suggests the presence of trapping levels. Such traps could increase the majority carrier lifetime and thereby increase the photoconductive sensitivity according to Eq. (5). Further details of a model based on this mechanism will be discussed in a following paper.[17]

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[17] J. N. Humphrey and R. L. Petritz (to be published).

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Modified Deformable Potential for Thermal Scattering of Electrons*

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In order to study thermal scattering of moderately bound electrons in a metal, corrections are considered to a deformable scattering potential. A constant multiple of the dilatation is derived that must be added to account for the correct zero of potential in a homogeneously deformed crystal. In an inhomogeneously deformed crystal (a crystal undergoing thermal vibrations), a function of the strain must be added to take care of charge redistribution. The deformable potential must also be modified to treat umklapp processes consistently. The modification provides that as the phonon wave vector increases in magnitude, some umklapp character must gradually be added to the scattering amplitude.

1. INTRODUCTION

In calculating the thermal scattering of electrons in a metal, one considers each electron to be approximately describable by a Bloch wave function. The thermal distortions of the crystal alter the potential felt by the electrons, and thus scatter the electrons from one Bloch state to another. A central problem in the theory of thermal scattering is to estimate the scattering potential V_{sc}, which is the difference between the actual potential V_d in a thermally deformed crystal and the potential V of an undeformed crystal.

$$V_{\text{sc}}(\mathbf{r})=V_d(\mathbf{r})-V(\mathbf{r}). \tag{1.1}$$

In a vibrating crystal, the displacement $\mathbf{S}_n$ of the ionic core, whose equilibrium position is at $\mathbf{r}_n$, can be expanded in normal modes of the lattice (phonons), as

$$\mathbf{S}_n(\mathbf{r}_n)=N^{-\frac{1}{2}}\sum_{qj}\boldsymbol{\varepsilon}_{qj}[a_{qj}\exp(i\mathbf{q}\cdot\mathbf{r}_n)+a_{qj}^*\exp(-i\mathbf{q}\cdot\mathbf{r}_n)]. \tag{1.2}$$

Here a_{qj} and a_{qj}^* are respectively proportional to the destruction and creation operators for the phonon with wave vector $\mathbf{q}$ and polarization vector $\boldsymbol{\varepsilon}_{qj}$; N is the number of unit cells in the crystal. (Discussion is limited to the case of a single atom per unit cell.) One can also consider Eq. (1.2) as defining a general displacement function $\mathbf{S}(\mathbf{r})$ by replacing $\mathbf{r}_n$ in that equation by the continuous variable $\mathbf{r}$.

Bloch,[1] in his early work on the conductivity of metals, assumed that the potential deforms along with the crystal. That is,

$$V_d(\mathbf{r}+\mathbf{S}(\mathbf{r}))=V(\mathbf{r}). \tag{1.3}$$

The potential in the deformed crystal at the displaced point is equal to the potential of the undeformed crystal at the corresponding equilibrium point. Nordheim[2] used an alternative assumption that the potential in a deformed crystal is the sum of the contributions from the several ion cores, and that each contribution to the potential moves rigidly with the corresponding core. Probably the most satisfactory calculation of the scattering potential to date is Bardeen's self-consistent formulation,[3] but Bardeen's method seems limited to metals whose conduction electrons are nearly free.

The object of the present paper is to find a scattering potential that would also be applicable to moderately tightly bound electrons, such as the d electrons of transition metals. We base our work on the deformable potential, but we suggest three important modifications. (1) In a crystal with a small homogeneous strain, it is necessary to add a constant to the deformable potential in order to maintain the energy of the crystal independent of the strain (to terms linear in the strain). (2) In a crystal with locally varying strain, such as the sinusoidal deformation corresponding to a phonon of finite wavelength, some redistribution of charge takes place to keep the Fermi level constant throughout the crystal. The calculation of this second effect follows closely the work of Hunter and Nabarro.[4] (Bardeen's

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[1] F. Bloch, Z. Physik **52**, 555 (1928); **59**, 208 (1930).

[2] L. Nordheim, Ann. Physik **9**, 607 (1931).

[3] J. Bardeen, Phys. Rev. **52**, 688 (1937).

[4] S. C. Hunter and F. R. Nabarro, Proc. Roy. Soc. (London) **A220**, 542 (1953).

method also involves a redistribution of charge.) Finally, (3) it is necessary to modify the description of the deformable potential to treat umklapp processes.

