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PHONON SPECTRUM OF A SHOCKED SOLID

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ABSTRACT: The Boltzmann equation for the phonon distribution function is derived for a medium undergoing large strains in the hydrodynamic approximation (driving frequency less than the collision frequency). The phase space in which the Boltzmann equation holds is found to be different from that phase space composed of ordinary position and "crystal momentum" spaces common to the linear theory. A transformation, involving the volume dependence of the sound speed, is shown to relate the two different spaces.

Existing linear theory is reexamined with the idea of developing a firm understanding of the physics of amplitude independent phonon-phonon sound absorption in insulators. This understanding of the linear theory is used to develop a collision term which is valid in the presence of large strains. It is shown that, in the large strain hydrodynamic approximation, it is valid to neglect umklapp processes.

Finite strain theory is used to develop a Hamiltonian for a single phonon in the presence of large amplitude deformations. Using the Hamiltonian and the collision term, the Boltzmann equation is solved in the long wave length approximation with temperature and strain as independent variables. The solution so obtained is shown to reduce to the linear theory in the limit of small strains. The anisotropy of the large amplitude solution is discussed with respect to the anisotropy of the linear theory and from the point of view of the order of the phonon-phonon interactions.

Thermoelastic equations are developed, and the Burgers equation is investigated with the hope of finding simultaneous solutions for the strain and temperature (as functions of position and time) for substituting into our solution of the microscopic physics Boltzmann equation. The concept of an irreversible contribution to the stress tensor, $T_{ij}^{(I)}$, is used in the thermoelastic equations and $T_{ij}^{(I)}$ is found for the special case of dislocation induced linear internal friction in the limit of large time. The thermal part of the thermoelastic equations is developed for arbitrary strain, although only a first order perturbation mechanical equation is found.

Based upon our understanding of linear theory, and other simple considerations, it is shown that the phonon drift is large only in the region of the shock front. The most fruitful area for future work is discussed.

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This report treats the problem of predicting the mutual interaction between a large amplitude shock wave and the phonon spectrum of the host solid. The principal result is a relation giving the distribution of phonons among the various phonon states as a function of temperature, strain, strain gradient, Gruneisen parameter, and the angle which the phonon propagation vector makes with respect to the direction of shock propagation.

The work, theoretical in nature, was carried out in the Explosion Dynamics Division, Explosions Research Department, under FR-52 the Dynamic Properties of Solids, and is based upon a thesis submitted to the University of Maryland in partial fulfillment of the requirements of the degree of Doctor of Philosophy. It is hoped that this work will be of interest to those concerned with the shock loading of solids, both from a research and an applications point of view.

The author wishes to thank all of his colleagues at NOL who may have read and/or commented on various parts of the work presented here. In addition, special thanks go to Drs. R. F. Greene and Z. I. Slawsky for encouragement and many useful discussions.

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By direction

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List of Important Symbols

a	Lattice constant
a_0	Lattice constant for zero strain
a^*	Sound speed for zero strain
$\hbar$	Planck's constant divided by 2π
k	Boltzmann's constant
u	Particle displacement in the z direction
u_k	Particle displacement in the k^{th} direction
$\vec{q}$	2π divided by phonon wave length
u_p	Particle velocity in the laboratory coordinate system
u'_p	Particle velocity with respect to a moving coordinate system
x_k	Position coordinate in the k direction. $x_3 = z$
E	Energy of lattice vibrations
$N_u(\vec{q})$	Number of phonons with polarization u in state $\vec{q}$
P	Pressure
Q	Heat energy density in Lagrangian coordinates
S	Entropy density in Lagrangian coordinates
T	Absolute temperature
T_{ij}	Stress tensor
U	Internal energy density in Lagrangian coordinates
V	Volume
γ_c	Ratio of constant pressure to constant volume specific heats
ξ_e	Strain energy density in Lagrangian coordinates
$\delta_{u\ell}$	1 if $u=\ell$, 0 otherwise

ζ_1	Shear viscosity coefficient
ζ_2	Volume viscosity coefficient
η	Geometrical strain. $\eta = \frac{\partial u}{\partial z}$
κ	Thermal conductivity
$\bar{\kappa}$	Compressibility
K_d	Thermal diffusivity
ρ	Mass density
χ'	Viscosity like coefficient
τ	Phonon-phonon relaxation time
τ_N	Phonon-phonon relaxation time for normal processes
τ_u	Phonon-phonon relaxation time for umklapp processes
χ_1	Viscosity coefficient
$\hbar\omega(\vec{q})$	Energy of phonon in state $\vec{q}$
Ω_p	2π times the frequency at which the Fourier spectrum of the strain peaks
ϵ	The zz component of the Lagrangian finite strain tensor

FORWARD

To date there has been no known attempt to describe a shock wave in a solid from the point of view of modern solid state physics. There had been no attempt to relate the spectrum of the thermal excitation quasi-particles (phonons) to the time dependent large amplitude strain existing in the medium. With few exceptions those interested in the theory of shock waves had concerned themselves with a study of hydrodynamics, while solid state physicists have only rarely been interested in amplitude dependent sound propagation.

A description of shock wave phenomena in the vocabulary of modern solid state physics seems very appropriate at the present time. It has become apparent that pressure is a parameter to be varied in the same sense that temperature is varied in solid state experiments, and shock waves are a means of arriving at very high pressures. Furthermore shock waves occur widely in nature: A few causes of shock waves are earthquakes, meteor impact on space satellites, and various ordnance related effects. Included in the latter group of manmade shocks are earth waves due to underground nuclear explosions, the detection of which has recently become a very important politico-scientific problem. It was, of course, hoped that a better understanding of the basic phenomena involved in shock propagation in solids would lead to corresponding advances in the related technology. We must also mention that an understanding of the phonon spectrum of a deforming solid is an important first step in the treatment of such problems as the galvanomagnetic effects in the presence of shock waves.

In the development of the theory presented in this thesis we have found it necessary to do both macroscopic and microscopic physics simultaneously. This was because we were unable to find a completely self consistent treatment on the microscopic level and found it necessary to develop and use macroscopic thermoelastic equations as an aid in predicting microscopic behavior. Even this simultaneous macro-micro approach left something to be desired in that we were forced to limit our mechanical part of the thermoelastic equations to amplitudes so small that perturbation techniques remained valid (the primarily thermal equation was under no such restriction). It is because of this perturbation limitation that our microscopic treatment of large strain phenomena is rather incomplete - i.e. the corresponding macroscopic treatment is lacking.

We believe the most fruitful areas for future research in this field to be (a) the derivation of "macro" thermoelastic equations which are explicitly consistent with the microscopic approach, and (b) the development of thermoelastic equations which are valid for large strains.

At this time, unfortunately, we are unable to give hints on how one should proceed.

The author would like to acknowledge the assistance and encouragement of his mentor, Prof. Zaka I. Slawsky. In addition, Dr. Richard F. Greene of the Naval Ordnance Laboratory has been an always available sounding board and a constant source of beneficial criticism. This work was only possible because of the generous funding by the Naval Ordnance Laboratory under their Foundational Research Program.

I. INTRODUCTION

The thermal energy of a crystalline solid is representable in terms of elementary excitations known as phonons. For a uniform isotropic harmonic solid that representation takes the form[1],[*] [‡]

$$E(T) = \hbar \sum_{\vec{q},\mu} \omega_\mu(\vec{q}) \left[N_\mu(\vec{q},T) + \tfrac{1}{2} \right] , \qquad \text{Eq.(1-1a)}$$

$$\omega_\mu(\vec{q}) = q \left[\frac{\alpha \delta_{\mu\ell} + \beta}{\rho} \right] , \qquad \text{Eq.(1-1b)}$$

where the summation is over allowed values[1,2] of $\vec{q}$ and the polarization μ. Longitudinal is indicated by ℓ in Eq. (1-1b), $N_\mu(\vec{q},T) \equiv N_\mu(\vec{q}) \equiv N$ is the number of phonons in the state $(\mu,\vec{q})$ and α and β are elastic constants.

Elastic constants are functions of crystal structure (i.e. lattice parameter), and the allowed values of q are also structure sensitive. Thus it is obvious that a disturbance in the density also results in a disturbance in $N_\mu(\vec{q})$ and $\omega_\mu(\vec{q})$. One would consequently expect to be able to represent the propagation of an elastic strain pulse by an equivalent propagation of disturbances in $N_\mu(\vec{q})$ and $\omega_\mu(\vec{q})$. It is that concept which has motivated the work described in this paper.

In Chapter II linear theory is used to calculate $N_\mu(\vec{q})$ as a function of position and time. Chapter III presents the macroscopic treatment of strain propagation in a nonlinear thermoviscous medium. In Chapter IV we

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[*] See list of important symbols.
[‡] References are on page 71.

solve the Boltzmann equation in the presence of large amplitude strains and consider the attenuation of large amplitude shock waves. A discussion and suggestions for future work are found in Chapter V.

II. LINEAR THEORY

A. The Boltzmann Equation

In 1961 Woodruff and Ehrenreich[3] successfully explained the observed[4],[5] decay of small amplitude hypersonic waves in insulators by employing phonon relaxation times appropriate to the phonon-phonon interaction. In the process of arriving at expressions for the attenuation they developed a formalism for the disturbance of $N_\mu(\vec{q})$ and $\omega_\mu(\vec{q})$ as a function of time and position. We will present that formalism here, but in a form modified to admit strains of arbitrary position and time. We consider only isotropic solids.

Let us restrict ourselves to a one dimensional longitudinal strain type of problem such that particle velocity and propagation are both in the z direction and all physical quantities depend only upon z and t. We drop the polarization index μ and consider only the distribution function for longitudinal acoustic phonons. The effect of strain propagation on other polarizations and branches is mentioned in Chapter VI. As our propagating strain can, at least intuitively at the outset, be thought of as composed of a drifting cloud of longitudinal acoustic phonons restricting ourselves to a study of the distribution function for such phonons should not be frowned upon.

It is useful to define three phonon distribution functions.

$$N_o(\omega_o,T_o)=\left[\exp\left(\frac{\hbar\omega_o}{kT_o}\right)-1\right]^{-1}\equiv N_o(\omega_o)$$ Eq. (2-1a)

$$N_o(\omega,T)=\left[\exp\left(\frac{\hbar\omega}{kT}\right)-1\right]^{-1}\equiv N_o(\omega)$$ Eq. (2-1b)

and $N(\vec{q};\ z,t)$. The first, $N_0(\omega_0,T_0)$, is a Planck type distribution function and gives the probability of finding a phonon in the state $(\omega_0,T_0)$where the subscript zero refers to the undisturbed medium. The second, $N_0(\omega_0,T)$, is also Planck type and gives a similar probability for a solid which has been deformed and has reached a new equilibrium configuration characterized by the temperature T(as well as the strain). By assuming a phonon mean free path small compared to the shock front thickness we will be able to use $N_0(\omega,T)$locally - i.e. we will assume that as a shock wave passes over a differential volume of our solid that differential volume passes through a succession of equilibrium states which are described by Eq.(2-1b). This restriction on the phonon mean free path being small compared to the shock front thickness is known as the hydrodynamic approximation and is employed throughout this paper. $N(\vec{q};z,t)$ gives the instantaneous distribution function.

The difference between $N(\vec{q};z,t)$ and $N_0(\omega,T)$ is controlled by the relaxation processes of importance and has prompted[8] the invention of a function $\Phi(\vec{q};\eta,u)$. u is the particle displacement in the z direction, $\eta \equiv \frac{\partial u}{\partial z}$, and

$$N(\vec{q};z,t) \equiv N_0(\omega) - \frac{N_0'}{kT_0}\,\Phi(\vec{q};\eta,u) , \qquad \text{Eq. (2-2a)}$$

$$N_0' \equiv \frac{dN_0(\omega_0)}{d\left(\frac{\hbar\omega_0}{kT_0}\right)} = -N_0^2(\omega_0)\exp\left(\frac{\hbar\omega_0}{kT_0}\right) . \qquad \text{Eq. (2-2b)}$$

Let us next consider the Hamiltonian for a single phonon*

$$H(\vec{q};z,t) = H_0(\vec{q}) + H_1(\vec{q};z,t) \equiv \hbar\omega(\vec{q};z,t) , \qquad \text{Eq. (2-3a)}$$

$$H_1(\vec{q};z,t) \equiv a(\vec{q};\eta,u)H_0(\vec{q}) , \qquad \text{Eq. (2-3b)}$$

where H_1 is the perturbation resulting from strain. The functional dependence contained in Eq. (2-3b) is consistent as η and u are functions of z and t. As $N_0(\omega)$ is a Planck type distribution function we have to first order in $\left(\frac{H_1}{kT}\right)$

$$N_0(\omega) = \left[\exp\left(\frac{\hbar\omega}{kT}\right) - 1\right]^{-1} = \left[\left(1 + \frac{H_1}{kT}\right)\exp\left(\frac{\hbar\omega_0}{kT}\right) - 1\right]^{-1} , \qquad \text{Eq. (2-4a)}$$

$$N_0(\omega) = N_0(\omega_0) - N_0^2(\omega_0)\left(\frac{H_1}{kT}\right)\exp\left(\frac{\hbar\omega_0}{kT}\right) . \qquad \text{Eq. (2-4b)}$$

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*The ability to consider the Hamiltonian of a single phonon, the justification of Eq. (2-7), and the identification of the collision term in the Boltzmann equation is treated and made valid in Appendix A.

