\partial\epsilon_i}+e^2\tau^2(\mathbf{E}\cdot\mathbf{v}_i)^2\frac{\partial^2\tilde{f}_i}{\partial\epsilon_i^2}+\cdots\,, \tag{2.6}$$

where $\mathbf{v}_i(\mathbf{k})=\hbar(1/\mathbf{m}_i^*)$. $\mathbf{k}$ is the electron velocity and τ is the net relaxation time [Eq. (B8)].

Combining (2.5) and (2.6) we find f_i to second order in $\mathbf{E}$ and first order in $\delta\epsilon_{0i}$.

$$f_i=f_i^0+[g_{1i}+g_{2i}]+(\delta\epsilon_{0i})[h_{0i}+h_{1i}+h_{2i}]\,, \tag{2.7}$$

where g_{1i} and g_{2i} are of first order and second order in $\mathbf{E}$, respectively:

$$g_{1i}=e\tau(\mathbf{E}\cdot\mathbf{v}_i)\frac{\partial f_i^0}{\partial\epsilon_i}\,, \tag{2.8}$$

$$g_{2i}=e^2\tau^2\mathbf{E}\cdot\frac{1}{\mathbf{m}_i^*}\cdot\mathbf{E}\frac{\partial f_i^0}{\partial\epsilon_i}+e^2\tau^2(\mathbf{E}\cdot\mathbf{v}_i)^2\frac{\partial^2 f_i^0}{\partial\epsilon_i^2} \tag{2.9}$$

and similarly for h_{0i}, h_{1i}, and h_{2i}

$$h_{0i}=\frac{\partial f_i^0}{\partial\epsilon_i}\,, \tag{2.10}$$

$$h_{1i}=e\tau(\mathbf{E}\cdot\mathbf{v}_i)\frac{\partial^2 f_i^0}{\partial\epsilon_i^2}\,, \tag{2.11}$$

$$h_{2i}=e^2\tau^2\mathbf{E}\cdot\frac{1}{\mathbf{m}_i^*}\cdot\mathbf{E}\frac{\partial^2 f_i^0}{\partial\epsilon_i^2}+e^2\tau^2(\mathbf{E}\cdot\mathbf{v}_i)^2\frac{\partial^3 f_i^0}{\partial\epsilon_i^3}\,. \tag{2.12}$$

The free energy of this nonequilibrium distribution of electrons is given by[5]

$$F=\sum_{i=1}^{l}F_i\,, \tag{2.13}$$

$$F_i=2\sum_{\mathbf{k}(i)}f_i(\mathbf{k})\epsilon_i(\mathbf{k})+2\beta^{-1}\sum_{\mathbf{k}(i)}[f_i\ln f_i+(1-f_i)\ln(1-f_i)]\,. \tag{2.14}$$

Inserting Eq. (2.7) and expanding to second order in $\mathbf{E}$ and to first order in ϵ_{0j} we find (see Appendix C)

$$F_i=F_i^0+(1/l)N\epsilon_{0i}+G_{2i}+(\delta\epsilon_{0i})[H_{0i}+H_{2i}]\,, \tag{2.15}$$

where

$$G_{2i}=\beta^{-1}\sum_{\mathbf{k}(i)}\frac{g_{1i}^2}{f_i^0(1-f_i^0)}\,, \tag{2.16}$$

$$H_{0i}=2\mu_0\sum_{\mathbf{k}(i)}h_{0i}\,, \tag{2.17}$$

$$H_{2i}=2\beta^{-1}\sum_{\mathbf{k}(i)}\frac{g_{1i}h_{1i}}{f_i^0(1-f_i^0)}+\beta^{-1}\sum_{\mathbf{k}(i)}\frac{2f_i^0-1}{[f_i^0(1-f_i^0)]^2}h_{0i}g_{1i}^2\,. \tag{2.18}$$

The functions G_{2i} and H_{2i} are second order in $\mathbf{E}$, whereas H_{0i} is zero order.

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[5] L. D. Landau and E. M. Lifshitz, *Statistical Physics* (Pergamon Press Ltd., London, 1958), p. 155.

As we shall see, the function H_{2i} is the only one of these functions which we must evaluate explicitly. Inserting the value of h_{0i}, h_{1i}, and g_{1i}, and noting that

$$\frac{\partial f_i^0}{\partial \epsilon_i} = -\beta f_i^0(1-f_i^0), \quad \frac{\partial^2 f_i^0}{\partial \epsilon_i^2} = \beta(2f_i^0-1)\frac{\partial f_i^0}{\partial \epsilon_i} \tag{2.19}$$

we find

$$H_{2i} = -e^2\tau^2 \sum_{\mathbf{k}(i)} (\mathbf{E}\cdot\mathbf{v}_i)^2 \frac{\partial^2 f_i^0}{\partial \epsilon_i^2}. \tag{2.20}$$