2. HOMOGENEOUSLY STRAINED CRYSTAL

In this section, we consider the ion cores as rigidly fixed at lattice points. In an unstrained crystal, the Bloch wave functions for the conduction electrons satisfy a Schrödinger equation

$$[-(\hbar^2/2m)\nabla^2+V(\mathbf{r})-E(\mathbf{k})]\psi(\mathbf{r},\mathbf{k})=0. \tag{2.1}$$

Now apply a homogeneous deformation $\mathbf{S}(\mathbf{r})$ to the entire crystal:

$$\begin{aligned}\mathbf{r}\rightarrow\mathbf{r}'&=\mathbf{r}+\mathbf{S}(\mathbf{r})\\&=(\mathbf{I}+\boldsymbol{\eta})\cdot\mathbf{r},\end{aligned} \tag{2.2}$$

where $\mathbf{I}$ is the identity tensor, and the strain,

$$\eta_{ij}=\tfrac{1}{2}(\partial S_i/\partial r_j+\partial S_j/\partial r_i),$$

is independent of position. Since the crystal is still a perfectly periodic structure, the electrons will again be described by Bloch functions satisfying the equation

$$[-(\hbar^2/2m)\nabla'^2+V_h(\mathbf{r}')-E_h(\mathbf{k}')]\psi_h(\mathbf{r}',\mathbf{k}')=0. \tag{2.3}$$

The subscript h is used to emphasize a homogeneous strain.

It is useful to change the independent variable in Eq. (2.3) from $\mathbf{r}'$ to $\mathbf{r}$ as defined in Eq. (2.2).

Since

$$\nabla^2=\nabla'^2+2\nabla'\cdot\eta\cdot\nabla',$$

the Schrödinger equation for the strained crystal becomes

$$\begin{aligned}[-(\hbar^2/2m)(\nabla^2-2\nabla\cdot\eta\cdot\nabla)+V_h(\mathbf{r}+\mathbf{S}(\mathbf{r}))&\\-E_h(\mathbf{k}')]\psi_h(\mathbf{r}'(\mathbf{r}),\mathbf{k}')&=0.\end{aligned} \tag{2.4}$$

Terms quadratic in the strain have been neglected. We now introduce the fundamental assumption that the potential felt by an electron in a uniformly strained crystal is the deformed potential of the unstrained crystal plus an additive constant (proportional to the strain):

$$V_h(\mathbf{r}+\mathbf{S}(\mathbf{r}))=V(\mathbf{r})+C. \tag{2.5}$$

It is an immediate consequence of this assumption and of Eqs. (2.1) and (2.4) that, to the first order in the strain, the energy of an electron with wave vector $\mathbf{k}'$ in a uniformly strained crystal is related to the energy of an electron with wave vector $\mathbf{k}$ in the unstrained crystal by

$$E_h(\mathbf{k}')-E(\mathbf{k})=C+(\hbar^2/m)\langle k|\nabla\cdot\eta\cdot\nabla|k\rangle \tag{2.6}$$

provided that $\mathbf{k}$ and $\mathbf{k}'$ are connected by the relation

$$\mathbf{r}'\cdot\mathbf{k}'=\mathbf{r}\cdot(\mathbf{I}+\boldsymbol{\eta})\cdot\mathbf{k}'=\mathbf{r}\cdot\mathbf{k}. \tag{2.7}$$

During the process of straining the crystal, as the wave vectors of the individual electrons change from $\mathbf{k}$ to $\mathbf{k}'$, the energies of the electrons will change according to Eq. (2.6). So the total change in energy of the conduction electrons is obtained by summing the right hand side of Eq. (2.6) over all the occupied states of the conduction band (in the unstrained crystal). [Since all of the electrons do not change energy by the same amount, there will be some jumping by electrons near the Fermi level into states of different wave vectors. But the number of electrons that jump will be small, and proportional to the strain. Unless there is a band degeneracy in the immediate neighborhood of the Fermi level—in which case Eq. (2.6) is itself not valid—the energy lost by each electron will also be linear in the strain. So the effect of electron jumps is quadratic in the strain and negligible for the present calculations.]

If (and only if) the crystal is cubic, then in summing the energy changes over the occupied states all shear terms will vanish, and only dilatations will contribute a net change in energy. Since the dilatation is expressed as

$$\Delta=\eta_{xx}+\eta_{yy}+\eta_{zz}, \tag{2.8}$$

the average change in energy per conduction electron can be written as

$$\begin{aligned}\langle E_h-E\rangle_{\mathrm{Av}}&=C+(\hbar^2\Delta/3m)\langle k|\nabla^2|k\rangle_{\mathrm{Av}}\\&=C-(2\Delta/3)(\mathrm{K.E.})_B,\end{aligned} \tag{2.9}$$

where $(\mathrm{K.E.})_B$ is the electron kinetic energy averaged over the occupied states of the conduction band. An almost identical argument indicates that strain produces a shift in the Fermi level F equal to

$$G\Delta=F_h-F=C-(2\Delta/3)(\mathrm{K.E.})_F, \tag{2.10}$$

where the kinetic energy is now to be averaged over the Fermi surface.