In Eqs. (2-4) we have used $H_0(\vec{q}) = \hbar\omega_0(\vec{q})$. Combining Eqs. (2-2) and (2-4) gives

$$N(\vec{q}\,; z,t) = N_0(\omega_0) + \left(\frac{N_0'}{kT}\right)(H_1 - \Phi), \qquad \text{Eq. (2-5)}$$

or

$$N(\vec{q}\,; z,t) \equiv N_0(\omega_0) + N_1(\vec{q}\,; z,t), \qquad \text{Eq. (2-6)}$$

where $N_1(q; z,t)$ is the perturbation in phonon occupation number. In order to solve for N_1, which is now our task, we must have an equation of motion for the phonon distribution. From Eq. (A-16) that equation of motion is given by

$$\frac{\partial N}{\partial t} + \frac{1}{\hbar}\left[\frac{\partial N}{\partial z_1}\frac{\partial H}{\partial q_3} - \frac{\partial N}{\partial q_3}\frac{\partial H}{\partial z_1}\right] = \frac{\partial N}{\partial t}\bigg|_{coll}, \qquad \text{Eq. (2-7a)}$$

or to first order

$$\frac{\partial N_1}{\partial t} + \frac{1}{\hbar}\left[\frac{\partial N_1}{\partial z}\frac{\partial H}{\partial q_3} - \frac{\partial N_0}{\partial q_3}\frac{\partial H_1}{\partial z}\right] = \frac{\partial N}{\partial t}\bigg|_{coll}, \qquad \text{Eq. (2-7b)}$$

where H_1 denotes the effect of strain upon a single phonon state. In Eq. (2-7a) z_1 is not an external variable in the sense of size, but rather an internal (dummy) variable which is canonically conjugate[6] to the internal (dummy) variable q_3. In transforming from z_1 to position in a fixed coordinate system one uses the sound speed which, for large strains, is position dependent (see Appendix A). For first order theory, however, it is valid to consider z_1 as a position coordinate. Thus, in Eq. (2-7b) z may be interpreted as the position of a phonon wave packet.

Aside from the $\frac{\partial N_1}{\partial t}$ term we see that inhomogeneities must be present in N_1 and H_1 in order to have a non zero effect. This is equivalent to saying that the presence of a shock (wave) front results in scattering, and is in agreement with our introductory ideas. $\frac{\partial N_1}{\partial t}$ is non zero only in the presence of an explicit time dependence in the perturbed phonon density. Since, in principal, we are interested here in a strongly time dependent problem the $\frac{\partial N_1}{\partial t}$ term must be retained. If we can now equate $\left.\frac{\partial N}{\partial t}\right|_{coll.}$ to a known expression for a particular scattering mechanism then, since H_1 is assumed known, we can find Φ .

A theoretical expression[7] for the effect of phonon-phonon interactions is

$$\left.\frac{\partial N}{\partial t}\right|_{coll.} = -\frac{N(\vec{q}; z, t) - N_0(\omega; T', \lambda)}{\tau_N(\vec{q})} - \frac{N(\vec{q}; z, t) - N_0(\omega, T'', 0)}{\tau_u(\vec{q})}, \text{ Eq. (2-8)}$$

which assumes that the return to equilibrium follows an exponential law. τ_N and τ_u are relaxation times for the so-called[1,2,7] normal and "umklapp" processes respectively, and $N_0(\omega; T', \lambda)$ is the distribution function which the normal scattering processes relax towards with T' being the equilibrium temperature. The normal processes conserve "crystal momentum" so that it is possible for the phonon "gas" to have $\left[\sum_i \vec{q}_i\right]$ a constant of the motion, where the sum is over the allowed values of $\vec{q}_i$. One thus associates[7,8,9] a phonon "gas" drift velocity, λ, with the equilibrium density function*

$$N_0(\omega; T', \lambda) = \left[\exp\left(\frac{\hbar\omega - \lambda q_3}{kT'}\right) - 1\right]^{-1}. \qquad \text{Eq. (2-9)}$$

In Eq. (2-8), by writing two different temperatures T' and T'', we have allowed for the possibility of the normal and the umklapp processes relaxing to different equilibrium temperatures as well as to different drift velocities. By this we mean that an umklapp gas and a normal collision gas must necessarily have different equations of state. If, however, we allow the possibility that $(T' - T'')$ is proportional to the drift velocity λ then, as shown in Chapter IV, $\left(\frac{T' - T''}{T'}\right)$ is small compared to unity in the hydrodynamic approximation. We thus set $T' = T''$ in the remainder of this chapter.

Let $T' = T_0 + (\Delta T)$ in Eq. (2-9) and expand to first order

$$N_0(\omega, T', \lambda) \cong \left[\exp\left\{\frac{\hbar\omega}{kT_0}\left(1 - \frac{\Delta T}{T_0}\right)\right\} \exp\left\{-\frac{\lambda q_3}{kT_0}\left(1 - \frac{\Delta T}{T_0}\right)\right\} - 1\right]^{-1}, \qquad \text{Eq. (2-10a)}$$

$$N_0(\omega; T', \lambda) \cong \left[\exp\left\{\frac{\hbar\omega}{kT_0}\right\} \left\{1 - \frac{\hbar\omega}{kT_0}\left(\frac{\Delta T}{T_0}\right)\right\}\left\{1 - \frac{\lambda q_3}{kT_0}\right\} - 1\right]^{-1}, \qquad \text{Eq. (2-10b)}$$

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*Conserving "crystal momentum" means conserving $\vec{q}$ so that for a three phonon process the normal processes insure $\vec{q}_1 + \vec{q}_2 = \vec{q}_3$, where the numerical subscripts refer to individual phonons. On the other hand "umklapp" processes satisfy $\vec{q}_1 + \vec{q}_2 = \vec{q}_3 + \vec{G}$, where $\vec{G}$ is a non-zero vector in the reciprocal lattice. In Eq.(2-8) $\lambda=0$ is taken for the "umklapp" part since λ results from a Lagrange's Multiplier type of argument which only occurs for conserved quantities.

$$N_0(\omega;T',\lambda) \cong \frac{N_0(\omega;T_0,0)}{1-N_0(\omega;T_0,0)\left\{\frac{\hbar\omega}{kT_0}\left(\frac{\Delta T}{T_0}\right)+\frac{\lambda q_3}{kT_0}\right\}} , \qquad \text{Eq. (2-10c)}$$

and

$$N_0(\omega;T',\lambda) \cong N_0(\omega;T_0,0) - \left(\frac{N_0'}{kT_0}\right)\left[\hbar\omega_0\left(\frac{\Delta T}{T_0}\right)+\lambda q_3\right] . \qquad \text{Eq. (2-10d)}$$

In keeping with our first order desires we have substituted ω_0 for ω in the second term on the right in Eq. (2-10d). We also recognize that $N_0(\omega;T,o)$ is identical with the distribution function given by Eq. (2-4). Substituting Eq. (2-2a) and Eq. (2-10d) into Eq. (2-8) yields

$$\left.\frac{\partial N}{\partial t}\right|_{\text{coll.}} = -\frac{1}{\tau}\left(\frac{N_0'}{kT_0}\right)\left[\hbar\omega_0\left(\frac{\Delta T}{T_0}\right)-\Phi\right] - \frac{1}{\tau_n}\left(\frac{N_0'}{kT_0}\right)\lambda q_3 , \qquad \text{Eq. (2-11)}$$

where $\frac{1}{\tau(\vec{q})} \equiv \frac{1}{\tau_n(\vec{q})} + \frac{1}{\tau_u(\vec{q})}$ has been used.

The following calculations are useful for substitution into Eq. (2-7c);

$$\frac{\partial H_0}{\partial q_3} = \hbar\frac{\partial\omega_0}{\partial q_3} = \hbar c_3(\vec{q}) \equiv \hbar c_3 , \qquad \text{Eq. (2-12a)}$$

$$\frac{\partial N_0}{\partial q_3} = -N_0^2(\omega_0)\frac{\hbar c_3}{kT_0}\exp\left(\frac{\hbar\omega_0}{kT_0}\right) = N_0'\,\frac{\hbar c_3}{kT_0} . \qquad \text{Eq. (2-12b)}$$

Thus from Eqs. (2-6a), (2-7c), and (2-12)

$$\left.\frac{\partial N}{\partial t}\right|_{\text{coll.}} = \left(\frac{N_0'}{kT_0}\right)\left[\frac{\partial H_1}{\partial t} - \frac{\partial\Phi}{\partial t} - c_3\frac{\partial\Phi}{\partial z}\right] . \qquad \text{Eq. (2-13)}$$

And, upon equating Eq. (2-11) and Eq. (2-13) we find

$$\frac{\partial H_1}{\partial t} - \frac{\partial\Phi}{\partial t} - c_3\frac{\partial\Phi}{\partial z} = -\frac{1}{\tau}\left[\hbar\omega_0\left(\frac{\Delta T}{T_0}\right)-\Phi\right] - \frac{\lambda q_3}{\tau_n} . \qquad \text{Eq. (2-14)}$$

Thus we can solve for Φ in terms of (ΔT), λ, and a model for the perturbation Hamiltonian, H_1. We note that Eq. (2-14) is exact to first order. Let us now develop a model for H_1.

Since the energy change associated with a volume change is of the form PdV we expect that, for an isotropic solid[a],

$$\Delta\omega(\vec{q}\,; z,t) = \omega_o(\vec{q}) \sum_{m,n=1}^{3} \gamma_{mn}(\vec{q})\, u_{mn}(z,t), \qquad \text{Eq. (2-15a)}$$

or from Eq. (2-3a)

$$H_1(\vec{q}\,; z,t) = \hbar\omega_o(\vec{q}) \sum_{m,n=1}^{3} \gamma_{mn}(\vec{q})\, u_{mn}(z,t), \qquad \text{Eq. (2-15b)}$$

where $u_{mn}(z,t)$ is the strain tensor[a,10] for small strains.

$$u_{mn}(z,t) = \frac{1}{2}\left(\frac{\partial u_m}{\partial x_n} + \frac{\partial u_n}{\partial x_m}\right), \qquad \text{Eq. (2-16a)}$$

and[10]

$$u_{11} + u_{22} + u_{33} \cong \left(\frac{\Delta V}{V}\right). \qquad \text{Eq. (2-16b)}$$

Since we are only interested in 1-D wave propagation in the z direction, Eq. (2-15b) becomes

$$H_1(\vec{q}\,; z,t) = \hbar\omega_o(\vec{q})\, \gamma_{33}(\vec{q})\, \eta(z,t) \equiv \hbar\omega_o \gamma_{33} \eta, \qquad \text{Eq. (2-17)}$$

where Eq. (2-2c) has been used. γ_{zz}, however, can be related[a] to the Grüneisen constant by $\gamma_{zz} \approx -\gamma$ as is shown below.

The Free Energy[11] density, f, of a strained anharmonic solid can be written[2] as

$$f(z,t) = \frac{1}{2!}\sum_{ijk\ell} G_{ijk\ell}\, u_{ij}\, u_{k\ell} + \frac{1}{3!}\sum_{\substack{ijk\ell\\mn}} G_{ijk\ell mn}\, u_{ij}\, u_{k\ell}\, u_{mn} + \qquad \text{Eq. (2-18)}$$

$$+\left(\frac{kT}{V_0}\right)\sum_{\vec{q}} \ln\left[2\sinh\frac{\hbar\omega(\vec{q},u_{mn})}{2kT}\right],$$

where the strain dependence of the allowed frequencies has been explicitly indicated. V_0 is the unstrained volume, and $G_{ijk\ell}$ and $G_{ijk\ell mn}$ are second and third order elastic constants[2] respectively. If we are able to consider a differential volume of our solid as being in thermal equilibrium then[11], for a given temperature and strain, $\frac{\partial f}{\partial u_{mn}} = 0$. Such an equilibrium condition is possible providing that

(1) $\lambda_p \gg q_{th}^{-1}$. The wavelength at which the Fourier spectrum of the strain peaks, λ_p, is large compared to the wavelength of the most abundant phonons. q_{th} denotes the wave vector for thermal phonons.

(2) $\Omega\tau \ll 1$. Ω_p is the frequency at which the Fourier spectrum of the strain peaks. This allows for the definition of a local temperature.

Assuming thermal equilibrium then gives

$$\sum_{ij} G_{ijmn}\, u_{ij} = -\left(\frac{\hbar}{2V_0}\right) \sum_{\vec{q}} \left(\frac{\partial \omega}{\partial u_{mn}}\right) \coth\left[\frac{\hbar\omega(\vec{q})}{2kT}\right] , \qquad \text{Eq. (2-19)}$$

where only first order terms in the strain have been considered, and $G_{ijk\ell} = G_{k\ell ij}$ has been employed*. And, upon using

$$T_{mn} = \sum_{ij} G_{mnij}\, u_{ij} , \qquad \text{Eq. (2-20a)}$$

$$T_{mn} = -\left(\frac{\hbar}{2V_0}\right) \sum_{\vec{q}} \left(\frac{\partial \omega}{\partial u_{mn}}\right) \coth\left[\frac{\hbar\omega(\vec{q})}{2kT}\right] . \qquad \text{Eq. (2-20b)}$$

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*The symmetry relation $G_{ijk\ell} = G_{k\ell ij}$ is practically a matter of definition. Let us split $G_{ijk\ell}$ into symmetric and anti-symmetric parts

$$G_{ijmn} = G^{(1)}_{ijmn} + G^{(2)}_{ijmn}$$

$$G^{(1)}_{ijmn} \equiv \frac{1}{2}\left(G_{ijmn} + G_{mnij}\right) , \qquad G^{(2)}_{ijmn} \equiv \frac{1}{2}\left(G_{ijmn} - G_{mnij}\right)$$

But the anti-symmetric part, $G^{(2)}_{ijmn}$, is easily shown to contribute nothing to the strain energy density function $\mathcal{E}_e$

$$\mathcal{E}_e = \frac{1}{2} G_{ijk\ell}\, u_{ij}\, u_{k\ell} .$$

Thus in Eq. (2-18) and beyond we shall only mean the symmetrical part of $G_{ijk\ell}$.