Following a procedure similar to that leading to Eq. (B9)

$$H_{2i} = -\tfrac{1}{2}e^2\tau^2\left(\mathbf{E}\cdot\frac{1}{\mathbf{m}_i^*}\cdot\mathbf{E}\right)\frac{2}{3}\frac{1}{2\pi^2}\left(\frac{2m_e}{\hbar^2}\right)^{3/2} \times \int_0^\infty \epsilon_i^{3/2}\frac{\partial^2 f_i^0}{\partial \epsilon_i^2}d\epsilon_i, \tag{2.21}$$

where we have utilized the familiar density-of-states function

$$g(\epsilon_i) = \frac{1}{2\pi^2}\left(\frac{2m_e}{\hbar^2}\right)^{3/2}\epsilon_i^{1/2} \tag{2.22}$$

with m_e as the "density-of-states" effective mass

$$m_e^3 = \det|m_i^*| = m_1 m_2 m_3. \tag{2.23}$$

Integrating by parts,

$$H_{2i} = \tfrac{1}{2}e^2\tau^2\left(\mathbf{E}\cdot\frac{1}{\mathbf{m}_i^*}\cdot\mathbf{E}\right)\frac{1}{2\pi^2}\left(\frac{2m_e}{\hbar^2}\right)^{3/2} \times \int_0^\infty \epsilon_i^{1/2}\frac{\partial f_i^0}{\partial \epsilon_i}d\epsilon_i, \tag{2.24}$$

$$H_{2i} = -\tfrac{1}{2}e^2\tau^2\left(\mathbf{E}\cdot\frac{1}{\mathbf{m}_i^*}\cdot\mathbf{E}\right)\frac{1}{2\pi^2}\left(\frac{2m_e}{\hbar^2}\right)^{3/2} \times \frac{\partial}{\partial\mu}\int_0^\infty \epsilon_i^{1/2} f_i^0 d\epsilon_i, \tag{2.25}$$

$$H_{2i} = -\tfrac{1}{2}e^2\tau^2\left(\mathbf{E}\cdot\frac{1}{\mathbf{m}_i^*}\cdot\mathbf{E}\right)\frac{\partial N_i}{\partial\mu}. \tag{2.26}$$

3. THE QUASI-EQUILIBRIUM CONDITION

For a cubic semiconductor with l valleys the total free energy is

$$F = \sum_{i=1}^{l} F_i + \tfrac{1}{2}\mathbf{\Sigma}:\mathbf{c}:\mathbf{\Sigma}, \tag{3.1}$$

where $\mathbf{\Sigma}$ is the 2nd-rank strain tensor and $\mathbf{c}$ is the 4th-rank elastic modulus tensor. This tensor has only three independent components

$$c_{11}(\equiv c_{xx,xx} = c_{yy,yy} = c_{zz,zz}),$$

$$c_{12}(\equiv c_{xx,yy} = c_{xx,zz} = c_{yy,zz}),$$

and

$$c_{44}(\equiv c_{xy,xy} = c_{yz,yz} = c_{xz,xz}).$$

Mixed components such as $c_{xx,xy}$ vanish. The quantity $\mathbf{\Sigma}:\mathbf{c}:\mathbf{\Sigma}$ denotes $\Sigma_{\mu\nu}c_{\nu\mu'\mu'\nu'}\Sigma_{\nu'\mu'}$ summed over all indices.

The coupling between the electronic energy and the strain energy is characterized by the deformation potential. In particular, the energy ϵ_{0i} of the ith valley is given by,

$$\epsilon_{0i} = \mathbf{\Xi}^{(i)}:\mathbf{\Sigma}, \tag{3.2}$$

where $\mathbf{\Xi}^{(i)}$ is a 2nd-rank tensor, so that ϵ_{0i} is equal to $\Xi^{(i)}{}_{\mu\nu}\Sigma_{\nu\mu}$ summed over μ and ν. The deformation potential $\mathbf{\Xi}^{(i)}$ for germanium or silicon-type semiconductors (i.e., for [111] or [100] valleys) is given by

$$\Xi^{(i)} = \Xi_d\mathbf{1} + \Xi_u(\hat{k}_i\hat{k}_i). \tag{3.3}$$

Here Ξ_d and Ξ_u are constants, $\mathbf{1}$ is the unit tensor, $\hat{k}_i$ is the unit vector in $\mathbf{k}$ space in the direction of the ith valley, and $(\hat{k}_i\hat{k}_i)$ is the diadic tensor product.[6]

It should be noted that the strain not only shifts the energy minima ϵ_{0i}, but that it also alters the effective mass tensor m_i^*. The magnitude of this effect has been evaluated by Hensel, Hasegawa and Nakayama[7] by cyclotron resonance; for Si they find $\Delta m^*/m^* \simeq 5\Sigma$. This effect consequently is too small to affect our results appreciably and has been omitted in our analysis.

Recalling that F_i is a function of the energy minima ϵ_{0i}, Eq. (3.1) now expresses the total free energy F as a function of the strain components.

Unfortunately, statistical mechanics does *not* provide us with a general prescription for finding the expectation values of the strain components. In equilibrium ($\mathbf{E}=0$) the strain components would be found by minimizing F, but the steady state ($\mathbf{E}\neq 0$) is not an equilibrium state. It is quite obvious, for instance, that the $f_i(\mathbf{k})$ of Eqs. (2.7) and (2.12) are not those which minimize the free energy, although they would do so in equilibrium. On the other hand we have seen [Eq. (B11)] that the N_i do take the values $\bar{N}_i$ which minimize F. There is an important and fundamental difference between variables such as the $f_i(\mathbf{k})$ and those such as N_i or the strain components $\Sigma_{\mu\nu}$. Whereas the electric field directly induces transitions which alter $f_i(\mathbf{k})$ within a valley it does not directly induce transitions which alter the N_i. Similarly the direct effect of $\mathbf{E}$ on the strain components $\Sigma_{\mu\nu}$ is negligibly small; in fact this direct effect is precisely the ionic polarization discussed in the first paragraph of the Introduction. *The mechanism of change of the strain components consists of the same spontaneous*

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[6] H. Brooks, in *Advances in Electronics and Electron Physics* (Academic Press Inc., New York, 1955), Vol. 7, p. 85.