So far, no attempt has been made to evaluate the constant C in the potential. This constant is now determined in accord with a stationary property of the energy of the crystal. The work of straining a solid is proportional to the square of the strain produced. So to the first power of strain, the energy of the crystal must be independent of the strain. Presumably in a correct calculation, this stationary property would follow automatically. With an approximate potential such as the deformable potential assumed in Eq. (2.5), the additive constant C may be so chosen to keep the energy constant.

In order to assign a value to C, it would be necessary to know how the separate components of energy (exchange, correlation, and core effects as well as the single-particle energies of the valence electrons) vary with volume. Lacking this information, we propose to determine C so that the direct electronic energy is itself stationary. This then gives for C the value

$$C=(2\Delta/3)(\mathrm{K.E.})_B. \tag{2.11}$$

3. THERMALLY VIBRATING CRYSTAL

Because the lattice motion is slow compared to electronic motions, it is reasonable to treat the lattice motions as adiabatic. Further, in any particular electron scattering process only a single mode of lattice vibration is involved. So we assume that there is a slowly varying local deformation determined by the particular lattice mode doing the scattering. The conduction electrons feel the same potential as in a homogeneously deformed crystal, deformed to the local deformation.

Landauer[5] has pointed out, however, that there is a further correction. If a metal is given a hypothetical nonuniform deformation, without allowing any redistribution of charge, the Fermi level will not be uniform throughout the metal. Hunter and Nabarro[4] have determined the charge redistribution required to equalize the Fermi level, if without any flow of charge the Fermi level fluctuates by an amount $G\Delta$. Let the density of electrons added to any region be $n'(\mathbf{r})$. If this density oscillates with a wave vector $\mathbf{q}$, then it gives rise to an additional Coulomb potential

$$V_C=-4\pi n'e/q^2. \qquad (3.1)$$

The extra electrons added locally to the conduction band raise by an amount $n'/2\rho_F$ the energy level to which states are occupied, where ρ_F indicates density of states per energy interval for a particular spin direction, at the Fermi energy. The condition that the conduction band is everywhere filled to the same energy is that

$$G\Delta+4\pi n'e^2/q^2+n'/2\rho_F=0. \qquad (3.2)$$

From this it follows that

$$n'=-(q^2G\Delta/4\pi e^2)L(q), \qquad (3.3)$$

and so the added potential energy per electron is

$$-eV_C=-G\Delta L(q), \qquad (3.4)$$

where $L(q)$ is an abbreviation for

$$L(q)=[1+(q^2/8\pi e^2\rho_F)]^{-1}. \qquad (3.5)$$

The shift in Fermi level without charge redistribution, $G\Delta$, has already been indicated in Eq. (2.10).

The result of combining Eqs. (1.1), (2.5), and (3.4) can be written as

$$V_{\mathrm{sc}}=V(\mathbf{r}-\mathbf{S}(\mathbf{r}))-V(\mathbf{r})+J(q)\Delta, \qquad (3.6)$$

where $J(q)$ stands for

$$J(q)=(C/\Delta)-GL(q). \qquad (3.7)$$

Except in the immediate neighborhood of core positions $V(\mathbf{r}-\mathbf{S}(\mathbf{r}))$ can reasonably be approximated as $-\mathbf{S}(\mathbf{r})\cdot\mathrm{grad}V$. If for a particular phonon the displacement is written as

$$\mathbf{S}(\mathbf{r})=N^{-\frac{1}{2}}\boldsymbol{\varepsilon}[a\exp(i\mathbf{q}\cdot\mathbf{r})+a^*\exp(-i\mathbf{q}\cdot\mathbf{r})], \qquad (3.8)$$

and the dilatation as

$$\Delta(\mathbf{r})=iN^{-\frac{1}{2}}(\mathbf{q}\cdot\boldsymbol{\varepsilon})[a\exp(i\mathbf{q}\cdot\mathbf{r})-a^*\exp(-i\mathbf{q}\cdot\mathbf{r})], \qquad (3.9)$$

