Frequency Dependence of High-Frequency Transport Properties of Cubic Crystals*

KEITH S. CHAMPLIN
Electrical Engineering Department, University of Minnesota, Minneapolis, Minnesota
(Received 2 January 1963).

To the first and second orders in electric and magnetic fields, respectively, isothermal transport properties of a uniform cubic crystal are described by five coefficients. With sinusoidally varying electric field, the coefficients are complex functions of frequency. This paper discusses the frequency dependence of the coefficients for the case of electrons occupying states near nondegenerate energy minima arranged with cubic symmetry. The frequency dependence is found to be strongly influenced by the mechanism of the electron-lattice interaction.

I. INTRODUCTION

It has been shown by Seitz,[1] using a phenomenological argument, that the five coefficients of the equation

$$\mathbf{J}=\sigma\mathbf{E}+\alpha(\mathbf{E}\times\mathbf{B})+\beta(\mathbf{B}\cdot\mathbf{B})\mathbf{E}+\gamma(\mathbf{E}\cdot\mathbf{B})\mathbf{B}+\delta\{E_xB_x^2\hat{\imath}+E_yB_y^2\hat{\jmath}+E_zB_z^2\hat{k}\} \quad (1)$$

describe the isothermal transport properties of a uniform crystal with cubic symmetry to the first and second orders in electric and magnetic fields, respectively. The orthogonal xyz axes in Eq. (1) are aligned with the cubic axes of the crystal. Although the five coefficients defined above are directly calculable from the Boltzmann equation, dc experiments generally measure the components of a resistivity tensor inverse to (1). Comparison between theory and experiment then involves intermediate calculations relating the coefficients of the resistivity and conductivity tensors.[2]

When the electric field is varied as $e^{i\omega t}$, the five coefficients are complex functions of frequency. As in the dc case, the complex coefficients are not directly observed in a high-frequency (hf) experiment but must be related to measured quantities through intermediate calculations. These calculations embrace a variety of forms because of the extreme diversity of experimental techniques employed at the frequencies of interest,[3] generally in the microwaves.

The present paper discusses the frequency dependence of the five coefficients for the case of electrons occupying nondegenerate energy minima arranged with cubic symmetry. The frequency dependence is shown to be substantially affected by the mechanism of the electron-lattice interaction. This sensitivity to the details of the interaction mechanism is seen to increase with ascending powers of the magnetic field and suggests that hf transport properties can be used to study scattering processes in solids. Microwave techniques for measuring the zero- and first-order coefficients, σ and α, have recently been described by the author.[4,5] A companion technique for measuring the second-order coefficients will be the subject of a forthcoming paper.

II. Hf TRANSPORT PROPERTIES

If the electron-lattice interaction can be described by a relaxation time τ, the hf, low-field transport properties follow from the dc properties by the substitution of $\tau'=\tau/(1+i\omega\tau)$ for τ. This well-known result of the Boltzmann equation is the basis of the work that follows.

A. Many-Valley Model

Herring and Vogt[6] have formulated a transport theory for the nondegenerate, many-valley model based on a relaxation time tensor with energy-dependent principal components $\tau_\perp(\epsilon)$ and $\tau_{\parallel}(\epsilon)$. Their results can be generalized to the hf case[7] by replacing these components by $\tau_\perp'(\epsilon)$ and $\tau_{\parallel}'(\epsilon)$, where

$$\tau_\perp'(\epsilon)=\frac{\tau_\perp(\epsilon)}{1+i\omega\tau_\perp(\epsilon)} \quad (2)$$

and

$$\tau_{\parallel}'(\epsilon)=\frac{\tau_{\parallel}(\epsilon)}{1+i\omega\tau_{\parallel}(\epsilon)}. \quad (3)$$

In terms of the weighted average

$$\langle x\rangle=\int_0^\infty f_0(\epsilon)[1-f_0(\epsilon)]\epsilon^{3/2}x(\epsilon)d\epsilon \Big/ \int_0^\infty f_0(\epsilon)[1-f_0(\epsilon)]\epsilon^{3/2}d\epsilon, \quad (4)$$

in which $f_0(\epsilon)$ is the Fermi function, the frequency-dependent coefficients are written

$$\sigma(\omega)=\frac{nq^2}{3}\left(2\frac{\langle\tau_\perp'\rangle}{m_\perp^*}+\frac{\langle\tau_{\parallel}'\rangle}{m_{\parallel}^*}\right), \quad (5)$$

* Supported by AF Office of Scientific Research of the Office of Aerospace Research, under Contract No. AF 49(638)-747.