[7] J. C. Hensel, H. Hasegawa and M. Nakayama, Phys. Rev. 138, A225 (1965).

TABLE I. Dependence of $\partial N/\partial\mu$ on the number of electrons in the conduction-band valleys. Here $\beta=(k_BT)^{-1}$, m_0 is the free-electron mass, m_e is the density-of-states electron mass, l is the number of valleys. The Fermi energy μ is given, for convenience, in the third column.

$\frac{1}{\beta N}\frac{\partial N}{\partial\mu}$	$10^{-19}\frac{N}{l}\left(\frac{m_0}{m_e}\right)^{3/2}$ (cm^{-3})	$\beta\mu$
0.973	0.0457	−4.0
0.989	0.0750	−3.5
0.983	0.123	−3.0
0.973	0.200	−2.5
0.956	0.324	−2.0
0.932	0.520	−1.5
0.897	0.823	−1.0
0.850	1.274	−0.5
0.827	1.506	−0.3
0.815	1.635	−0.2
0.803	1.773	−0.1
0.791	1.920	0.0
0.764	2.243	0.2
0.723	2.804	0.5
0.652	3.954	1.0
0.582	5.383	1.5
0.519	7.086	2.0
0.462	9.052	2.5
0.413	11.262	3.0
0.371	13.697	3.5
0.336	16.340	4.0

transition probabilities which are effective in equilibrium. Accordingly, we again assume that the steady-state values of the strain components are those which minimize the nonequilibrium free energy (3.1).

Minimizing F with respect to $\Sigma_{\nu\mu}$

$$\sum_{i=1}^{l}\sum_{j=1}^{l}\frac{\partial F_i}{\partial\epsilon_{0j}}\Xi_{\nu\mu}{}^{(j)}+(\mathbf{c}:\,\mathbf{\Sigma})_{\nu\mu}=0 \tag{3.4}$$

or inserting Eq. (2.15).

$$N\langle\Xi_{\nu\mu}\rangle+l\langle(H_0+H_2)\Xi_{\nu\mu}\rangle-l\langle H_0+H_2\rangle\langle\Xi_{\nu\mu}\rangle +(\mathbf{c}:\mathbf{\Sigma})_{\nu\mu}=0\,, \tag{3.5}$$

where we use the notation $\langle\cdots\rangle$ to denote an average over valleys

$$\langle\Xi_{\nu\mu}\rangle\equiv\frac{1}{l}\sum_{i=1}^{l}\Xi_{\nu\mu}{}^{(i)}\,. \tag{3.6}$$

TABLE II. Constants of silicon.

Constants	Values	References
c_{11}	1.66×10^{12} dyn cm^{-2}	a
c_{12}	0.64×10^{12} dyn cm^{-2}	a
m_l	$0.91m_0$	b
m_t	$0.19m_0$	b
μ_d	1100 cm^2 V^{-1} sec^{-1}	c
μ_H	1600 cm^2 V^{-1} sec^{-1}	c
τ	2.1×10^{-13} sec	From Eq. (D4)
Ξ_u	1.5×10^{-11} ergs	d

[a] C. Kittel, *Introduction to Solid State Physics* (John Wiley & Sons, Inc., New York, 1956), 2nd ed., p. 93.
[b] G. Dresselhaus, A. F. Kip, and C. Kittel, Phys. Rev. **98**, 368 (1955).
[c] F. J. Morin and J. P. Maita, Phys. Rev. **96**, 28 (1954).
[d] I. Balslev, Phys. Rev. **143**, 636 (1966).

In principle we should have expanded F_i to second order in ϵ_{0j} rather than to first order. Then the first term in Eq. (3.4) would contain a first-order correction in $\Sigma_{\nu\mu}$. However, such a term could be absorbed into the $(\mathbf{c}:\mathbf{\Sigma})$ term in Eq. (3.4), merely altering the effective elastic constants. This contribution to the elastic constants has been calculated by Keyes,[8] and his result can be recovered by the method indicated above. The change in the elastic constants is very small (of the order of 10^{-4} for reasonable values of N) and we henceforth ignore this correction.