Eq. (2-20b) gives the stress in terms of the frequency spectrum and the derivative of the frequency spectrum with respect to strain. And using Eq. (2-15a) in Eq. (2-20b) gives

$$T_{mn} = -\frac{1}{2V_0}\sum_{\vec{q}} \hbar\omega(\vec{q})\,\gamma_{mn}(\vec{q})\coth\left[\frac{\hbar\omega(\vec{q})}{2kT}\right]. \qquad \text{Eq. (2-21)}$$

But it is simply shown[12] that the mean vibrational energy in mode $\vec{q}$, $\overline{E(\vec{q})}$, is given by

$$\overline{E(\vec{q})} = \frac{1}{2}\hbar\omega(\vec{q})\coth\left[\frac{\hbar\omega(\vec{q})}{2kT}\right], \qquad \text{Eq. (2-22a)}$$

$$\therefore T_{mn} = -\frac{1}{V_0}\sum_{\vec{q}} \gamma_{mn}(\vec{q})\,\overline{E(\vec{q})}. \qquad \text{Eq. (2-22b)}$$

And, to the extent that $\gamma_{mn}(\vec{q})$ is independent of $\vec{q}$,

$$T_{mn}(T) = -\frac{\gamma_{mn}}{V_0}\sum_{\vec{q}} \overline{E(\vec{q})} = -\frac{\gamma_{mn}}{V_0}E_{vib}(T). \qquad \text{Eq. (2-22c)}$$

Considering Eq. (2-22c) at some temperature, T_0, allows us to write

$$T_{mn}(T) - T_{mn}(T_0) = -\frac{\gamma_{mn}}{V_0}\left[E_{vib}(T) - E_{vib}(T_0)\right], \qquad \text{Eq. (2-22d)}$$

where in this and all the succeeding formulae the temperature dependence of γ_{mn} has been neglected. Eq. (2-22d) compares with the equation of state[12] for solids in the hydrostatic approximation

$$P(T) - P_K = \frac{\gamma}{V}\left(E_{vib} - E_K\right), \qquad \text{Eq. (2-23)}$$

where γ is Grüneisen's "constant", and P_k and E_k are the pressure and energy at the volume V and some reference temperature, say T_k. In Eq. (2-22d) V_0 is the unstrained volume for both $T_{mn}(T)$ and $T_{mn}(T_\theta)$ to first order in the phonon-phonon coupling (i.e. to first order in γ_{mn}). If we were considering four phonon processes then this approximation would not be possible. A similar statement holds for Eq. (2-23). Furthermore, we are not concerning ourselves with the volume dependence of γ_{mn} since we are considering strains of less than 10^{-3}. We now wish to compare Eqs. (2-22d) and (2-23).

Let us define a pressure, P', by

$$P' = \frac{1}{3}\left[T_{11} + T_{22} + T_{33}\right]. \qquad \text{Eq. (2-24)}$$

P' as defined by Eq. (2-24) is the lowest order non-trivial rotationally[14] invariant quantity of elastic theory, and is thus equal to the pressure of Eq. (2-23) to first order. If we now take the trace of Eq. (2-22d) we find

$$P'(T) - P'_K = -\left(\frac{\gamma_{11} + \gamma_{22} + \gamma_{33}}{3V_0}\right)\left[E_{vib}(T) - E_K\right], \qquad \text{Eq. (2-25)}$$

where Eq. (2-24) has been used. Since we are assuming an isotropic solid it is true that

$$\gamma_{11} = \gamma_{22} = \gamma_{33}, \qquad \text{Eq. (2-26a)}$$

which gives upon equating P to P'

$$\gamma_{33} = -\gamma \qquad \text{Eq. (2-26b)}$$

by comparison with Eq. (2-23). Eq. (2-26b) must hold regardless of the type of strain[15] (one dimensional strain, one dimensional stress, or hydrostatic conditions) as to first order γ is independent of volume and only a function of the medium. In passing let us mention that the theory of the Grüneisen constant (or perhaps better called the Grüneisen tensor*) is very complicated. Indeed one of the experimental facts which must be taken into consideration is its strong temperature dependence[16]; at low temperatures certain materials are known to exhibit a negative thermal expansion coefficient[16] and thus a negative Grüneisen constant.

Using Eqs. (2-14), (2-17), and (2-26b) thus gives

$$\frac{\partial \Phi}{\partial t} + C_3 \frac{\partial \Phi}{\partial z} + \frac{\Phi}{\tau} = \qquad \text{Eq. (2-27)}$$

$$= \frac{\hbar \omega_0}{\tau}\left[\left(\frac{\Delta T}{T_0}\right) - \gamma \tau \frac{\partial \eta}{\partial t}\right] + \frac{\lambda q_3}{\tau_n}.$$

But for the most part Φ follows the frequency spectrum of the applied elastic pulse so that $\left(\frac{\partial \Phi}{\partial t}\right) < \left(\frac{\Phi}{t}\right)$

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* The tensor character of γ_{mn} has been considered by Brugger. See K. Brugger, Phys. Rev. 137, A1826 (1965).

except at the lowest temperatures* where $(\omega\tau)$ approaches unity from below. Also $C_z \frac{\partial\Phi}{\partial z}$ is of equal magnitude as compared to $\frac{\partial\Phi}{\partial t}$ so that

$$\left|\frac{\partial\Phi}{\partial t} + C_3 \frac{\partial\Phi}{\partial z}\right| << \left|\frac{\Phi}{\tau}\right|, \qquad \text{Eq. (2-28)}$$

and

$$\Phi = \hbar\omega_0\left[\left(\frac{\Delta T}{T_0}\right) - \gamma\tau\frac{\partial\eta}{\partial t}\right] + \left(\frac{\tau}{\tau_n}\right)\lambda q_3 . \qquad \text{Eq. (2-29)}$$

And by substituting Eq. (2-29) into Eq. (2-6)

$$N_1(\vec{q}\,; z,t) = \frac{N_0'}{kT_0}\left[\hbar\omega_0\gamma\left(\tau\frac{\partial\eta}{\partial t} - \eta\right) + \right.$$

$$\left. - \hbar\omega_0\left(\frac{\Delta T}{T_0}\right) - \left(\frac{\tau}{\tau_n}\right)\lambda q_3\right].$$

Assuming that a model for $\tau(q)$ and $\tau_n(q)$ exists then the conservation principals for energy and crystal momentum allow one to determine λ and (ΔT) in terms of the impressed variables η and $\frac{\partial\eta}{\partial t}$ (see Appendix B). To be consistent we will neglect the $\tau\frac{\partial\eta}{\partial t}$ term as compared to η for the same reasons as we neglected $\tau\frac{\partial\Phi}{\partial t}$ as compared to Φ .

$$N_1(\vec{q}\,; z,t) = -\frac{N_0'}{kT_0}\left[\hbar\omega_0\gamma\eta + \hbar\omega_0\left(\frac{\Delta T}{T_0}\right) + \left(\frac{\tau}{\tau_n}\right)\lambda q_3\right].$$

Eq. (2-30a)

---

*From thermal conductivity measurements and[8] $\kappa = \frac{1}{3} C\cdot a\cdot \ell$ where κ is the heat conductivity, C the specific heat, a the sound speed, and ℓ the mean free path it is found that temperatures for which $\tau = 10^{-10}$ sec. are

Solid Helium:	2°K	Sapphire:	200°K
Quartz :	50°K	Diamond :	400°K

Let us stop for a moment and attempt to justify the sign of the dependence of N_1 upon η as given by Eq. (2-30a). The sign of its dependence upon (ΔT) is obviously correct. By using Eqs. (2-12b) and (2-30) along with $\eta = \frac{\partial u}{\partial z}$ gives for the strain part of Eq. (2-30a)

$$\frac{N_1(\vec{q};z,t)}{N_0(\omega_0)} = \gamma\left(\frac{\partial u}{\partial z}\right) N_0(\omega_0)\left\{\frac{\hbar\omega_0}{kT_0}\right\}\exp\left\{\frac{\hbar\omega_0}{kT_0}\right\}.$$

Compressional Wave*: $\frac{N_1(\vec{q};z,t)}{N_0(\omega_0)} < 0,$

Rarefaction Wave: $\frac{N_1(\vec{q};z,t)}{N_0(\omega_0)} > 0.$

This makes sense since, according to Eqs. (2-17) and (2-26b), a compression increases the energy associated with each state and $N_0(\omega_0)$ is a decreasing function of energy.

Equation (2-27) can be solved by an alternate procedure. As at this stage we are considering a first order perturbation theory our problem is linearized. Thus it is valid to seek solutions via Fourier analyzing Eq. (2-27) with respect to the time. But this

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*The sign of the strain dependence found here is the same as found by T. H. K. Barron for the corresponding static isothermal problem. See T. H. K. Barron, Phys. Rev. <u>137</u>, A487 (1965).

is in essence the method of Woodruff and Ehrenreich who consider the driving strain to have a single frequency component, $\left(\frac{\Omega}{2\pi}\right)$, and thus derive for their equation corresponding to Eq. (2-30a)

$$N_1(\vec{q};z,t) = -N_0' \frac{\hbar\omega_0}{kT_0} \left[\frac{(1 - ic_3k\tau)\gamma\eta + \left(\frac{\Delta T}{T_0}\right) + \frac{\tau}{\tau_n}\left(\frac{\lambda q_z}{\hbar\omega_0}\right)}{1 - i(\Omega - c_3k)\tau} \right],$$

Eq. (2-30b)

where k is the wave number for the applied strain. It is understood that, in Eq. (2-30b), η, (ΔT), and λ are all given by a modulus times a running wave factor $\exp[i(kz-\Omega t)]$. If we now take the limit $(\Omega\tau) \rightarrow 0$ we arrive at Eq. (2-30a) exactly. Thus, as one would expect for the low amplitude part of the problem, we are in agreement with Woodruff and Ehrenreich.

B. The Conservation Relations

There is not very much practical value in considering conservation relations for our linear theory in the limit $(\Omega_p\tau) \rightarrow 0$. This is because, as shown in Appendix B, for the linear theory in the limit mentioned $\Delta T \rightarrow -\gamma T_0\eta$ and $\lambda_s \rightarrow 0$. It is precisely the value of these variables which one hopes to derive from the conservation relations. Practicality, however, has never been a good physicist's virtue. By studying some general aspects of the conservation relations, but not quite going to the limiting case of the approximations considered above, we hope to learn something for future use. Further mention is made of conservation relations in Chapter V. during the discussion of phonon drift in the presence of large amplitude shock waves.

Consider the crystal momentum $\vec{P}(z,t)$ and the strain energy $E(z,t)$ in our local picture

$$\vec{P}(z,t) \equiv \hbar \int \vec{q}\, N(\vec{q}, z, t)\, d\vec{q} \ , \qquad \text{Eq. (2-31a)}$$

$$E(z,t) \equiv \hbar \int \omega(\vec{q}; z,t)\, N(\vec{q}, z, t)\, d\vec{q} - \hbar \int \omega_0(\vec{q})\, N_0(\vec{q})\, d\vec{q} \ , \qquad \text{Eq. (2-31b)}$$

where E(z,t) represents the strain energy contribution to the crystal energy as well as any time dependent effects contained in $N(q;z,t)$. Integrating Eqs. (2-31) over z gives

$$\vec{P}(t) \equiv \int_{-\infty}^{\infty} \vec{P}(z,t)\, dz, \qquad \text{Eq. (2-32a)}$$

$$E(t) \equiv \int_{-\infty}^{\infty} E(z,t)\, dz. \qquad \text{Eq. (2-32b)}$$

$E(t)$ and $\vec{P}(t)$ are nice functions because

$$\frac{dE(t)}{dt} = \left.\frac{dE(t)}{dt}\right|_{coll.} = \left.\frac{\partial E}{\partial t}\right|_{coll.} \ , \qquad \text{Eq. (2-33a)}$$

and

$$\frac{d\vec{P}(t)}{dt} = \left.\frac{d\vec{P}(t)}{dt}\right|_{coll.} = \left.\frac{\partial \vec{P}}{\partial t}\right|_{coll.} \ , \qquad \left.\frac{\partial \vec{P}}{\partial t}\right|_{n} = 0 \ , \ \text{Eq. (2-33b)}$$

where Eqs. (2-33) assume that there are no external forces acting on the crystal at the time of observation (strain pulse completely contained within crystal). Setting $\frac{\partial E(t)}{\partial t} = 0$ expresses the conservation of energy while the second part of Eq. (2-33b) is a matter of definition; normal processes conserve crystal momentum.

It is understood that a sum over the different branches is contained in the integrations over $\vec{q}$.