[1] F. Seitz, Phys. Rev. **79**, 372 (1950).
[2] G. L. Pearson and H. Suhl, Phys. Rev. **83**, 768 (1951).
[3] See, for example, T. S. Benedict and W. Shockley, Phys. Rev. **89**, 1152 (1953); J. K. Furdyna and S. Broersma, *ibid.* **120**, 1995 (1960); N. Watanabe, J. Phys. Soc. Japan **16**, 1979 (1961); T. Fukuroi and M. Date, Sci. Rept. Res. Inst. Tohoku Univ. **A9**, 190 (1957).
[4] K. S. Champlin, Physica **28**, 1143 (1962).
[5] K. S. Champlin and D. B. Armstrong, IEEE Trans., **MTT-11**, 73 (1963).
[6] C. Herring and E. Vogt, Phys. Rev. **101**, 944 (1956).
[7] J. K. Furdyna and M. E Brodwin, Phys. Rev. **124**, 740 (1961).

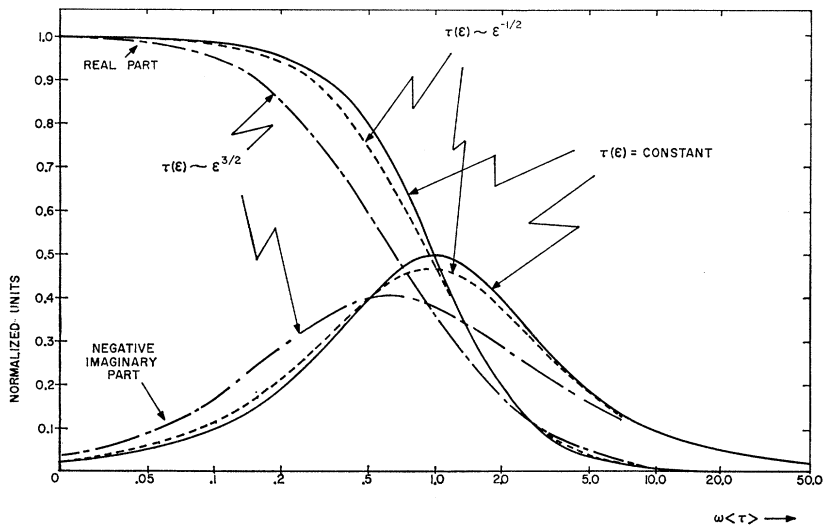

FIG. 1. Real and negative imaginary parts of $\sigma(\omega)/\sigma(0)$ for $\tau_\perp(\epsilon)=\tau_{\parallel}(\epsilon)=\tau(\epsilon)$ and nondegenerate statistics.

$$\alpha(\omega)=\frac{nq^3}{3}\left(\frac{\langle\tau_\perp'^2\rangle}{m_\perp^{*2}}+2\frac{\langle\tau_\perp'\tau_{\parallel}'\rangle}{m_\perp^*m_{\parallel}^*}\right), \tag{6}$$

$$\left.\begin{matrix}\beta(\omega)\\ \gamma(\omega)\\ \delta(\omega)\end{matrix}\right\}=\frac{nq^4}{3}\left(K_1\frac{\langle\tau_\perp'^3\rangle}{m_\perp^{*3}}+K_2\frac{\langle\tau_\perp'^2\tau_{\parallel}'\rangle}{m_\perp^{*2}m_{\parallel}^*}+K_3\frac{\langle\tau_\perp'\tau_{\parallel}'^2\rangle}{m_\perp^*m_{\parallel}^{*2}}\right), \tag{7}$$

where n and q are the electron density and charge, respectively, and $m_\perp^*$ and $m_{\parallel}^*$ are principal components of the effective mass tensor. The constants in Eq. (7) are tabulated in Table I for the two cases which occur in crystals with cubic symmetry.