Similarly, the terms involving H_{0i} and the first term in Eq. (3.5) represent contributions to $\Sigma_{\nu\mu}$ which are field-independent. They give a volume dilatation dependent on the number of conduction electrons. We write

$$\mathbf{\Sigma}=\mathbf{\Sigma}_0+\delta\mathbf{\Sigma}\,, \tag{3.7}$$

where

$$\mathbf{c}:\mathbf{\Sigma}_0=-N\langle\boldsymbol{\Xi}\rangle+l\langle H_0\rangle\langle\boldsymbol{\Xi}\rangle-l\langle H_0\boldsymbol{\Xi}\rangle\,. \tag{3.8}$$

Of course, H_{0i} is independent of i, so the last two terms cancel. Then, inverting the matrix $\mathbf{c}$ and invoking Eq. (2.26) for H_{2i},

$$\delta\mathbf{\Sigma}=\tfrac{1}{2}e^2\tau^2\frac{\partial N}{\partial\mu}\mathbf{c}^{-1}: \left[\left\langle\left(\mathbf{E}\cdot\frac{1}{\mathbf{m}^*}\cdot\mathbf{E}\right)\boldsymbol{\Xi}\right\rangle-\left\langle\mathbf{E}\cdot\frac{1}{\mathbf{m}^*}\cdot\mathbf{E}\right\rangle\langle\boldsymbol{\Xi}\rangle\right]. \tag{3.9}$$

This is the basic equation of our theory and it remains only to evaluate $\partial N/\partial\mu$. This is a standard problem in semiconductor theory, which reduces to the numerical integration of certain Fermi functions. Numerical tables have been given by J. S. Blakemore.[9] We have abstracted Table I, recasting it in a form convenient for our purpose. We there give $(1/\beta N)(\partial N/\partial\mu)$ as a function of $(N/l)(m_0/m_e)^{3/2}$, where m_e is the free-electron mass.

It may be noted that in the nondegenerate limit where $f_i{}^0\simeq\exp\beta(\mu-\epsilon_i)$, we have immediately that

$$\partial N/\partial\mu=\beta N\text{ (nondegenerate)}\,. \tag{3.10}$$

Finally, we note that the relaxation time τ is ambiguous in the sense that measurements of the quantity by conductivity or Hall experiment give somewhat different results. The relationship of our relaxation time τ to the conventionally measured values is discussed in Appendix D. In applications we obtain τ from Hall and conductivity measurements according to Eq. (D4), although this relation is strictly true only in the nondegenerate case.

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[8] R. W. Keyes, IBM J. Res. Develop. **5**, 266 (1961).

[9] J. S. Blakemore, *Semiconductor Statistics* (Pergamon Press, Inc., New York, 1962), pp. 351, 352, 353.

4. APPLICATION TO SILICON

The simplest case is that of silicon, in which six valleys lie along the cube axes. Each valley has cylindrical symmetry, with a large effective mass m_l along the cube axes and with a small effective mass m_t transverse to the symmetry axes.

From Eq. (3.3) it follows that for the two valleys along the $\pm k_x$ axes

$$\Xi_{11}{}^{(x)}=\Xi_d+\Xi_u,\quad \Xi_{22}{}^{(x)}=\Xi_{33}{}^{(x)}=\Xi_d \tag{4.1}$$

and all other components vanish; similarly for the valleys along $\pm k_y$ and $\pm k_z$. Then

$$\langle\Xi_{\nu\mu}\rangle=(\Xi_d+\tfrac{1}{3}\Xi_u)\delta_{\nu\mu}\,, \tag{4.2}$$

$$\left\langle \mathbf{E}\cdot\frac{1}{\mathbf{m}^*}\cdot\mathbf{E}\right\rangle=\frac{1}{3}\left(\frac{1}{m_l}+\frac{2}{m_t}\right)E^2, \tag{4.3}$$

$$\left\langle \Xi_{\mu\nu}\mathbf{E}\cdot\frac{1}{\mathbf{m}^*}\cdot\mathbf{E}\right\rangle=\frac{1}{3}\left[\Xi_d\left(\frac{1}{m_l}+\frac{2}{m_t}\right)+\frac{\Xi_u}{m_t}\right]E^2\delta_{\mu\nu}+\tfrac{1}{3}\Xi_u\left(\frac{1}{m_l}-\frac{1}{m_t}\right)E_\mu{}^2\delta_{\mu\nu}\,, \tag{4.4}$$

whence

$$\left[\left\langle \Xi_{\mu\nu}\mathbf{E}\cdot\frac{1}{\mathbf{m}^*}\mathbf{E}\right\rangle-\langle\Xi_{\mu\nu}\rangle\left\langle \mathbf{E}\cdot\frac{1}{\mathbf{m}_1{}^*}\cdot\mathbf{E}\right\rangle\right]=\tfrac{1}{9}\Xi_u\left(\frac{1}{m_t}-\frac{1}{m_l}\right)(E^2-3E^2{}_\mu)\delta_{\mu\nu}. \tag{4.5}$$

Inverting the matrix for the elastic constants

$$\begin{aligned}(c^{-1})_{11}&=\frac{c_{11}+c_{12}}{(c_{11}-c_{12})(c_{11}+2c_{12})}\,,\\ (c^{-1})_{12}&=\frac{-c_{12}}{(c_{11}-c_{12})(c_{11}+2c_{12})}\,,\\ (c^{-1})_{44}&=1/c_{44}.\end{aligned} \tag{4.6}$$

Finally, we calculate the strain components by inserting Eq. (4.5) into (3.9),

$$\delta\Sigma_{xx}=\frac{1}{18}e^2\tau^2\frac{\partial N}{\partial\mu}\left(\frac{1}{m_t}-\frac{1}{m_l}\right)\times(c_{11}-c_{12})^{-1}\Xi_u(E^2-3E_x{}^2). \tag{4.7}$$

And similarly for $\delta\Sigma_{yy}$ and $\delta\Sigma_{zz}$. Also

$$\delta\Sigma_{xy}=\delta\Sigma_{xz}=\delta\Sigma_{yz}=0. \tag{4.8}$$

It follows from (4.7) and (4.8) that the volume dilatation ($=\delta\Sigma_{xx}+\delta\Sigma_{yy}+\delta\Sigma_{zz}$) vanishes, as do all shear components. An applied field simply produces an elongation along the field direction, with a volume-preserving contraction perpendicular to the field direction.