then in terms of Bloch functions of the form

$$\psi(\mathbf{r},\mathbf{k})=N^{-\frac{1}{2}}\exp(i\mathbf{k}\cdot\mathbf{r})u_k(\mathbf{r}),$$

the scattering amplitude between an initial state i and a final state f takes the form

$$\langle f|V_{\mathrm{sc}}|i\rangle=N^{-\frac{1}{2}}\int u_f^*\{[-\boldsymbol{\varepsilon}\cdot\mathrm{grad}V+iJ(q)(\mathbf{q}\cdot\boldsymbol{\varepsilon})]a \times\exp(i\mathbf{K}_+\cdot\mathbf{r})+[-\boldsymbol{\varepsilon}\cdot\mathrm{grad}V-iJ(q)(\mathbf{q}\cdot\boldsymbol{\varepsilon})]a^* \times\exp(i\mathbf{K}_-\cdot\mathbf{r})\}u_i d\mathbf{r}. \qquad (3.10)$$

The integration is over a unit cell of the crystal, and the K vectors, defined by

$$\mathbf{K}_\pm=\mathbf{k}_i\pm\mathbf{q}-\mathbf{k}_f, \qquad (3.11)$$

must be equal to 2π times a reciprocal lattice vector, or zero.

4. NORMAL AND UMKLAPP SCATTERING

A complete set of the wave vectors $\mathbf{k}$ and $\mathbf{q}$ is obtained by using reduced vectors, which are required to lie in some selected unit cell in reciprocal lattice space. This cell is conveniently (but not necessarily) chosen as the first Brillouin zone. Then processes in which $\mathbf{K}_\pm=0$ are called normal, and those in which $\mathbf{K}_\pm$ is equal to 2π times a small reciprocal lattice vector are called umklapp.

As the quantity $|\mathbf{k}_f-\mathbf{k}_i|$ gradually increases, a point is generally reached at which the scattering changes from normal to umklapp. There is no physical reason why the scattering amplitude should change markedly. In fact, which processes are called normal and which umklapp is essentially a matter of bookkeeping. (These remarks have no bearing on questions of the importance of umklapp processes in maintaining phonon equilibrium.) But Eq. (3.10) does predict a sudden change.

The difficulty arises in the expression (3.8) for the displacement of a general point $(\mathbf{r})$ While Eq. (3.8), or Eq. (1.2), describes the same displacement of ion cores if $\mathbf{q}$ is replaced by $\mathbf{q}\pm\mathbf{k}$, this is not true for the displacement of a general point in the crystal. But it is possible—and evidently necessary—to generalize the displacement to a form

$$\mathbf{S}(\mathbf{r})=N^{-\frac{1}{2}}\sum_{qjt}\boldsymbol{\varepsilon}_{qj}X_t\{a_{qj}\exp[i(\mathbf{q}+\mathbf{K}_t)\cdot\mathbf{r}] +a_{qj}^*\exp[-i(\mathbf{q}+\mathbf{K}_t)\cdot\mathbf{r}]\}. \qquad (4.1)$$

Provided only that for every mode

$$\sum_t X_t=1, \qquad (4.2)$$

Eq. (4.1) gives the same displacement for ion cores as the previous expressions for displacement.

The coefficients X_t can now be adjusted so that the

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[5] R. Landauer, Phys. Rev. 82, 520 (1951).

scattering potential of Eq. (3.6) is unaffected by replacing the phonon reduced wave vector $\mathbf{q}$ by an equivalent "expanded" wave vector $\mathbf{q}'=\mathbf{q}+\mathbf{K}$, where as usual $\mathbf{K}$ is 2π times a reciprocal lattice vector. A suggestion in line with the spirit of the deformable potential would be to require that X_t be a function of the magnitude of $|\mathbf{q}+\mathbf{K}_t|$, for example,

$$X_t \propto |\mathbf{q}+\mathbf{K}_t|^{-4}.$$

In calculating scattering amplitudes, it now becomes necessary to sum the contributions due to the various X_t's. For small q's, $X_0 \approx 1$ and all other coefficients are small. On the other hand, when q approaches a zone boundary, and $|\mathbf{q}| \approx |\mathbf{q}+\mathbf{K}_t|$ for some particular t, then $X_0 \approx X_t \approx \frac{1}{2}$. The character of the scattering—whether normal or umklapp—changes gradually as the magnitude of q changes.