TABLE I. Magnetoconductivity constants defined in Eq. (7) for valleys on the [100] and on the [111] symmetry axes, respectively.

	[100] valleys			[111] valleys		
	K_1	K_2	K_3	K_1	K_2	K_3
β	−1	−1	−1	−2/3	−5/3	−2/3
γ	0	3	0	2/3	5/3	2/3
δ	1	−2	1	−2/3	4/3	−2/3

Equations (5), (6), and (7) can be evaluated for specific cases by numerical integration of (4). The evaluation requires knowledge of $\tau_\perp(\epsilon)$ and $\tau_{\parallel}(\epsilon)$ which, in turn, are determined by the mechanism of the electron-lattice interaction. One sees that, in general, each of the five coefficients is a different function of frequency.

The frequency dependence has a simple form if the electrons interact with the lattice through neutral impurity scattering; through intervalley phonon scattering from either acoustic or optical modes; or, in nonpolar crystals, through intravalley optical mode scattering. For these cases,

$$\tau_\perp(\epsilon)=\tau_{\parallel}(\epsilon)=\tau(\epsilon) \tag{8}$$

is a good approximation[8] so that Eqs. (5)–(7) yield

$$\frac{\sigma(\omega)}{\sigma(0)}=\frac{\langle\tau/(1+i\omega\tau)\rangle}{\langle\tau\rangle}, \tag{9}$$

$$\frac{\alpha(\omega)}{\alpha(0)}=\frac{\langle\tau^2/(1+i\omega\tau)^2\rangle}{\langle\tau^2\rangle}, \tag{10}$$

$$\frac{\beta(\omega)}{\beta(0)}=\frac{\gamma(\omega)}{\gamma(0)}=\frac{\delta(\omega)}{\delta(0)}=\frac{\langle\tau^3/(1+i\omega\tau)^3\rangle}{\langle\tau^3\rangle}. \tag{11}$$

If the effective mass is highly anisotropic, Eqs. (9)–(11) may also apply quite well to intravalley acoustic mode scattering[8]; however, ionized impurity scattering is generally poorly described by[6] Eq. (8) thus requiring the more general form, Eqs. (5)–(7).

B. Single-Valley Model

When the many-valley model degenerates to the case of a single valley centered at $k=0$, cubic symmetry requires that

$$m_\perp^*=m_{\parallel}^*=m^*, \tag{12}$$

and requires further that

$$\tau_\perp(\epsilon)=\tau_{\parallel}(\epsilon)=\tau(\epsilon) \tag{13}$$

will apply to *every* type of scattering. Thus, Eq. (7) yields $\beta=-\gamma$, $\delta=0$; and from Eqs. (5)–(7),

$$\frac{\sigma(\omega)}{\sigma(0)}=\frac{\langle\tau/(1+i\omega\tau)\rangle}{\langle\tau\rangle}, \tag{14}$$

$$\frac{\alpha(\omega)}{\alpha(0)}=\frac{\langle\tau^2/(1+i\omega\tau)^2\rangle}{\langle\tau^2\rangle}, \tag{15}$$

$$\frac{\beta(\omega)}{\beta(0)}=\frac{\gamma(\omega)}{\gamma(0)}=\frac{\langle\tau^3/(1+i\omega\tau)^3\rangle}{\langle\tau^3\rangle}. \tag{16}$$

[8] C. Herring, Bell System Tech. J. 34, 237 (1955).