Combining Eqs. (2-31) to Eqs. (2-33) results in

$$\hbar \int_{-\infty}^{\infty} dz \int d\vec{q} \left[\omega(\vec{q};z,t) \frac{\partial N(\vec{q};z,t)}{\partial t} + \frac{1}{\hbar} \frac{\partial H_1(\vec{q};z,t)}{\partial t} N(\vec{q};z,t) \right] = 0, \qquad \text{Eq. (2-34a)}$$

where Eq. (2-3a) has been used. Rewriting Eq. (2-34a) to first order

$$\hbar \int_{-\infty}^{\infty} dz \int d\vec{q} \left[\omega_0(\vec{q}) \frac{\partial N_1(\vec{q};z,t)}{\partial t} + \frac{1}{\hbar} \frac{\partial H_1(\vec{q};z,t)}{\partial t} N_0(\vec{q}) \right] = 0. \qquad \text{Eq. (2-34b)}$$

Similarly for the momentum

$$\frac{\partial \vec{P}(t)}{\partial t} = \hbar \int_{-\infty}^{\infty} dz \int d\vec{q} \left[\vec{q} \frac{\partial N(\vec{q};z,t)}{\partial t} \right]. \qquad \text{Eq. (2-34c)}$$

Let us now consider the case when z is not a parameter explictly appearing in the problem*. Thus $N(\vec{q};z,t) \rightarrow N(\vec{q},t)$

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*Throughout the rest of this paper we shall neglect the $\frac{d\vec{q}}{dt}$ term in the partial derivative expansion of $\frac{dN(\vec{q};z,t)}{dt}$ under an integration over $\vec{q}$ and z. To prove this we consider

$$O_3 = \hbar \sum_{m=1}^{3} \int\int d\vec{q}\, dz \left[q_3 \frac{\partial N(\vec{q};z,t)}{\partial q_m} \frac{dq_m}{dt} \right]$$

to first order. Using Hamilton's equations[6] and Eqs. (2-17) and (2-26c) we find

$$O_3 = -\hbar^2 \gamma \int \frac{\partial \eta}{\partial z} \left[\int q_3 \omega_0(\vec{q}) \frac{\partial N(\vec{q};z,t)}{\partial q_3} d\vec{q} \right] dz,$$

or to first order

$$O_3 = -\hbar^2 \gamma \int \frac{\partial \eta}{\partial z} \left[\int q_3 \omega_0(\vec{q}) \frac{\partial N_0(\vec{q})}{\partial q_3} d\vec{q} \right] dz.$$

But to this order the integration over wave number is independent of z so that we need only show (con't next page) and Eq. (2-34c) becomes

$$\frac{\partial \vec{P}(t)}{\partial t} = \hbar \int_{-\infty}^{\infty} dz \int d\vec{q} \left[\vec{q} \, \frac{\partial N}{\partial t} \right] = \hbar \int_{-\infty}^{\infty} dz \int d\vec{q} \left[\vec{q} \, \frac{\partial N(\vec{q}; z, t)}{\partial t} \right], \qquad \text{Eq. (2-35a)}$$

so that

$$\left. \frac{d\vec{P}(t)}{dt} \right|_{n} = \hbar \int_{-\infty}^{\infty} dz \int d\vec{q} \left[\vec{q} \left. \frac{dN}{dt} \right|_{n} \right] = 0. \qquad \text{Eq. (2-35b)}$$

Similarly for the energy, from Eq. (2-34b),

$$\hbar \int_{-\infty}^{\infty} dz \int d\vec{q} \left[\omega_0(\vec{q}) \left. \frac{dN}{dt} \right|_{\text{Coll.}} + \frac{1}{\hbar} \frac{dH_1}{dt} N_0(\vec{q}) \right] d\vec{q} = 0. \qquad \text{Eq. (2-35c)}$$

If the $\frac{dH_1}{dt}$ term in Eq. (2-35c) is negligible than Eqs. (2-35b) and (2-35c) agree with the conservation conditions of Woodruff and Ehrenreich[3]. If Ω_p is the frequency at which the Fourier spectrum of the strain peaks

$$\omega_0 \left. \frac{dN}{dt} \right|_{\text{Coll.}} + \frac{1}{\hbar} \frac{dH_1}{dt} N_0 \simeq - \omega_0 \frac{N_0}{\tau} + \frac{\Omega_p}{\hbar} H_1 N_0 \qquad \text{Eq. (2-36a)}$$

(Con't from previous page)

$$\text{(a)} \quad \int \frac{\partial \eta}{\partial z} dz = 0, \qquad \text{or} \quad \text{(b)} \quad \int q_3 \omega_0(\vec{q}) \frac{\partial N_0(\vec{q})}{\partial q_3} d\vec{q} = 0.$$

Condition (a) is fulfilled in the case of a strain pulse of limited dimensions in an infinite crystal (the problem I am treating). Condition (b) is not fulfilled in the order considered as the integrand is an even function of q_z and the integration extends over both sides of the Brillouin zone. Thus the neglect of the $\frac{dq}{dt}$ term is valid to first order in the momentum condition. The analogous treatment for the energy conservation condition is fulfilled as the corresponding integrand in condition (b) is an odd function of q_z. In the case treated by Woodruff and Ehrenreich[3] the presence of a driver would seem to violate condition (a). Woodruff and Ehrenreich, however, still set the $\frac{dq}{dt}$ term in their energy condition equal to zero - fortunately this should only cause a numerical error in the adjustable and rather uncertain value of Y.

and from Eq. (2-15b) with $\gamma_{zz} = -\gamma$

$$\omega_0 \left.\frac{dN}{dt}\right|_{coll.} + \frac{1}{\hbar}\frac{dH_1}{dt} N_0 \simeq -\omega_0 \frac{N_0}{\tau} - \omega_0 N_0 \Omega_p \gamma \eta \, , \qquad \text{Eq. (2-36b)}$$

$$\therefore \ \omega_0 \left.\frac{dN}{dt}\right|_{coll.} + \frac{1}{\hbar}\frac{dH_1}{dt} N_0 \simeq -\Omega_p \omega_0 N_0 \left[\frac{1}{\Omega_p \tau} + \gamma\eta\right] . \qquad \text{Eq. (2-36c)}$$

Since γ is of the order of unity the $\frac{dH_1}{dt}$ term can be neglected for $\Omega_p\tau \ll 1$ and $\eta < 1$. One may not be able to throw the term away, however, for $\Omega_p\tau \sim 1$ although we shall not concern ourselves with this here. The presence of the $\frac{dH_1}{dt}$ term only means that changes in the energy levels, as well as changes in the occupation numbers are important in determining the energy of the perturbed system. We do not neglect the z dependence as Woodruff and Ehrenreich[3] have done because our strain pulse is allowed to have arbitrary shape, and because we do not wish to exclude the case of strong attenuation.

To sum up. In the absence of a z dependence the conservation conditions to be used with $\Omega_p\tau \ll 1$ and internal pulses are

$$\hbar \int_{-\infty}^{\infty} dz \int d\vec{q} \left[\vec{q} \, \left.\frac{dN(\vec{q}; z,t)}{dt}\right|_{n} \right] = 0 \, , \qquad \text{Eq. (2-35b)}$$

$$\hbar \int_{-\infty}^{\infty} dz \int d\vec{q} \left[\omega_0(\vec{q}) \left.\frac{dN(\vec{q}; z,t)}{dt}\right|_{coll.} \right] = 0 \, , \qquad \text{Eq. (2-37)}$$

where $\left.\frac{dN(\vec{q}; z,t)}{dt}\right|_{n}$ and $\left.\frac{dN(\vec{q}; z,t)}{dt}\right|_{coll.}$ are to be used from Eq. (2-8). In our case, however, we are interested in a problem with explicit z dependence so that we must consider, to first order,

$$\frac{\partial E(t)}{\partial t} = \hbar \int_{-\infty}^{\infty} dz \int d\vec{q} \left[\omega_0(\vec{q}) \frac{\partial N_1(\vec{q};z,t)}{\partial t} \right], \qquad \text{Eq. (2-38a)}$$

$$\frac{\partial \vec{P}(t)}{\partial t} = \hbar \int_{-\infty}^{\infty} dz \int d\vec{q} \left[\vec{q} \; \frac{\partial N_1(\vec{q};z,t)}{\partial t} \right], \qquad \text{Eq. (2-38b)}$$

where, in keeping with the previous footnote,

$$\frac{dN_1(\vec{q};z,t)}{dt} = \frac{\partial N_1(\vec{q};z,t)}{\partial t} + \frac{\partial N_1(\vec{q};z,t)}{\partial z} V(\vec{q};z,t) \qquad \text{Eq. (2-38c)}$$

$v(\vec{q};z,t)$ being the drift velocity for phonons in state $(\vec{q};z,t)$. With the method of attack presented in this paper a model is needed for $\eta(z,t)$ and $T(z,t)$ before further work can be done. We thus leave this chapter and go on to the next where such a model is sought.

III. MACROSCOPIC PHYSICS

In this chapter we would like to supplement our microscopic physics with macroscopic physics. By assuming a knowledge of coefficients (e.g. thermal conductivity and viscosity) in our macroscopic equations we might hope to solve for $\eta(z,t)$ and $T(z,t)$ for possible use in Eq. (2-30a) and subsequent large amplitude work. Ideally this should not be necessary as we might hope to express the strain and temperature as integrals over $N(\vec{q};z,t)$ so that Eq. (2-30a) would be transformed into an integro-differential equation in terms of the single independent variable $N(\vec{q};z,t)$. Unfortunately, at the present time, the recipe for calculating $\eta(z;t)$ and $T(z,t)$ from a given $N(\vec{q};z,t)$ is not known. Reverting to macroscopic physics is a practical necessity.

We consider two different methods of arriving at our macroscopic physics.

(a) The first combines thermodynamics in the presence of irreversible mechanical processes with the mechanical equation of motion for a nonlinear viscous medium. The result is what is usually known as thermoelastic[17] equations denoting a set of coupled strain and temperature equations. While our thermodynamic equations will be quite general we shall have to restrict our mechanical equation to a linear viscous and third order elastic system. In the process of carrying out these calculations we shall introduce an irreversible stress tensor, $T_{ij}^{(I)}$. The work done here differs from previous work in that we calculate $T_{ij}^{(I)}$ for a special case. We find the irreversible stress tensor in the large time limit for linear dislocation induced viscosity.

(b) The second method involves the application of the Burgers[18] equation to the problem of sound propagation in a viscous, thermally conducting, and third order elastic system. By using the strain energy relation for an anharmonic solid we find a number characterizing the nonlinearity of the system in terms of the ratio of a third order to a second order elastic constant. Experimental values of the elastic constants are used to find the nonlinearity factor, and whether weak steady state compressive disturbances will form shocks, in a variety of materials.

A. Thermoelasticity in Dissipative Systems

If we expand[19,20] the volume dependent part of the internal energy, U, to cubic terms in the Lagrangian[10,14] strain ϵ_{ij}, and also consider viscous and thermal effects

$$T_{ij} = \left.\frac{\partial U}{\partial\left(\frac{\partial u_i}{\partial x_j}\right)}\right|_T + T_{ij}\,(\text{viscous}) + \beta\,(\Delta T)\,\delta_{ij}\,, \qquad \text{Eq. (3-1)}$$

where all the quantities are written with respect to coordinates in the undeformed medium (see B. T. Chu, reference 17), and

$$\epsilon_{ij} = \frac{1}{2}\left[\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} + \sum_{k=1}^{3} \frac{\partial u_k}{\partial x_i}\,\frac{\partial u_k}{\partial x_j}\right]. \qquad \text{Eq. (3-2)}$$

We mean for Eq. (3-1) to be only a first order method of combining the different contributions to the total stress tensor. We shall use Eq. (3-1) to derive our mechanical equation. It is presented at the outset because it demonstrates the role of elasticity, viscosity, and thermal expansion in our calculations. We now consider the first law of thermodynamics[10,11]

$$\text{đ}Q = dU - T_{ij}\, d\left(\frac{\partial u_i}{\partial x_j}\right), \qquad \text{Eq. (3-3)}$$

$\text{đ}Q$ is the heat absorbed per unit volume in the differential process, and the barred differential sign before Q indicates that $\text{đ}Q$ may not be a complete differential (i.e. Q depends upon path as well as end points).

$$dS \equiv \frac{dQ^{(R)}}{T} = \frac{dU}{T} - \frac{T_{ij}^{(R)}}{T}\, d\left(\frac{\partial u_i}{\partial x_j}\right), \qquad \text{Eq. (3-4)}$$

where the superscript R means "reversible" and is indicative of the complete differential character of the entropy S (by definition). Our thermodynamic parameters (independent variables) are T and ϵ_{ij} where

$$T = T(z,t), \qquad \epsilon_{ij} = \epsilon_{ij}(z,t). \qquad \text{Eq. (3-5a)}$$

As the internal energy is independent of path

$$U = U(T, \epsilon_{mn}, t), \qquad \text{Eq. (3-5b)}$$

while a general thermodynamic quantity, say T_{ij}, is going to be path dependent so that

$$T_{ij} = T_{ij}(T, \epsilon_{mn}, t). \qquad \text{Eq. (3-5c)}$$

That is path dependence means explicit time dependence.