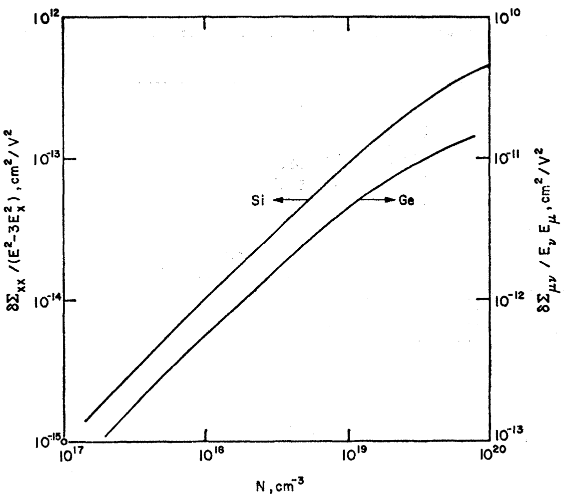

FIG. 1. The induced strain as a function of the electron concentration at room temperature.

The various constants necessary for calculating $\delta\Sigma_{xx}$ for silicon are given in Table II.

In Fig. 1 we plot $\delta\Sigma_{xx}/(E^2-3E_x{}^2)$ as a function of N for silicon. We note that for fields of the order of 10^2 V/cm, at room temperature, the dilatation has the very small value of $\approx 10^{-10}$.

5. APPLICATION TO GERMANIUM

In germanium there are eight valleys, lying along body diagonals. Again each valley has cylindrical symmetry, with a large effective mass m_l along the body diagonal and with a small effective mass m_t transverse to the symmetry axis.

From Eq. (3.3) we find that for the valleys along [111] the deformation potential is

$$\boldsymbol{\Xi}^{[111]}=\Xi_d\mathbf{1}+\tfrac{1}{3}\Xi_u\begin{bmatrix}1&1&1\\1&1&1\\1&1&1\end{bmatrix} \tag{5.1}$$

and for the valleys along $[\bar{1}11]$

$$\boldsymbol{\Xi}^{[\bar{1}11]}=\Xi_d\mathbf{1}+\tfrac{1}{3}\Xi_u\begin{bmatrix}1&-1&-1\\-1&1&1\\-1&1&1\end{bmatrix} \tag{5.2}$$

and similarly for valleys along $[1\bar{1}1]$ and $[11\bar{1}]$. Then

$$\langle\Xi_{\nu\mu}\rangle=(\Xi_d+\tfrac{1}{3}\Xi_u)\delta_{\nu\mu}\,, \tag{5.3}$$

$$\left\langle \mathbf{E}\cdot\frac{1}{\mathbf{m}^*}\cdot\mathbf{E}\right\rangle=\frac{1}{3}\left(\frac{1}{m_l}+\frac{2}{m_t}\right)E^2, \tag{5.4}$$

and

$$\left\langle \Xi_{\nu\mu}\mathbf{E}\cdot\frac{1}{\mathbf{m}^*}\cdot\mathbf{E}\right\rangle-\langle\Xi_{\nu\mu}\rangle\left\langle \mathbf{E}\cdot\frac{1}{\mathbf{m}^*}\cdot\mathbf{E}\right\rangle=\frac{1}{9}\left(\frac{1}{m_l}-\frac{1}{m_t}\right)\Xi_uE_\nu E_\mu(1-\delta_{\nu\mu})\,, \tag{5.5}$$

TABLE III. Constants of germanium.

Constants	Values	References
c_{44}	0.6×10^{12} dyn cm^{-2}	a
m_l	$1.6m_0$	b
m_t	$0.082m_0$	b
μ_d	3800 cm^2 V^{-1} sec^{-1}	c
μ_H	4200 cm^2 V^{-1} sec^{-1}	c
τ	5.3×10^{-13} sec	From Eq. (D4)
Ξ_u	3.0×10^{-11} erg	d

[a] C. Kittel, *Introduction to Solid State Physics* (John Wiley & Sons, Inc., New York, 1956), 2nd ed., p. 93.

[b] G. Dresselhaus, A. F. Kip, and C. Kittel, Phys. Rev. **98**, 368 (1955).

[c] F. J. Morin, Phys. Rev. **93**, 62 (1954).

[d] I. Balslev, Phys. Rev. **143**, 636 (1966).

and of course Eqs. (4.6) are again applicable. We now find that the linear dilatations vanish

$$\delta\Sigma_{xx}=\delta\Sigma_{yy}=\delta\Sigma_{zz}=0. \tag{5.6}$$

It should be recalled, however, that we have neglected a small contribution arising from the strain-induced change in the effective mass.(11) Similarly, we find shear strains.

$$\delta\Sigma_{\nu\mu}=\frac{1}{18}\tau^2e^2\frac{\partial N}{\partial\mu}c_{44}^{-1}\left(\frac{1}{m_t}-\frac{1}{m_l}\right)\Xi_uE_\nu E_\mu. \tag{5.7}$$

The various constants necessary for calculating $\delta\Sigma_{\nu\mu}$ are given in Table III.