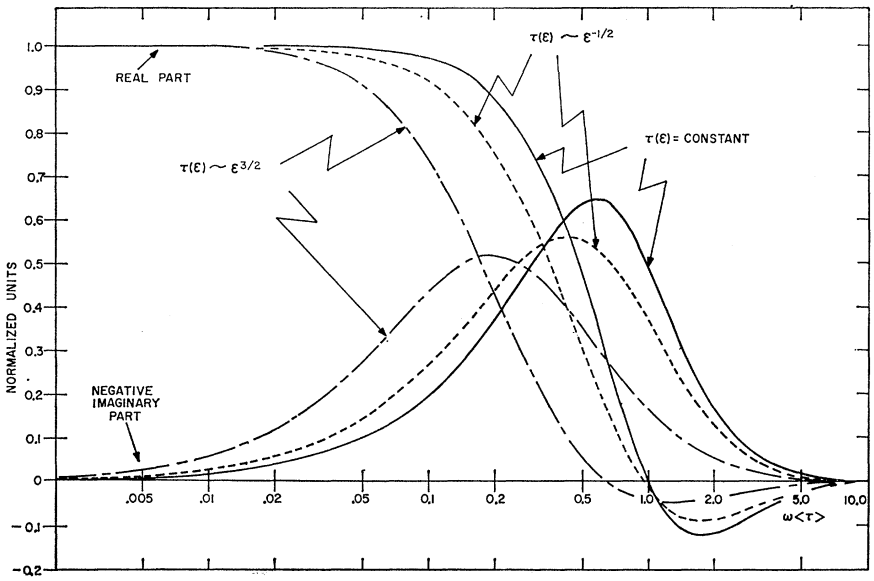

FIG. 2. Real and negative imaginary parts of $\alpha(\omega)/\alpha(0)$ for the same model. Note shift in frequency scale.

Intervalley scattering is, of course, nonexistent for the single-valley model; and for intravalley scattering from either the acoustic modes[9] or from dislocations[10] one has

$$\tau(\epsilon) \propto \epsilon^{-1/2}, \tag{17}$$

while for neutral impurity scattering[11]

$$\tau(\epsilon) = \text{const}, \tag{18}$$

and for ionized impurity scattering[12]

$$\tau(\epsilon) \propto \epsilon^{3/2}. \tag{19}$$

Equations (14)–(16) have been evaluated as functions of $\omega\langle\tau\rangle$ for the cases of nondegenerate statistics and $\tau(\epsilon)$ given by either (17), (18), or (19). For $\tau(\epsilon)$ proportional to $\epsilon^{-1/2}$ and $\epsilon^{3/2}$, the integrations were performed numerically with a digital computer. The results, shown in Figs. 1–3, also apply to the many-valley

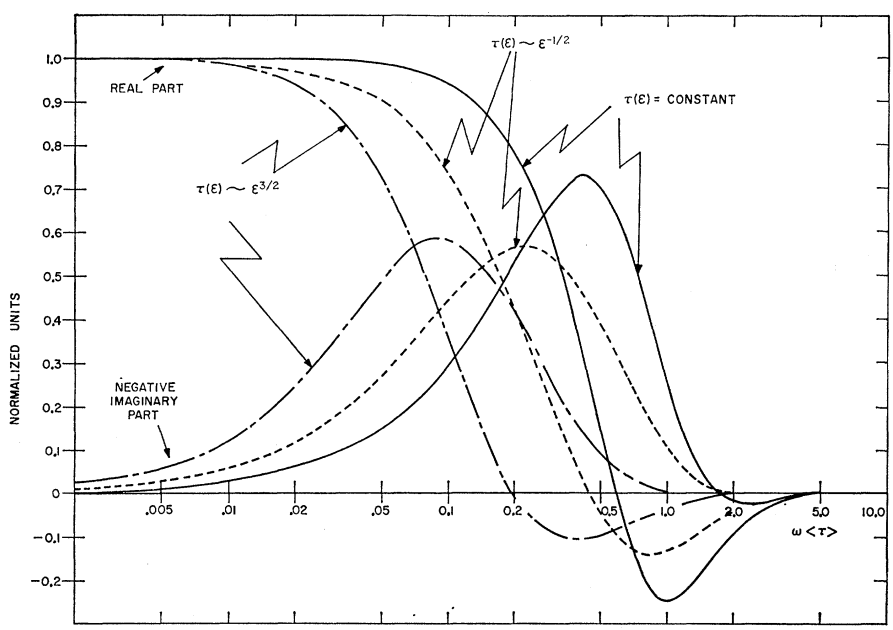

FIG. 3. Real and negative imaginary parts of $\beta(\omega)/\beta(0) = \gamma(\omega)/\gamma(0)$ for the same model.