5. DISCUSSION

Although the scattering potential developed in this paper is intended to be valid for any metal, it is of interest to examine the case of nearly free electrons, and to compare our results with those of Bardeen.[3] The potential V, which appears explicitly in expression (3.10) for the scattering amplitude, can be eliminated by use of the Schrödinger equation.[6] We write the resulting expression for that part of the scattering amplitude corresponding to phonon absorption:

$$\begin{aligned}\langle f|V_{\mathrm{sc}}|i\rangle = iN^{-\frac{1}{2}}a\Big\{&(\mathbf{q}\cdot\boldsymbol{\varepsilon})J(q)\int u_f^*\exp(i\mathbf{K}_+\cdot\mathbf{r})u_i d\mathbf{r}\\ &+i\{E_f-E_i-(\hbar^2/2m)[(\mathbf{k}_f+\mathbf{K}_+)^2-\mathbf{k}_i^2]\}\\ &\times\int u_i\boldsymbol{\varepsilon}\cdot\mathrm{grad}[u_f^*\exp(i\mathbf{K}_+\cdot\mathbf{r})]d\mathbf{r}-2(\hbar^2/2m)\\ &\times\int(\mathbf{q}\cdot\mathrm{grad}u_i)\boldsymbol{\varepsilon}\cdot\mathrm{grad}[u_f^*\exp(i\mathbf{K}_+\cdot\mathbf{r})]d\mathbf{r}\Big\}. \qquad (5.1)\end{aligned}$$

If we consider normal scattering, and neglect any dependence of the u's on k, then the first integral in Eq. (5.1) is just the normalization integral, and equal to unity. With the same approximation, the second integral vanishes, and the third integral is $[2m(\mathbf{q}\cdot\boldsymbol{\varepsilon})/3\hbar^2]$ times the kinetic energy of an electron with $\mathbf{k}=0$. So the normal scattering amplitude is

$$\begin{aligned}\langle f|V_{\mathrm{sc}}|i\rangle = iN^{-\frac{1}{2}}a(\mathbf{q}\cdot\boldsymbol{\varepsilon})\tfrac{2}{3}\{&(\mathrm{K.E.})_B-(\mathrm{K.E.})_0\\ &+L(q)[(\mathrm{K.E.})_F-(\mathrm{K.E.})_B]\}. \qquad (5.2)\end{aligned}$$

Of the subscripts on the several kinetic energies, B indicates an average over the occupied states of the band, F implies the average over the Fermi surface, and 0 refers to the $k=0$ state. For nearly free electrons, the band should have standard energy dependence, for which

$$(\mathrm{K.E.})_B-(\mathrm{K.E.})_0=\tfrac{3}{5}[(\mathrm{K.E.})_F-(\mathrm{K.E.})_0]=\tfrac{3}{5}\zeta. \qquad (5.3)$$

The bracket in Eq. (5.2) reduces to

$$[\tfrac{3}{5}+\tfrac{2}{5}L(q)]\zeta. \qquad (5.4)$$

A comparison with Bardeen's work now leads to the following conclusions. (1) Our expressions (5.2) and (5.4) agree precisely with Bardeen's result for forward scattering ($\mathbf{q}=0$). They decrease with increasing q, but less rapidly than Bardeen's work indicates. (2) There are minor differences in the q dependence of the correction $L(q)$ due to the potential of the redistributed charge. The constant ρ_F of our expression (5.4) replaces a slowly varying function $[N/W(K)]$ of q in Bardeen's paper. And this potential correction applies to the entire scattering potential in his work, instead of only $\frac{2}{5}$ of it, as in our expression (5.4). (3) But there is an essential difference in q dependence, which arises from our use of a deformable potential, in contrast to the use of a rigid-core potential as the basis of Bardeen's calculation. The rigid core introduces a phase factor $\exp(\pm i\mathbf{q}\cdot\mathbf{r})$ into the integrals corresponding to our Eqs. (3.10) or (5.1) even for normal scattering, and gives rise to a coefficient $[g(u)]$ in the scattering amplitude that decreases rapidly with q. Neither the deformable potential nor the rigid-core potential can be rigorously justified as correct starting points, and it is not obvious how to make an *a priori* choice between them.

The importance of $J(q)$ to Eqs. (5.1) and (5.2) should be pointed out. In the absence of $J(q)$, the bracket in Eq. (5.2) would become $-(\mathrm{K.E.})_0$. Rapid oscillations of the wave functions of the conduction electrons close to the nucleus, particularly for the larger principal quantum numbers, can make $(\mathrm{K.E.})_0$ several times as great as the Fermi energy ζ of Eqs. (5.3) and (5.4).

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[6] A. Sommerfeld and H. A. Bethe, *Handbuch der Physik* (Verlag Julius Springer, Berlin, 1933), Vol. 24, Part 2, p. 512.