The heat flow equation can be written

$$\frac{\partial Q}{\partial t} = \kappa \nabla^2 T + W, \qquad \text{Eq. (3-6a)}$$

where κ is the heat conductivity (thermal conductivity), and W is the heat power generated per unit volume by electrical, or chemical, forces (i.e. W is a source term). Let $Q = Q^{(R)} + Q^{(I)}$, where the superscript I means irreversible, so that

$$\frac{\partial Q^{(R)}}{\partial t} = \kappa \nabla^2 T + \left(W - \frac{\partial Q^{(I)}}{\partial t}\right). \qquad \text{Eq. (3-6b)}$$

In Eqs. (3-6) it is understood that the independent variables are (z,t). But from Eq. (3-3)

$$dQ^{(I)} = -T_{ij}^{(I)}\, d\left(\frac{\partial u_i}{\partial x_j}\right), \qquad \text{Eq. (3-7)}$$

where $T_{ij} = T_{ij}^{(R)} + T_{ij}^{(I)}$ has been used. Thus

$$\frac{\partial Q^{(R)}}{\partial t} = \mathcal{K}\,\nabla^2 T + \left[W + T_{ij}^{(I)} \frac{\partial\left(\frac{\partial u_i}{\partial x_j}\right)}{\partial t} \right]. \qquad \text{Eq. (3-8)}$$

We would like to eliminate $\frac{\partial Q}{\partial t}^{(R)}$ from Eq. (3-8). To do so we utilize the method standard to reversible thermoelasticity (see Nowacki, Reference 17). Since dU is a perfect differential

$$T\,dS = dQ^{(R)} = \left.\frac{\partial U}{\partial T}\right|_{\epsilon_{ij}} dT + \left[\frac{\partial U}{\partial\left(\frac{\partial u_i}{\partial x_j}\right)} - T_{ij}^{(R)} \right] d\left(\frac{\partial u_i}{\partial x_j}\right), \qquad \text{Eq. (3-9a)}$$

and upon using the perfect differential properties of dS we find

$$T_{ij}^{(R)} = T\,\frac{\partial T_{ij}^{(R)}}{\partial T} + \frac{\partial U}{\partial\left(\frac{\partial u_i}{\partial x_j}\right)}. \qquad \text{Eq. (3-9b)}$$

Combining Eqs. (3-9) with $\rho_0 C_v = \frac{\partial U}{\partial T}$, C_v is the specific heat at constant volume and ρ_0 is the mass density in the undeformed state, gives upon eliminating $\frac{\partial Q}{\partial t}^{(R)}$

$$\rho_0 C_v \frac{\partial T}{\partial t} - \mathcal{K}\,\nabla^2 T = \left[T_{ij}^{(I)} + T\,\frac{\partial T_{ij}^{(R)}}{\partial T} \right] \frac{\partial\left(\frac{\partial u_i}{\partial x_j}\right)}{\partial t} + W. \qquad \text{Eq. (3-10a)}$$

While setting W=0 (the only source of heat density being indirectly through an external mechanical **mechanism**) let us revert to one dimensional strain propagation in the z direction

$$\frac{\partial T}{\partial t} - \frac{1}{C_d^2}\nabla^2 T = \frac{1}{\rho_0 c_v}\left[T_{33}^{(I)} + T\,\frac{\partial T_{33}^{(R)}}{\partial T}\right]\frac{\partial \eta}{\partial t}, \qquad \text{Eq. (3-10b)}$$

where $C_d^2 = \frac{\rho_0 C_v}{\kappa}$ is the inverse of the thermal diffusivity. Eq. (3-10b) is the desired thermal part of the thermoelastic equations. Although Eq. (3-10b) has been derived elsewhere[21] we have not succeeded in finding a published calculation of $T_{33}^{(I)}$. We shall proceed to calculating $T_{33}^{(I)}$ for the a special case in a solid having dislocation induced viscosity.

By using[19]

$$\rho_0\frac{\partial^2 u_3}{\partial t^2} = \frac{\partial T_{33}}{\partial z}, \qquad \text{Eq. (3-11a)}$$

$$U = \mu\epsilon_{ik}^2 + \left[\frac{\bar{\kappa}}{2} - \frac{\mu}{3}\right]\epsilon_{mm}^2 + \frac{A}{3}\epsilon_{ik}\epsilon_{il}\epsilon_{kl} + B\epsilon_{ik}^2\epsilon_{ll} + \frac{C}{3}\epsilon_{ll}^3, \qquad \text{Eq. (3-11b)}$$

where μ is the rididity modulus, $\bar{\kappa}$ the compression modulus, A, B, and C are third order elastic constants, and Eq. (3-1) it is easily[19,20] shown that

$$\frac{\partial^2 u_3}{\partial t^2} - c_e^2\frac{\partial^2 u_3}{\partial z^2} = \chi_1\frac{\partial^3 u_3}{\partial z^2\partial t} + b\,\frac{\partial^2 u_3}{\partial z^2}\frac{\partial u_3}{\partial z} - \frac{\beta}{\rho_0}\frac{\partial T}{\partial z}, \qquad \text{Eq. (3-11c)}$$

where[22]

$$T_{ij}(\text{viscous}) = 2\mathcal{L}_1\left(\frac{\partial \epsilon_{ij}}{\partial t} - \frac{1}{3}\frac{\partial \epsilon_{mm}}{\partial t}\delta_{ij}\right) + \mathcal{L}_2\,\delta_{ij}\frac{\partial \epsilon_{mm}}{\partial t}, \qquad \text{Eq. (3-12a)}$$

$\mathcal{L}_1$ and $\mathcal{L}_2$ being the coefficients of shear and volume viscosity respectively. Also

$$\chi_1 = \rho_0^{-1}\left[\frac{4}{3}\mathcal{L}_1 + \mathcal{L}_2\right], \qquad \text{Eq. (3-12b)}$$

$$\rho_0 b = 3\left(\bar{\kappa} + \frac{4}{3}\mu\right) + 2A + 6B + 3C, \qquad \text{Eq. (3-12c)}$$

and

$$C_e^2 = \frac{\bar{\mathcal{K}} + \frac{4}{3}\mu}{\rho_0} \qquad \text{Eq. (3-12d)}$$

have been used. Taking the partial derivative of Eq. (3-11c) with respect to z gives

$$\frac{\partial^2 \eta}{\partial t^2} - C_e^2 \frac{\partial^2 \eta}{\partial z^2} = \chi_1 \frac{\partial^3 \eta}{\partial z^2 \partial t} + b\eta \frac{\partial^2 \eta}{\partial z^2} + b\left(\frac{\partial \eta}{\partial z}\right)^2 - \frac{\beta}{C_0} \frac{\partial^2 T}{\partial z^2} \cdot \text{Eq. (3-13)}$$

Equation (3-13) is the mechanical part of our thermoelastic equations and is to be used in conjunction with Eq. (3-10b). Eqs. (3-10b) and (3-13) taken together form our set of thermoelastic equations. Aside from simultaneous solution our thermoelastic equations are complete, for the given process under consideration, providing that suitable method of arriving at $T_{ij}^{(I)}$ is known. Such a method can be arrived at based upon the concept of path dependence.

Consider a non-uniform strain which is constant in time. From Eq. (3-7) we see that the problem is trivial for a uniform time independent strain. We expect that by $t = +\infty$ the stress will have stabilized to some constant value. Assuming that our static strain is turned on instantaneously (a highly non-hysical but useful model) at time $t = 0$ we can write

$$T_{33}(z,t) = \eta(z) \sum_{n=0}^{\infty} A_n(z) t^n , \qquad 0 \leq t < t_1 , \qquad \text{Eq. (3-14a)}$$

$$T_{33}(z,t) = \eta(z) \sum_{n=0}^{\infty} \frac{B_n(z)}{t^n} , \qquad t > t_2 , \qquad \text{Eq. (3-14b)}$$

where t_1 and t_2 are determined by the radii of convergence of the respective series. The coefficients A_n and B_n

are given a position dependence to allow for a variation of material properties with strain. One might hope to use Eqs. (3-14) to separate $T_{33}^{(R)}$ and $T_{33}^{(I)}$. Let us assume the following material behavior under the application of a non-uniform static stress at time t=0:

(a) There is a temperature change with the temperature approaching to $\left(\frac{1}{e}\right)$ of its final equilibrium value in a time τ corresponding to the phonon-phonon relaxation time.

(b) There is an irreversible heat flow, and a corresponding irreversible contribution to the stress tensor. The heat flow starts out at t= 0, at some time t_M reaches a local maximum value, and then decreases to zero.

For a dislocation induced viscosity t_M is related[23-25] to the fundamental vibrational frequency for dislocations. The material behavior enumerated above is illustrated in Fig. I and can always be achieved simply by making the dislocation density small enough. Our assumptions allow us to consider the viscosity process as being essentially isothermal for times greater than t_M. For a dislocation induced viscosity t_M is related[23-25] to the fundamental vibrational frequency for dislocations. t_M for most solids is in the 10^{-7} sec. range while we will consider temperatures high enough so that $\tau < 10^{-10}$ sec. Under such conditions Eq. (3-14b) gives

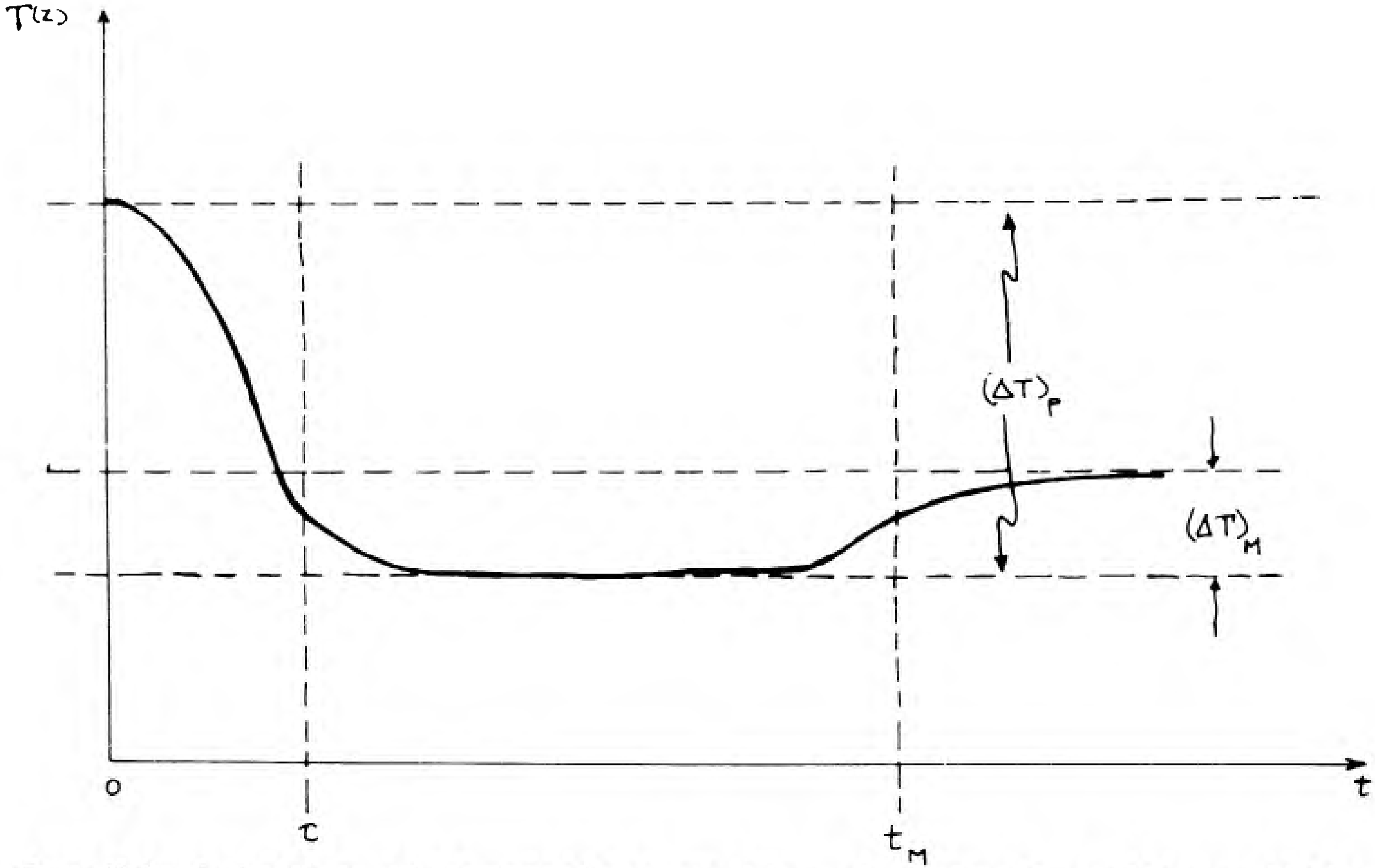

FIGURE I: Possible behavior of temperature vs time at a fixed position within the crystal. $(\Delta T)_p$ denotes the change in T due to phonon-phonon processes, while $(\Delta T)_M$ means the change in T due to dislocation induced viscosity. Our stated assumptions can be expressed as $(\Delta T)_p >> (\Delta T)_M$.

$$T_{33}^{(R)}(z) = \eta(z) B_0(z), \qquad t > t_2 = t_M, \qquad \text{Eq. (3-15a)}$$

$$T_{33}^{(I)}(z) = \eta(z) \sum_{n=1}^{\infty} \frac{B_n(z)}{t^n}, \qquad t > t_2 = t_M. \qquad \text{Eq. (3-15b)}$$

The separation made in Eqs. (3-15) is only possible because both of the independent thermodynamic variables, T and η, are essentially constant for $t > t_M$ so that $T_{33}^{(R)}$ is independent of time. We mean that changes in T are negligible in the time range $t > t_M$. If T as well as η were strictly independent of t one could not have a time varying $T_{33}^{(I)}$.

Thus we want a model for the viscosity which can be expanded in inverse powers of t as in Eq. (3-15b). Such a model gives the irreversible and reversible contributions to the large time stress unambiguously. For the case of isothermal dislocation induced viscosity, such a model has been developed by Harris and Greene[36],* from a memory function[36] point of view. In the small strain limit Harris and Greene find

$$T_{33}(z,t) = M\eta(z) + M_1\left[\tan^{-1}\left(\frac{T_1 - t}{T_M}\right) + \tan^{-1}\left(\frac{T_1 + t}{T_M}\right) - 2\tan^{-1}\left(\frac{T_1}{T_M}\right)\right], \qquad \text{Eq. (3-16a)}$$

---

*In Reference 4 stress was treated as the independent variable and strain the dependent variable. Thus one wants to interchange the roles of these variables in that paper before application to the problem being treated here. We feel that strain is a more fundamental variable than stress; an equation of motion is needed to relate stress to an observable.

where M is an elastic constant, M_1 is related to the dislocation content in the crystal, T_1 is the time constant associated with the viscous nature of the dislocation motion, and T_M is related to the resonant period associated with the vibrational motion of dislocations in the crystal. For $t > t_1 + T_M$ the inverse tangents in Eq. (3-16a) can be expanded as a power series in inverse time with the result

$$T_{33}^{(R)}(z) = \left[M - M_1 \tan^{-1}\left(\frac{T_1}{T_M}\right) \right] \eta(z), \qquad \text{Eq. (3-16b)}$$

$$T_{33}^{(I)}(z,t) = 2M_1 \frac{T_1 T_M}{t^2} \left[1 + \frac{T_1^2}{t^2} + \frac{T_M^2}{t^2} + \text{h.o.} \right] \eta(z), \qquad \text{Eq. (3-16c)}$$

where h.o. denotes higher order terms, and where Eqs. (3-15) have been used. Thus for this dislocation problem $T_{33}^{(I)}$ can be calculated leaving only a set of simultaneous equations to be solved. In general, however, it would seem like a difficult problem to solve for the irreversible part of the stress although the following points can be made

(a) A temperature type creep effect is to be expected (Coleman, Reference 26) for the same reasons that a creep effect exists for stress. Thus a non-isothermal theory adds many complications to Eqs. (3-16).