[9] W. Shockley and J. Bardeen, Phys. Rev. **77**, 407 (1949).
[10] W. T. Read, Phil. Mag. **45**, 775 (1954).
[11] C. Erginsoy, Phys. Rev. **79**, 1013 (1950).
[12] E. M. Conwell and V. F. Weisskopf, Phys. Rev. **77**, 388 (1950).

model if Eqs. (17)–(19) correctly describe the electron-lattice interaction.

III. CONCLUSIONS

From Figs. 1–3, one sees that the nature of the electron-lattice interaction becomes increasingly important in determining the frequency dependence with ascending powers of the magnetic field. It appears that any deviation from a constant relaxation time will move frequency-dependent effects to correspondingly lower frequencies. Indeed, with ionized impurity scattering, the imaginary part of $\beta(\omega)$ reaches its maximum when $\omega\langle\tau\rangle$ is less than one-tenth.

One would expect intervalley scattering to have a large effect on the frequency dependence for many-valley semiconductors because of the extreme way it influences $\tau(\epsilon)$.[8] Also, since the theory predicts that the three second-order coefficients have the same frequency dependence when the relaxation time is a scalar function of energy, comparison of these quantities should yield information concerning anisotropy of the relaxation time tensor.

PHYSICAL REVIEW VOLUME 130, NUMBER 4 15 MAY 1963

Calculated Vibrational Spectra and Specific Heats of Lithium and Vanadium*

JOHN B. HENDRICKS† AND HENRY N. RISER
Texas Instruments Incorporated and Southern Methodist University, Dallas, Texas

AND

CLIFTON BOB CLARK
Southern Methodist University, Dallas, Texas
(Received 3 January 1963)

Vibrational spectra and specific heats have been calculated for lithium and vanadium, from measured elastic constants, on the basis of three different models. Two of the models are of the Born-von Kármán type. One of these considers only central forces between nearest and next-nearest neighbors; the other includes noncentral forces between nearest neighbors and central forces between next-nearest neighbors. The third model is due to de Launay. The calculated quantities from all models are compared with the available empirical values and values calculated by others. It is concluded that none of the models is a satisfactory representation of either metal.

INTRODUCTION

THE availability of measured elastic constants for vanadium and lithium now permits the computation of the vibration spectra of these two metals without having to resort to derived elastic constants. The vibration spectra have been determined using three well-known force models.

In one model the atomic interactions are assumed to be central forces between nearest and next-nearest neighbors in the bcc lattice structure. This model is called the *central model* in this paper. The calculated frequency spectra for 18 values of the ratio of the next-nearest-neighbor force constant to that for nearest neighbors have been reported previously by Clark,[1] and calculations for the specific heats of seven bcc elements were reported later.[2]

In a second model, interactions of a noncentral nature between nearest neighbors are considered as well as central interactions between next-nearest neighbors. The model is characterized, then, by 3 force constants. This model has been described by Leibfried,[3] for example, and was employed by Singh and Bowers[4] for the calculation of the spectrum of vanadium; however, their calculations employed elastic constants deduced from low-temperature specific-heat data. This model is referred to as the *noncentral model* in this paper.

The third phenomenological model is due to de Launay.[5] In this model it is presumed that the conduction electrons in a metal respond in-phase to longitudinal components of lattice waves, but are not influenced by transverse components. This response modifies the force constants so that one set is effective for transverse components and a different set is effective for longitudinal components. This model will be called the *de Launay model* in this paper. (It should be pointed out that de Launay proposed a model which would reduce to this

* Some of the work reported here formed parts of the theses presented by Hendricks and Riser to the Faculty of the Graduate School of Southern Methodist University in partial fulfillment of the requirements for the degree of Master of Science.

† Present address: Physics Department, Rice University, Houston, Texas.

[1] C. B. Clark, J. Grad. Res. Center **29**, 10 (1961).

[2] C. B. Clark, Phys. Rev. **125**, 1898 (1962).

[3] G. Leibfried, in *Handbuch der Physik*, edited by S. Flügge (Springer-Verlag, Berlin, 1955), Vol. 7, Pt. 1, p. 104.

[4] D. N. Singh and W. A. Bowers, Phys. Rev. **116**, 279 (1959).

[5] J. de Launay, in *Solid State Physics*, edited by F. Seitz and D. Turnbull (Academic Press Inc., New York, 1956), Vol. 2, p. 219.