In Fig. 1 we plot $\delta\Sigma_{\nu\mu}/E_\nu E_\mu$ as a function of N for germanium. For fields of the order of 10^2 V/cm at room temperature and in the nondegenerate limit, the induced shear strains are of the order of 10^{-8}.

CONCLUSION

We have calculated that fields of 100 Volts/cm. should produce strains of the order of 10^{-8} in germanium with $N\simeq10^{18}/\text{cm}^3$. This is to be compared with strains of the order of 10^{-12} to be expected in homopolar crystals. The theory also predicts that the strain should be 100 times smaller in silicon. More detailed predictions of angular and temperature dependence also emerge from the theory. Comparison of theory and experiment is, however, premature. We are now extending the calculations to include the effects of impurities and of p-type conductivity. These results and detailed comparisons will be given in a subsequent publication.

APPENDIX A

We show that the total number of electrons in the conduction-band valleys is independent of the ϵ_{0i}, to first order in the ϵ_{0i}.

We assume a set of donor states of s symmetry. This implies that the Wannier functions of the donor states have equal admixture of the Bloch waves from all valleys. It then follows that the energy of the impurity state shifts symmetrically with the valley energies:

$$\epsilon_{\text{impurity}}=\epsilon^0{}_{\text{impurity}}-\frac{1}{l}\sum_{i=1}^{l}\epsilon_{0i}. \tag{A1}$$

Similarly the density of electrons in all l valleys is

$$N=2\sum_{i=1}^{l}\sum_{\mathbf{k}(i)}\tilde{f}_i(\mathbf{k})=2\sum_{i}\sum_{\mathbf{k}(i)}\times[\exp\beta(-\tilde{\mu}+\epsilon_{0i}+\epsilon_{1i})+1]^{-1}. \tag{A2}$$

Since the several mass tensors are simply rotated relative to each other, the sum over $\mathbf{k}(i)$ is independent of i, and we can drop the subscript on ϵ_{11}. Then Eq. (A2) can equally well be written, to first order in the ϵ_{0i}, as

$$N=2l\sum_{\mathbf{k}}\left[\exp\beta\left(-\tilde{\mu}+\frac{1}{l}\sum_{i}\epsilon_{0i}+\epsilon_1\right)+1\right]^{-1}. \tag{A3}$$

Comparison of Eqs. (A1) and (A3) shows that all energies in the problem are simply shifted by $(1/l)\sum_{i=1}\epsilon_{0i}$; these include the energy of the impurity state and the *effective* energy of the bottom of the conduction band. Hence $\tilde{\mu}$ also shifts by this amount, and the total density N of electrons in the conduction band stays constant.

If impurity states of symmetry other than s symmetry play a role, then N is not invariant. This case will be treated in a subsequent publication.

APPENDIX B

Within each valley the electric field changes the distribution function at the rate

$$[f_i(\mathbf{k})]_E=-\frac{e}{h}\mathbf{E}\cdot\nabla_{\mathbf{k}}f_i(\mathbf{k}). \tag{B1}$$

The intervalley scattering relaxes $f_i(\mathbf{k})$ towards $\tilde{f}_i(\mathbf{k})$

$$[\dot{f}_i(\mathbf{k})]_{\text{intervalley}}=-(1/\tau_r)[f_i(\mathbf{k})-\tilde{f}_i(\mathbf{k})]. \tag{B2}$$

Finally, the intravalley scattering relaxes $f_i(\mathbf{k})$ towards the local distribution function $f_i{}^*(\mathbf{k})$

$$[\dot{f}_i(\mathbf{k})]_{\text{intravalley}}=-(1/\tau_a)[f_i(\mathbf{k})-f_i{}^*(\mathbf{k})], \tag{B3}$$

where

$$f_i{}^*(\mathbf{k})=[\exp\beta(\epsilon_i(\mathbf{k})-\mu_i)+1]^{-1} \tag{B4}$$

and where μ_i is determined by

$$\sum_{\mathbf{k}(i)}f_i{}^*(\mathbf{k})=\tfrac{1}{2}N_i\equiv\sum_{\mathbf{k}(i)}f_i(\mathbf{k}). \tag{B5}$$

The Boltzmann equation is, then,

$$\frac{1}{\tau_r}[f_i(\mathbf{k})-\tilde{f}_i{}^0(\mathbf{k})]+\frac{1}{\tau_a}[f_i(\mathbf{k})-f_i{}^*(\mathbf{k})]=\frac{e}{h}\mathbf{E}\cdot\nabla_{\mathbf{k}}f_i(\mathbf{k}). \tag{B6}$$