(b) The non-linear effects are expected to contribute to $T_{33}^{(I)}$ in the case of a time dependent strain. This makes sense because a change in distribution function is not a reversible effect and because the higher order processes change the distribution of phonons among the states.

In summary Eqs. (3-10b) and (3-13) form a set of thermoelastic equations for our nonlinear viscous system. If it made sense to do the problem in the isothermal approximation then a memory function[25] could easily be found* which gives rise to the stress-strain law of a first order anharmonic medium. And, by using this memory function, the characteristics for the problem can be found[25] which when integrated (on a machine or otherwise) completely solve the problem.

When we calculated $T_{33}^{(I)}$ in the dislocation viscosity case we were forced to consider large time

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*If we consider the problem of 1-D strain and write the stress-strain law in the form (from Eq. (2-18) or Reference 2)

$$T_{33} = G^{33}_{33}\eta + G^{333}_{333}\eta^2 \equiv G^{33}_{33}(\eta)\eta ,$$

where

$$G^{33}_{33}(\eta) \cong \frac{G^{33}_{33}}{1 - \frac{G^{333}_{333}\eta}{G^{33}_{33}}} .$$

We wish to compare the above expression for $G^{33}_{33}(\eta)$ with Eq. (13) of Reference 25. Upon this comparison we see that if the only source of creep present is phonon-phonon coupling than the only nonvanishing memory function is $A_2(t-\tau)$ with a possible solution

$$A_2(t-\tau) = \frac{G^{333}_{333}}{2G^{33}_{33}}\delta(t-t'-\tau) ,$$

where t' is the relaxation time for the system. And upon employing Eqs. (8) and (9) from Reference 25 this completely solves the isothermal problem.

behavior so that the temperature would be essentially constant (although the irreversible contribution to the stress tensor remains nonzero). Thus, even in the case of dislocation induced viscosity we are unable to find the small time behavior of $T_{33}^{(I)}$. Consequently either we generate a new recipe for calculating the stress tensor or we must approach the problem through other than thermoelasticity. At this point it seems wise to take the latter course.

B. The Burgers Equation and Weak Shock Propagation

It can be shown[27] that a compressible thermoviscous fluid can be described, for first order disturbances, by the so-called[18] Burgers equation

$$\frac{\partial \xi}{\partial t} + \xi \frac{\partial \xi}{\partial z_0} = \frac{\nu}{2} \frac{\partial^2 \xi}{\partial z_0^2}, \qquad \text{Eq. (3-17a)}$$

for a disturbance propagating in the z direction with particle velocity in the z direction (one dimensional strain propagation), viscosity-like coefficient, ν, velocity-like dependent variable, ξ, and time, t. The coordinate z_0 is the distance of a particle with respect to the origin of a coordinate system moving at the constant velocity a* (the zero strain adiabatic sound speed) in the positive z direction. In addition, because we shall use experimentally determined elastic constants in this section, the z direction is chosen parallel to a cube axis for those cubic crystal structures considered. The dependent variable ξ is given by

$$\xi \equiv u_p' + a \equiv \Gamma(u_p' + a^*) \equiv \Gamma u_p$$

where u_p is the particle velocity with respect to the laboratory coordinate system, u_p' is the particle with respect to the moving coordinate system, a is the volume dependent adiabatic sound speed, and Γ is a constant determining the nonlinear properties of the medium through the equation of state.

Blackstock[28] has investigated the problem of wave propagation in an arbitrary fluid by considering a number of different numerical values for Γ. In this paper, however, we will be concerned both with what values of Γ exist in representative solids as well as with what these values mean in terms of allowed sound propagation. We assume* that the viscosity-like coefficient, ν, is known and positive.

One of the reasons this is interesting is, as first shown by Hopf[29],

$$\xi = -\frac{\nu}{\Gamma}\frac{1}{\chi_a}\frac{\partial \chi_a}{\partial z_0} \qquad \text{Eq. (3-17b)}$$

transforms Eq. (3-17a) into

$$\frac{\partial \chi_a}{\partial t} = \frac{\nu}{2}\frac{\partial^2 \chi_a}{\partial z_0^2}, \qquad \text{Eq. (3-17c)}$$

---

* ν is known from the work of others. See Woodruff and Ehrenreich (Reference 3) or DeVault and Mclennan. G. P. DeVault and J. A. Mclennan, Phys. Rev. 138, A856 (1965).

to within an arbitrary time dependent factor in χ_a. Since such a multiplicative factor does not affect u_p as given by Eq. (3-17b) it is neglected throughout the rest of this paper. Eq. (3-17c) is the well known diffusion equation of heat conduction. Two possible solutions of Eq. (3-17c) are

$$\chi_a = \exp\left[\frac{\Gamma^2 A^2 t}{2\nu}\right] \cosh\left[\frac{\Gamma A z_0}{\nu}\right], \qquad \text{Eq. (3-18a)}$$

$$\chi_a = (e^R+1) - (e^R-1)\int_0^{z_0/\sqrt{2\nu t}} \frac{e^{-s^2}}{(\frac{1}{2})!}\, ds, \qquad \text{Eq. (3-18b)}$$

where $R \equiv \ln \dfrac{\chi_a(z_0 = -\infty)}{\chi_a(z_0 = +\infty)}$. R can be identified[37] as the Reynolds number for the flow in question. That Eqs. (3-18a) and (3-18b) are solutions is easily checked by substitution into Eq. (3-17c). Corresponding to Eqs. (3-18a) and (3-18b), from Eq. (3-17b), are

$$\xi = -A \tanh\left[\frac{\Gamma A z_0}{\nu}\right], \qquad \text{Eq. (3-18c)}$$

and

$$\xi = +\left[\frac{\nu(e^R-1)}{\Gamma\sqrt{2\nu t}} \exp\left(-\frac{z_0^2}{2\nu t}\right)\right] \otimes$$

$$\otimes \left[\left(\frac{1}{2}\right)! (e^R+1) - (e^R-1)\int_0^{z_0/\sqrt{2\nu t}} e^{-s^2}\, ds\right]^{-1}. \qquad \text{Eq. (3-18d)}$$

u_p is the particle velocity with respect to a coordinate system at rest. By transforming Eqs. (3-18c) and (3-18d) with

$$z = z_0 + a^* t$$

we have, respectively,

$$u_p = -\Gamma^{-1} A \tanh\left[\frac{\Gamma A (z - a^* t)}{\nu}\right], \qquad \text{Eq. (3-18e)}$$

$$u_p = \Gamma^{-1}\left[\frac{\nu (e^R - 1)}{\Gamma\sqrt{2\nu t}} \exp\left[-\frac{(z - a^* t)^2}{2\nu t}\right]\right] \otimes$$
$$\otimes \left[\left(\frac{1}{2}\right)!\,(e^R + 1) - (e^R - 1)\int_0^{(z - a^* t)/\sqrt{2\nu t}} e^{-s^2}\, ds\right]^{-1}. \qquad \text{Eq. (3-18f)}$$

Upon considering the behavior of Eqs. (3-18e) and (3-18f) we see that (3-18e) can represent a weak steady shock propagating in an infinite medium while (3-18f) can represent the nonsteady propagation of a pulse in an infinite medium. Because of the mathematical complexity of Eq. (3-18f) we will consider the case of the steady shock, Eq. (3-18c), in the rest of the calculations. This is justified as the concepts involved in the propagation of the phonon distribution are more important than the form of the strain governing that distribution.

For finite t we require

$$\lim_{z \to +\infty} u_p = 0 \qquad \text{Eq. (3-19a)}$$

$$\lim_{z \to -\infty} u_p = u_p^{(f)} \qquad \text{Eq. (3-19b)}$$

$$u_p(z,t) = \frac{u_p^{(f)}}{2} - \frac{u_p^{(f)}}{2} \tanh\left[\frac{\Gamma u_p^{(f)}}{2\nu} (z - a^* t) \right], \qquad \text{Eq. (3-20)}$$

where $u_p^{(f)}$ is the particle velocity associated with the boundary at $-\infty$. Since Eq. (3-17) represents only a single shock one cannot choose $u_p^{(f)} = 0$ in Eq. (3-20) as that would represent a trivial solution. But

$$\frac{\partial \eta}{\partial t} = \frac{\partial u_p}{\partial z} = \frac{\Gamma}{\nu} \left(\frac{u_p^{(f)}}{2} \right)^2 \operatorname{sech}^2 \left[\frac{\Gamma u_p^{(f)} (z - a^* t)}{2\nu} \right] . \qquad \text{Eq. (3-21)}$$

$$\therefore \quad \eta(z,t) = \frac{\Gamma}{\nu} \left(\frac{u_p^{(f)}}{2} \right)^2 \int_{-\infty}^{t} \operatorname{sech}^2 \left[\frac{\Gamma u_p^{(f)} (z - a^* \ell)}{2\nu} \right] d\ell, \qquad \text{Eq. (3-22a)}$$

or

$$\eta(z,t) = \frac{\Gamma}{8\nu} \left(\frac{G_{33}^{33}}{\rho_0 a^*} \right)^2 \eta_f^2 \int_{-\infty}^{t} \operatorname{sech}^2 \left[\frac{\Gamma G_{33}^{33} \eta_f}{2 \rho_0 a^* \nu} (z - a^* \ell) \right] d\ell . \qquad \text{Eq. (3-22b)}$$

In Eqs. (3-22) $\lim_{t \to -\infty} \eta(z,t) = 0$ has been used along with the approximation[30]

$$\eta = - \frac{u_p a^* \rho_0}{G_{33}^{33}} \qquad \text{Eq. (3-23)}$$

η_f is the strain corresponding to $u_p^{(f)}$. Eq. (3-22b) can be integrated to give

$$\eta(z,t) = \left[\frac{\eta_f G_{33}^{33}}{2 \rho_0 a^{*2}} \right] \left[1 - \tanh\left\{ - \frac{\Gamma \eta_f G_{33}^{33}}{2\nu} (z - a^* t) \right\} \right] . \qquad \text{Eq. (3-24)}$$

Aside from Γ we now have all the necessary ingredients for determining $N_1 (\vec{q}; z,t)$ from Eq. (2-30a).

We now wish to consider the dimensionless factor Γ which has been claimed to control the nonlinearity of the medium. I should like to show that to a first approximation, Γ can be written* as

$$\Gamma = 1 + \frac{\rho}{a}\left(\frac{\partial a}{\partial \rho}\right)_S , \qquad a \equiv \left(-\frac{\partial T_{33}}{\partial \rho}\right)_S^{1/2} , \tag{Eq. (3-25)}$$

Using $\Gamma(u'_p + a^*) = (u'_p + a)$ and Eq. (3-25) yields

$$a - a^* = \frac{\rho}{a}\left(\frac{\partial a}{\partial \rho}\right)_S (u'_p + a^*) . \tag{Eq. (3-26)}$$

But the conservation of mass can be written

$$\rho_0 (u'_p)_0 = \rho u'_p \tag{Eq. (3-27a)}$$

where the subscript zero refers to unperturbed values. Rewriting Eq. (3-27a) to first order yields

$$u'_p = \frac{\rho_0}{\rho}(u'_p)_0 \cong -\frac{\rho_0}{\rho} a^* \tag{Eq. (3-27b)}$$

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*The adiabatic sound speed, a, is usually written as $a = \left(\frac{\partial p}{\partial \rho}\right)_S^{\frac{1}{2}}$. The form given in Eq. (3-25), however, is valid for our special case of one dimensional strain propagation. As an example of this consider the revised set of Maxwell's thermodynamic equations (the starred functions are not the conventional functions).

$dU = TdS - T_{33}dV$, $\quad \therefore \left.\frac{\partial T}{\partial V}\right|_S = -\left.\frac{\partial T_{33}}{\partial S}\right|_V .$

$H^* = U + T_{33}V$, $\quad dH^* = TdS + VdT_{33}$, $\quad \therefore \left.\frac{\partial T}{\partial T_{33}}\right|_S = \left.\frac{\partial V}{\partial T}\right|_{T_{33}} .$

$F = U - TS$, $\quad dF = -T_{33}dV - SdT$, $\quad \therefore \left.\frac{\partial T_{33}}{\partial T}\right|_V = \left.\frac{\partial S}{\partial V}\right|_T .$

$G^* = H^* - TS$, $\quad dG^* = VdT_{33} - SdT$, $\quad \therefore \left.\frac{\partial V}{\partial T}\right|_{T_{33}} = -\left.\frac{\partial S}{\partial T_{33}}\right|_T .$

The correctness of this revised set of Maxwell's equations rests only on U,H*,F and G* being valid thermodynamic variables-which of course they are. These revised equations also lead[11], in a natural manner, to revised First and Second TdS equations. Similarly T_{33} takes the place of P in the equations of motion. This line of reasoning leads directly to a as given by Eq. (3-25).