We proceed by the standard iteration technique, substituting $\tilde{f}_i(\mathbf{k})$ in the right-hand-member and iterating twice, to find

$$f_i=\left[\frac{\tau}{\tau_a}f_i^*+\frac{\tau}{\tau_r}\tilde{f}_i\right]+e\tau(\mathbf{E}\cdot\mathbf{v}_i)\left[\frac{\tau}{\tau_a}\frac{\partial f_i^*}{\partial\epsilon_i}+\frac{\tau}{\tau_r}\frac{\partial\tilde{f}_i}{\partial\epsilon_i}\right]$$
$$+e^2\tau^2\left[(\mathbf{E}\cdot\mathbf{v}_i)^2\frac{\partial^2\tilde{f}_i}{\partial\epsilon_i^2}+\mathbf{E}\cdot\frac{1}{\mathbf{m}_i^*}\cdot\mathbf{E}\frac{\partial\tilde{f}_i}{\partial\epsilon_i}\right],\quad\text{(B7)}$$

where $v_i(\mathbf{k})=(1/\hbar)\nabla_{\mathbf{k}}\epsilon_i(\mathbf{k})$ is the electron velocity and where τ is the net relaxation time

$$\frac{1}{\tau}=\frac{1}{\tau_r}+\frac{1}{\tau_a}.\quad\text{(B8)}$$

We now sum Eq. (B7) over $\mathbf{k}(i)$. The second term on the right vanishes because the square bracket is even under inversion through the center of the valley, whereas $\mathbf{E}\cdot\mathbf{v}_i$ is odd. Consider the first term arising from the last bracket on the right of Eq. (B7).

$$I=\sum_{\mathbf{k}(i)}(\mathbf{E}\cdot\mathbf{v}_i)^2\frac{\partial^2\tilde{f}_i^*}{\partial\epsilon_i^2}=\sum_{\mathbf{k}(i)}\left(\mathbf{E}\cdot\frac{\hbar}{\mathbf{m}_i^*}\cdot\mathbf{k}_i\right)^2\frac{\partial^2\tilde{f}_i}{\partial\epsilon_i^2}=\sum_{\mathbf{k}(i)}\sum_{\nu i\mu}\left(E_\nu\frac{\hbar}{m_\nu}k_{i\nu}\right)\left(E_\mu\cdot\frac{\hbar}{m_\mu}k_{i\mu}\right)\frac{\partial^2\tilde{f}_i}{\partial\epsilon_i^2}$$
$$=2\sum_\nu\left(E_\nu\frac{1}{m_\nu}E_\nu\right)\sum_{\mathbf{k}(i)}\frac{\hbar^2k_{i\nu}^2}{2m_\nu}\frac{\partial^2\tilde{f}_i}{\partial\epsilon_i^2}=\tfrac{2}{3}\sum_\nu\left(E_\nu\frac{1}{m_\nu}E_\nu\right)\sum_{\mathbf{k}(i)}\epsilon_{1i}\frac{\partial^2\tilde{f}_i}{\partial\epsilon_i^2}=\tfrac{2}{3}\mathbf{E}\cdot\frac{1}{\mathbf{m}_i^*}\cdot\mathbf{E}\int g(\epsilon_{1i})\epsilon_{1i}\frac{\partial^2\tilde{f}_i}{\partial\epsilon_i^2}d\epsilon_i$$
$$=-\left(\mathbf{E}\cdot\frac{1}{\mathbf{m}_i^*}\cdot\mathbf{E}\right)\int g(\epsilon_{1i})\frac{\partial\tilde{f}_i}{\partial\epsilon_i}d\epsilon_i=-\mathbf{E}\cdot\frac{1}{\mathbf{m}_i^*}\cdot\mathbf{E}\sum_{\mathbf{k}(i)}\frac{\partial\tilde{f}_i}{\partial\epsilon_i},\quad\text{(B9)}$$

where the transition to the last line is accomplished by inserting $g(\epsilon_{1i})\sim\epsilon_{1i}^{1/2}$ and integrating by parts. The result (B9) ensures that the sum over $\mathbf{k}(i)$ of the last term in (B7) vanishes. Hence, the sum over $\mathbf{k}(i)$ of Eq. (B7) gives

$$2N_i(\mathbf{E})=\left[2\frac{\tau}{\tau_0}N_i(\mathbf{E})+2\frac{\tau}{\tau_r}\tilde{N}_i\right],\quad\text{(B10)}$$

$$N_i(\mathbf{E})=\tilde{N}_i,\quad\text{(B11)}$$

where $N_i(E)$ is the number of electrons in the ith valley in the presence of a field.

APPENDIX C

Let f_i^0 equal $f_i^0+\eta_i$. Then by a straightforward expansion of Eq. (2.14) we immediately find

$$F_i=F_i^0+\sum_{k(i)}\left[2\eta_i\epsilon_i+2\beta^{-1}\eta_i\ln\frac{f_i^0}{1-f_i^0}\right.$$
$$\left.+\beta^{-1}\frac{\eta_i^2}{f_i^0(1-f_i^0)}+\tfrac{1}{3}\beta^{-1}\eta_i^3\frac{2f_i^0-1}{f_i^{02}(1-f_i^0)^2}\right].\quad\text{(C1)}$$