It is to be remembered that u_p is the particle velocity with respect to a coordinate system moving to the right at the velocity a*. Substituting Eq. (3-27b) into Eq. (3-26) yields

$$a - a^* \cong \left(\frac{a^*}{a}\right)\left(\frac{\partial a}{\partial \rho}\right)_s (\rho - \rho_0), \qquad \text{Eq. (3-28a)}$$

$$a - a^* \cong \left(\frac{\partial a}{\partial \rho}\right)_s (\rho - \rho_0) \cdot \qquad \text{Eq. (3-28b)}$$

Eq. (3-28b) is the first order version of Eq. (3-28a). Eq. (3-28b) is obviously the correct first order Taylor's expansion of the sound velocity about the unperturbed density ρ_0. Consequently, Eq. (3-25) is correct to first order. Thus if the equation of state is known so is Γ.

To evaluate Γ we consider from Eqs. (2-18) and (3-1)

$$T_{33} = G^{33}_{33}\, u_{33} + \frac{1}{2}\, G^{333}_{333}\, u^2_{33}, \qquad \text{Eq. (3-29)}$$

where we are using subscripts and superscripts interchangeably on the elastic constants. It can be shown[31] that

$$\eta = \frac{\partial U_3}{\partial z} = u_{33} = \frac{\rho_0}{\rho} - 1, \qquad \text{Eq. (3-30a)}$$

which gives upon expansion to third order in $\left(\frac{\Delta\rho}{\rho_0}\right)$

$$\eta = -\left(\frac{\Delta\rho}{\rho_0}\right)\left[1 - \left(\frac{\Delta\rho}{\rho_0}\right) + \left(\frac{\Delta\rho}{\rho_0}\right)^2\right]. \qquad \text{Eq. (3-30b)}$$

Then, upon usings Eqs. (3-25), (3-29), and (3-30b) we find

$$\Gamma = 1 - \frac{G^{333}_{333}}{G^{33}_{33}}. \qquad \text{Eq. (3-31)}$$

Were we interested in a gas the expression corresponding to Eq. (3-31) would be[28]

$$\Gamma = 1 + \frac{B'}{2A'}, \qquad \text{Eq. (3-32)}$$

where $\frac{B'}{2A'}$ is the coefficient of the first nonlinear term in an assumed pressure-density relation. It is interesting to note that $\Gamma = -1$ for a harmonic solid, while $\Gamma = \frac{C_p + C_v}{2C_p}$ for a perfect gas. The specific heat at constant pressure, and at constant volume, is denoted by C_p and C_v respectfully.

It is easily seen, in the process of arriving at Eq. (3-20) from Eq. (3-18c), that $\nu > 0$ (as expected) requires $\Gamma > 0$. Experimentally weak shock propagation has been observed[32]. Thus $\Gamma > 0$ is expected to hold, for at least some materials, from the known volume dependence of the elastic constants. Values of Γ for representative materials[33] are

	KCℓ	Cu	Ge	Fused SiO_2
Γ	23	9	4	-10

We thus see that steady compressive weak shock propagation can occur in all of the representative materials except for SiO_2. It would appear, however, that in amorphous SiO_2 rarefactions will shock up*. In conclusion, for $\nu > 0$ and $\Gamma > 0$, we have found

$$u_p = \frac{u_p^{(f)}}{2} - \frac{u_p^{(f)}}{2} \tanh \left\{ \frac{\Gamma u_p^{(f)}}{2\nu} \left[z - (a^* t) \right] \right\} \qquad \text{Eq. (3-33)}$$

for the solution corresponding to steady weak shock propagation in a anharmonic, viscous, and thermally conducting medium.

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*For a disturbance moving to the right $u_p^{(f)} < 0$ requires $\Gamma < 0$ in order to apply the weak steady solution demonstrated by Eq. (3-18a). $\nu > 0$ is assumed.

IV. LARGE STRAINS

In the two previous sections we have been content to analyze the strain-phonon spectrum interaction from a perturbation (first order) point of view. We now intend to widen our horizons and consider the effect of an arbitrarily large compressive strain on the phonon distribution.

In the course of our calculations we shall continually make two assumptions. These assumptions are:

(1) As in the first order theory, $\Omega_p \tau < 1$.

(2) We assume that at each equilibrium state characterized by the thermodynamic variables of finite Lagrangian[31] strain and temperature the material is linear with respect to small disturbances (i.e., the material is harmonic). This means that at each equilibrium state it is valid to speak of eigenfrequencies of non-interacting phonons.

The second assumption is justified here as we are concerned primarily with low frequency phonons ($\omega < 10^{11}$ cycles per sec). The long wavelength higher order elastic constants are well defined quantities. The high frequency difficulty arises because the high frequency modes essentially see the nearest neighbor interatomic potential which, under compression, may become highly anharmonic. The long wavelength phonons reflect a potential which is smeared out over many atoms.

With the above two assumptions it becomes valid to use Eq. (2-7a) for large amplitudes* providing that we substitute a position like coordinate z_1, for the laboratory position coordinate z.

$$\frac{\partial N}{\partial t} + \frac{1}{\hbar}\left[\frac{\partial N}{\partial z_1}\frac{\partial H}{\partial q_3} - \frac{\partial N}{\partial q_3}\frac{\partial H}{\partial z_1}\right] = \frac{\partial N}{\partial t}\bigg|_{\text{coll.}} , \qquad \text{Eq. (A-16)}$$

with $H=H(\vec{q};z,t)=\hbar\omega(\vec{q};z,t)$. So that this equation becomes usable we must derive expressions for H and for $\frac{\partial N}{\partial t}\Big|_{\text{coll.}}$ in terms of strain and temperature (which in turn are functions of z, and t). Let us first consider $\frac{\partial N}{\partial t}\Big|_{\text{coll.}}$.

A. Large Strain Collision Term

Aside from the definition[8] involving the conservation of $\vec{q}$, normal processes may be characterized by their ability to maintain[8,9] a drift velocity for phonons. In our case this is meant in the local $(\Omega_p\tau<1)$ sense so that at any instant the drift is position dependent. The so-called unklapp processes would tend to randomize such a drift to zero. Thus were one able to show that the effects of such a phonon drift were small regardless of the strain amplitude when compared to the effects of strain and temperature variation, then the distinction between normal and

---

*Both assumptions are used in Appendix A in the process of arriving at Eq. (A-16) which is similar to Eq. (2-7a). In that Appendix the second assumption allows us to write for the Hamiltonian of a single phonon $\tilde{m}(\vec{q}) = \hbar\omega(\vec{q};z,t)$.

umklapp processes could be neglected with the result

$$\left.\frac{\partial N}{\partial t}\right|_{\text{coll.}} = - \frac{N(\vec{q}, z_1, t) - N_0(\omega, T)}{\tau(\vec{q}, \eta)} , \qquad \text{Eq. (4-1)}$$

where the relaxation time $\tau(\vec{q},\eta)$ is, in general[24], strain dependent. However, because the $\vec{q}$ dependence over-complicates matters, we will consider τ to be only a function of η.

In the limit $(\Omega_p \tau) \to 0$, and for small strains (linearized theory) we have seen that existing theory leads to

$$N(\vec{q}, z_1, t) = N_0(\omega_0, T_0) - \frac{dN_0(\omega_0, T_0)}{d\left(\frac{\hbar\omega_0}{kT_0}\right)} \otimes$$

$$\otimes \left[\left(\frac{\hbar\omega_0}{kT_0}\right)\left(\gamma\eta + \frac{\Delta T}{T_0}\right) + \frac{\lambda_3 q_3}{kT_0}\left(\frac{\tau}{\tau_\eta}\right) \right] , \qquad \text{Eq. (2-30a)}$$

where $\vec{\lambda}$ is defined by Eq. (2-9). One can show that when the applied strain is sinusoidal in time existing theory[8] leads to

$$\lambda_3 = -i \frac{\hbar c \gamma (\Omega_p \tau_u) \eta}{i(\Omega_p \tau_u) - 1} , \qquad \text{Eq. (4-2)}$$

and similarly

$$\left(\frac{\Delta T}{T_0}\right) = -\gamma\eta , \qquad \text{Eq. (4-3)}$$

with the result that

$$\left(\frac{\Delta T}{T_0}\right) \hbar\omega_0 \left(\frac{\lambda_3 q_3 \tau}{\tau_n}\right)^{-1} < \frac{i(\Omega_p \tau_u) - 1}{(\Omega_p \tau_u)} . \qquad \text{Eq. (4-4)}$$

Thus if we assume that $(\Omega_p \tau_u) \to 0$, then the drift term can be ignored in comparison to the effect of temperature variation. This assumption is made throughout the paper.

But it is to be noted that when Eq. (4-3) is substituted into Eq. (2-30a) the only first order contribution to $N(\vec{q};z,t)$ is that due to the phonon drift term[35]. However, if we further assume that the effects of temperature variation and energy shift do not cancel at large strain amplitudes, we can safely assert that Eq. (4-1) can be employed in the large strain limit. This reasoning is based upon Eq. (2-7) being independent of strain.

B. Large Strain Hamiltonian

Using our assumption that it is valid to describe the equilibrium state thermal vibrations as phonons, we have for the change in phonon frequency due to a volume variation about an equilibrium point

$$d\omega = -\omega(\vec{q};V,T)\,\gamma(V,T)\,\frac{dV}{V}, \qquad \text{Eq. (4-5)}$$

where $\gamma(V,T)$ is the Grüneisen constant associated with the state (V,T). Multiplying and dividing the right side of Eq. (4-5) by V_0 and transforming[14,31] from volume to Lagrangian strain via

$$V = V_0\,(1+2\epsilon)^{\frac{1}{2}}, \qquad \text{Eq. (4-6)}$$

gives

$$\omega(\vec{q};z,t) = \omega_0(\vec{q})\exp\left[-\int_0^{\epsilon}\frac{\gamma(E,T)}{1+2E}\,dE\right]. \qquad \text{Eq. (4-7)}$$

For later convenience we rewrite this as

$$\omega(\vec{q};z,t) = \omega_0(\vec{q})\,R(z,t), \qquad \text{Eq. (4-8a)}$$

$$R(z,t) \equiv R \equiv \exp\left[- \int_0^{\epsilon} \frac{\gamma(\xi,T)}{1+2\xi} \, d\xi \right] . \qquad \text{Eq. (4-8b)}$$

We note that R is independent of q. Eq. (4-8a) gives us a Hamiltonian for use in Eq. (2-7a). Neglecting its temperature dependence $\gamma(V)$ can be found in principle by fitting shock wave data[13] or by using assumed interatomic potentials[38]. In the classical limit of high temperature it is valid[13] to neglect the temperature dependence of γ.

C. Solutions

Using Eqs. (4-1) and (4-8a) we will now seek to solve Eq. (A-16) for $N(\vec{q};z,t)$ as a function of $\vec{q}$, η, and T with the idea that η and T may be found by setting up and solving macroscopic thermoelastic equations for a material exhibiting phonon-phonon viscosity.

Rewriting Eq. (4-1) in the long wavelength limit gives

$$\left.\frac{\partial N}{\partial t}\right|_{\text{Coll.}} = - \frac{N_1}{\tau} + \frac{1}{\tau}\left(\frac{kT}{\hbar\omega_0 R}\right)\left(1 - R\,\frac{T_0}{T}\right), \qquad \text{Eq. (4-9)}$$

where Eq. (2-6) has been used. Substituting Eqs. (4-8a) and (4-9) into Eq. (A-16) gives

$$- \frac{N_1}{\tau} - \left[\frac{\partial N_1}{\partial t} + R C_3^0 \frac{\partial N_1}{\partial z_1}\right] = - \left[N_0' \frac{\hbar C_3^0}{kT_0} + \frac{\partial N_1}{\partial q_3}\right] \omega_0 \frac{\partial R}{\partial z_1} + - \frac{1}{\tau}\left(\frac{kT}{\hbar\omega_0 R}\right)\left[1 - R\,\frac{T_0}{T}\right], \qquad \text{Eq. (4-10)}$$

where Eqs. (2-12) have been used and C° refers to the

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shock propagation

$$N_1(q,\theta;z_1,t) = B \exp\left[\beta \cos\theta \ln q\right] + \frac{N_0(\omega_0,T_0)}{1+\beta\cos\theta}\left[\beta\left(1-\frac{T}{RT_0}\right)\cos\theta - \cos^2\theta\right], \qquad \text{Eq. (4-12a)}$$

with values of θ restricted so that $1+\beta\cos\theta \neq 0$, where $\beta \equiv \dfrac{\left(\frac{\partial R}{\partial z_1}\right)^{-1}}{C^\circ \tau}$, and B is a constant of integration such that

$$B = N_1(q, \tfrac{\pi}{2}; z_1, t). \qquad \text{Eq. (4-12b)}$$

For our one dimensional strain, phonons with $\vec{q}$ normal to the direction of shock propagation do not have their energy states shifted although they are scattered to a new distribution function in the process of thermalizing the states having non zero q_3. This means that

$$B = N_0(\omega_0, T^*) - N_0(\omega_0, T_0), \qquad \text{Eq. (4-13)}$$

where the temperature T^* is characterized by $T_0 \leq T^* \leq T$, and determined by the Boltzmann equation

$$\frac{\partial}{\partial t}\left[B + N_0(\omega_0,T_0)\right] = -\frac{1}{\tau}\left[B + N_0(\omega_0,T_0) - N_0(\omega_0,T)\right]. \qquad \text{Eq. (4-14)}$$

In Eq. (4-14) $N_0(\omega_0, T)$ represents the distribution function towards which the transverse q's want to relax and the sign in front of the right hand side has been chosen so that the density of phonons of a given frequency is increasing as a function of time. Combining Eqs. (4-13) and (4-14) gives in the long wavelength approximation

$$\frac{\partial T^*}{\partial t} - \frac{T^*}{\tau} = - \frac{T}{\tau} , \qquad \text{Eq. (4-15)}$$

which requires solutions to the thermoelastic equations, and a knowledge of the strain dependence of τ, before solving. But from Eq. (4-14) we see that in the limit $(\Omega_p \tau) \to 0$ we have $T = T^*$. Thus combining Eqs. (4-12a) and (4-13) gives

$$N_1(q,\theta;z_1,t) = N_0(\omega_0,T_0)\left[\left(\frac{T}{T_0} - 1\right) \exp(\beta \cos\theta \ln q) + \frac{\beta\left(1 - \frac{T}{RT_0}\right)\cos\theta - \cos^2\theta}{1 + \beta\cos\theta}\right]. \qquad \text{Eq. (4-16)}$$

This equation is correct for each mode of each branch. One must simply remember to use the Grüneisen constant and relaxation time appropriate for the mode and branch in question. The most interesting thing about Eq. (4-16) is the presence of directionality effects ($\cos\theta$). Such directionality does not occur in the low amplitude first order calculations as given by Eq. (2-30a), for $\lambda_3 = 0$, as directionality represents the scattering (at least first order) of q_1 and q_2 phonons by nonequilibrium (at least first order) q_3 phonons which results in at least a second order process. This directionality is quite important physically as it means that the strain gradient causes the two halves of the Brillouin zone, $\pm q_3$, to be occupied differently. In the small amplitude case this only occurs for nonzero λ_3 and is simply understood.