Taking η_i to be given in (2.7) we then obtain an equation of the form (2.15), but G_{2i}, H_{0i}, and H_{2i} are replaced by G_{21}', H_{0i}', and H_{2i}', where

$$G_{2i}'=2\sum_{\mathbf{k}(i)}g_{2i}\left[\epsilon_{1i}+\beta^{-1}\ln\frac{f_i^0}{1-f_i^0}\right]+G_2,\quad\text{(C2)}$$

$$H_{0i}'=2\sum_{\mathbf{k}(i)}h_{0i}\left[\epsilon_{1i}+\beta^{-1}\ln\frac{f_i^0}{1-f_i^0}\right],\quad\text{(C3)}$$

$$H_{2i}'=2\sum_{\mathbf{k}(i)}h_{2i}\left[\epsilon_{2i}+\beta^{-1}\ln\frac{f_i^0}{1-f_i^0}\right]$$
$$+2\beta^{-1}\sum_{\mathbf{k}(i)}\frac{h_{1i}g_{1i}}{f_i^0(1-f_i^0)}$$
$$+\beta^{-1}\sum_{\mathbf{k}(i)}\frac{2f_i^0-1}{f_i^{02}(1-f_i^0)^2}h_{0i}g_{1i}^2.\quad\text{(C4)}$$

However, inserting

$$f_i^0=[\exp\beta(\epsilon_{1i}-\mu_0)+1]^{-1}.\quad\text{(C5)}$$

The square brackets in Eqs. (C2)–(C4) become μ_0. We then note that Eq. (B9) implies

$$\sum_{\mathbf{k}(i)}g_{2i}=0\quad\text{(C6)}$$

whence, Eq. (C2) reduces to (2.16). By an analysis exactly paralleling that leading to Eq. (B9) (in which $\tilde{f}_i$ is replaced by $\partial f_i/\partial\epsilon_i$) we similarly find

$$\sum_{\mathbf{k}(i)}h_{2i}=0\quad\text{(C7)}$$

and Eq. (C4) thereby reduces to (2.18).

APPENDIX D

The relaxation time τ requires some comment, as there are two distinctly different values in common use, one associated with the drift mobility μ_d, and the other associated with the Hall mobility μ_H. The conductivity relaxation time τ_c is related to the drift mobility by[10,11]

$$\tau_c=\int_0^\infty \tau\epsilon^{3/2}f^0 d\epsilon \Big/ \int_0^\infty \epsilon^{3/2}f^0 d\epsilon = \mu_d/\tfrac{1}{3}e\left(\frac{1}{m_1^*}+\frac{1}{m_2^*}+\frac{1}{m_3^*}\right). \tag{D1}$$

Similarly, the Hall relaxation time τ_H is related to the Hall mobility $\mu_H(=R\sigma_0)$ by

$$\tau_H=\int_0^\infty \tau^2\epsilon^{3/2}f^0 d\epsilon \Big/ \int_0^\infty \tau\epsilon^{3/2}f^0 d\epsilon = \frac{\mu_H}{e}\left(\frac{1}{m_1^*}+\frac{1}{m_2^*}+\frac{1}{m_3^*}\right) \Big/ \left(\frac{1}{m_1^*m_2^*}+\frac{1}{m_2^*m_3^*}+\frac{1}{m_1^*m_2^*}\right). \tag{D2}$$

If we now re-examine our formalism, we note that in the nondegenerate limit, H_{2i} of Eq. (2.21) is proportional to

$$\int_0^\infty \epsilon_i^{3/2} f_i^0 d\epsilon_i .$$

Thus, our τ should be defined as

$$\tau^2\equiv\int_0^\infty \tau^2\epsilon_i^{3/2}f_i^0 d\epsilon_i \Big/ \int_0^\infty \epsilon_i^{3/2}f_i^0 d\epsilon_i \tag{D3}$$

which can also be obtained from (D1) and (D2) by

$$\tau^2=\tau_c\tau_H=\frac{3\mu_H\mu_d}{e^2}\Big/ \left(\frac{1}{m_1^*m_2^*}+\frac{1}{m_2^*m_3^*}+\frac{1}{m_1^*m_2^*}\right). \tag{D4}$$

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Hall Mobility in $SrTiO_3$†

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Electron mobilities in reduced and doped $SrTiO_3$ have been deduced from measurements of the conductivity and Hall coefficient between 1 and 1000°K. Above room temperature, scattering by the highest two longitudinal optical modes determines the mobility. Expressions based on intermediate electron-phonon coupling yield good agreement with experimental results. Below 10°K experiments indicate that ionized impurity scattering is the dominant collision process. Using a screened Coulomb potential, one obtains mobility values of the right order of magnitude.

INTRODUCTION

The quantitative understanding of electron scattering[1] in polar semiconductors has progressed somewhat less than that of scattering in covalent semiconductors.[2] This lag is caused by a number of inherent difficulties. At high temperatures, the mobility of electrons in polar semiconductors is often limited by optical mode scattering, which is governed by an electron-phonon coupling constant α.[3,4] The parameters that appear in α are the effective mass of the electron m^*, the energy of the phonon $\hbar\omega_{\text{ph}}$, and the high- and low-frequency dielectric constants of the medium, ϵ_{op} and ϵ_{stat}. So far, very little has been done theoretically to take into account the energy and wave-vector dependence of these quantities. Moreover, the electrons in a polar material have an effective mass different from that calculated on the basis of a rigid lattice. In a polar crystal an electron will cause a local polarization, which will "dress" the electron. Hence the electron— when moving—will take this "polarization-dressing" along. The

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[1] It is noteworthy that the *Proceedings of the International Conference on the Physics of Semiconductors, Kyoto, 1966* [J. Phys. Soc. Japan Suppl. 21 (1966)] do not contain a single paper (experimental or theoretical) dealing with phonon- or impurity-limited Hall mobilities in semiconductors.

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