A nonzero λ_3 means that it is possible to maintain a net crystal momentum.

It is interesting to note that, regardless of amplitude, a strain gradient is necessary in order to have an asymmetry*; in the absence of a strain gradient Eq. (4-12) becomes

$$N_1(q,\theta,z,t) = N_0(\omega_0,T_0)\left[\frac{T}{RT_0}-1\right]. \qquad \text{Eq. (4-17)}$$

D. The Attenuation

To the student of shock waves in solids one of the more interesting theoretical quantities is the attenuation of shock (strain) amplitude with propagation distance[37,38,39]. By using relatively simple experimental techniques (e.g. measuring free surface velocity as a function of sample thickness) the attenuation can usually be measured. In order for phonon-phonon attenuation of a shock wave (at least for small amplitudes) to be important it is necessary[4,5,40] that Ω_p, the angular velocity at which the Fourier spectrum of the strain peaks, be in the hypersonic range (greater than $2\pi \times 10^9$ radians per sec). This implies that the

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*We are suggesting here that λ_3 is proportional to $\frac{\partial n}{\partial z}$ in the small amplitude case similar to the case of pure thermal conduction where it is shown that λ_3 is proportional to $\frac{\partial T}{\partial z}$ (see reference 8). This is derived in Appendix B.

rise time of the shock be less than 10^{-9} secs. Such rise times, however, are near the current limits of experimental high speed camera techniques[41]. Perhaps electronic means such as probes or piezoelectric gauges will better serve the purpose. In any event comparison between theory and experiment is presently not possible. Experimentalists should note that if two sources of viscosity with different relaxation times are present, say dislocation induced viscosity and anharmonic processes in an otherwise perfect crystal, the observations must be made before the weaker process (here assumed to be the dislocation viscosity) controls the thickness of the shock front.

By attenuation we mean the rate at which kinetic energy is converted into thermal energy - i.e., the rate at which average particle velocity is transferred into vibrational energy of the lattice. The instantaneous rate of energy density thermalization can be simply written as

$$Q(z,t) = -\frac{1}{(2\pi)^3}\int H(\vec{q}\,;z,t)\left.\frac{\partial N}{\partial t}\right|_{\text{coll.}} d\vec{q} \qquad \text{Eq. (4-18)}$$

where the factor $(2\pi)^{-3}$ converts from total number of particles to the number of particles per unit volume of phase space*. It is understood that a sum over all

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*The total number of phonons per unit (size) volume can be written

$$\frac{N}{V} = \int G(\vec{q})\, f(\vec{q})\, d\vec{q}$$

Continued on next page.

branches and polarizations is to be included in Eq. (5-1). However, if W(z,t) is the instantaneous kinetic energy associated with the strain wave, the really important[†] physical quantity is the number

$$\alpha(z,t) = \tau \frac{Q(z,t)}{W(z,t)} . \qquad \text{Eq. (4-19)}$$

$\alpha(z,t)$ is a nice number because $\alpha \sim 1$ means that the phonon-phonon processes are important for determining the shape of the shock front, with the shape being <u>relatively</u> stable, while $\alpha >> 1$ means that the phonon-phonon processes are extremely important for determining the rise time with an extremely unstable shape associated with the shock front.

W(z,t) can be written

$$W(z,t) = \frac{1}{2} \rho(z,t) \left(\frac{\partial U_s}{\partial t}\right)^2 . \qquad \text{Eq. (4-20)}$$

Using Eq. (4-6) we find that Eq. (4-20) can be rewritten

$$W(z,t) = \frac{\rho_0}{2} (1+2\epsilon)^{-\frac{1}{2}} \left[\int_0^z \left(\frac{\partial \epsilon}{\partial t}\right) \frac{dz}{\sqrt{1+2\epsilon}} + u_p(0,t) \right]^2 , \qquad \text{Eq. (4-21)}$$

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[*] Continued from previous page.

where $F(\vec{q})$ is the probability that the state $\vec{q}$ is occupied, and $G(\vec{q})$ is the density of states per unit volume of phase space. We thus find for the number of phonons per unit size volume between $\vec{q}$ and $(\vec{q}+d\vec{q})$

$$(2\pi)^{-3} f(\vec{q}) \chi$$

where χ takes units into account and $\left(\frac{1}{2\pi}\right)^3$ has been used for G(q).

[†] Rather than the usual attenuation coefficient $(Q(z,t)W^{-1}(z,t)U^{-1}(z,t))$, familiar to linear theories. U(z,t) is the propagation velocity of the kinetic energy.

where $u_p(o,t)$ is the particle velocity in the z direction at z=0. Assuming solutions to the thermoelastic equations and a knowledge of the indicated boundary conditions thus means that W(z,t) is known. From Eqs. (4-1), (4-8a) and (4-18)

$$Q(z,t) = \frac{\hbar R(z,t)}{(2\pi)^3} \int \omega_0(\vec{q}) \left[\frac{N(\vec{q};z,t) - N_0(\omega,T)}{\tau(\epsilon)} \right] d\vec{q} \quad \text{Eq. (4-22)}$$

Upon using Eq. (4-18)

$$Q(z,t) = \frac{R(z,t)\,kT_0}{(2\pi)^3\,\tau(\epsilon)} \int \Bigg[\left(\frac{T}{T_0} - 1 \right) \exp(\beta \cos\theta \ln q) + \quad \text{Eq. (4-23)}$$

$$+ \frac{(1+2\beta\cos\theta)\left(1 - \frac{T}{RT_0}\right) - \cos^2\theta}{1+\beta\cos\theta} \Bigg] d\vec{q}$$

In order to integrate Eq. (4-23) we must have $\beta < 1$ because of our condition $1+\beta\cos\theta \neq 0$. Treating γ as a constant we find from Eq. (4-8b)

$$\frac{\partial R}{\partial z} = \gamma \frac{R \frac{\partial \epsilon}{\partial z}}{(1+2\epsilon)^2}, \quad \text{Eq. (4-24)}$$

so that $\left(\frac{\partial R}{\partial z}\right)$ is expected to be positive for $\frac{\partial \epsilon}{\partial z}$ positive. In the large strain limit $\epsilon \to -\frac{1}{2}$. One thus expects, for constant relaxation time, that β can be made as small as desired*. Thus assuming that the $|\beta| < 1$ we can integrate

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*Using Eq. (4-8b) we find that, for constant γ,

$$\frac{\partial R}{\partial z} = \frac{\partial \epsilon}{\partial z} \cdot \frac{1}{(1+2\epsilon)^{(2+\gamma)}},$$

so that $\beta \sim \frac{i}{(\Omega_p \tau)\epsilon} (1+2\epsilon)^{(2+\gamma)}$ results.

Eq. (5-7) to get

$$Q(z,t) = \frac{1}{12\pi^2} q_m^3 F(q_m, z, t) R(z,t) \frac{kT_0}{\tau(\epsilon)}, \qquad \text{Eq. (4-25)}$$

where $\frac{4\pi}{3} q_m^3 F(q_m; z,t)$ is equal to the integral in Eq. (5-7), and q_m is an average radius of the first Brillouin zone. If by q_m^0 we mean the isotropic radius in the undeformed medium, then

$$q_m = \frac{a_0}{a} q_m^0 = q_m^0 (1+2\epsilon)^{-\frac{1}{2}} \qquad \text{Eq. (4-26)}$$

where Eq. (4-8b) has been used. Thus combining Eqs. (4-19), (4-21), (4-25), and (4-26) gives

$$\alpha(z,t) = \left(\frac{1}{6\pi^2}\right) \frac{(q_m^0)^3 F(q_m; z,t)\, R k T_0}{\rho_0 (1+2\epsilon) \left[G(\epsilon) z + u_p(0,t)\right]^2}, \qquad \text{Eq. (4-27)}$$

where $G(\epsilon)$ is defined as the mean value of the integrand in Eq. (4-21). And for $z=0$ in the $\beta \to 0$ limit

$$\alpha(0,t) = \frac{b}{2\pi^2} (q_m^0)^3 \frac{\bar{R} kT}{\rho_0 (1+2\epsilon) u_p^2(0,t)}, \qquad \text{Eq. (4-28)}$$

where b denotes the number of phonon branches in the medium, and $\bar{R}$ an average value of R (necessitated because γ may depend upon branch and mode). In order to evaluate Eq. (4-28) we must be able to generate and solve thermoelastic equations for arbitrarily large strains. Since that cannot yet be done we will end our development here.

V. DISCUSSION

A. Thermoelastic Equations

We were forced to end our discussion of the phonon spectrum in the presence of large strains because we lacked thermoelastic equations which were valid in the presence of large amplitude mechanical disturbances. While it is not clear exactly how this situation can be alleviated there is an interesting possibility which must be mentioned. In a recent paper by Vedanov and Rudakov[43] a mechanical equation of motion was found in a manner explicitly consistent with the Boltzmann equation in the small strain isothermal approximation. Vedanov and Rudakov have arrived at their consistent equations by using variational techniques simultaneously on the particle position and the amplitude of the sound field. It seems to us that if one were also able to vary a property of the medium, simultaneously with the other two variables, then thermoelastic-like equations would automatically be generated which would be explicitly consistent with the Boltzmann equation. Perhaps in the end large amplitude thermoelastic equations which are explictly consistent will result. We hope to find out.

B. Validity of the Boltzmann Equation

Eventually we want to be able to treat the case $(\Omega_p\tau) \gtrsim 1$ as that would correspond to a shock wave before the high frequency components were dissipated out. Such a treatment would require a modification to our Boltzmann equation approach so as to take into account the off diagonal elements of the density matrix[43]. The reason for this is that if, for example, we consider a two level system such that $(\Omega_p\tau)>1$ then for a density matrix ρ_{ij} we cannot neglect $\frac{\partial\rho}{\partial t}$ as compared to $\frac{\rho}{\tau}$ because $\frac{\partial\rho}{\partial t}$ is given by[48]

$$\frac{\partial\rho_{11}}{\partial t} = -\frac{i}{\hbar}\left(V_{12}\,\rho_{21} - \rho_{12}V_{21}\right), \qquad \text{Eq. (5-1)}$$

where V_{12} is the interaction maxtrix taken between the states 1 and 2. Such a density matrix point of view has been successfully used by Kohn and Luttinger[44] in their treatment of the quantum theory of electrical transport and perhaps can be extended to phonon transport. Perturbation techniques exist for attacking the phonon transport problem. Landau and Rumer[45] worked the problem as early as 1937 and recently Maris[46] has given a Green's function approach which is valid for all $(\Omega_p\tau)$.

C. The Phonon Drift Velocity

The neglect, during the large amplitude considerations, of the phonon drift velocity was justified by an $(\Omega_p\tau) < 1$ condition. As we have just contemplated eventually considering $(\Omega_p\tau) > 1$ it seems logical at this point to attempt to extend the physics of the linearized theory to the non-linear with the hope of being able to better understand the effect of a shock on the phonon spectrum of the host solid.

Consider a material which has been subjected to external forces so that at the time some distribution of particle momentum p(z) exists in the medium. If we now Fourier analyze the p(z) distribution

$$A(q_3) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} p(z)\, e^{iq_3 z}\, dz \qquad \text{Eq. (5-2)}$$

we see that if p(z) is an even (odd) function of z then $A(q_3)$ is an even (odd) function of q_3. It also follows that if p(z) does not contain any symmetry then one should not expect $A(q_3)$ to have any obvious symmetry.

From Eq. (2-30a), for energy dependent relaxation times, we see that a nonzero λ_3 implies an antisymmetric contribution to $N_1(\vec{q};z,t)$ in q_3. For use at large amplitudes we shall generalize this to the statement that

> A lack of symmetry of $N_1(\vec{q};z,t)$ in q_i implies a nonzero λ_i.

This statement is less severe than simply taking the Eq. (5-2) result over to large amplitude strains and is made because we will be interested in $A^2(q_3)$ which is symmetric in q_3 for an antisymmetric $A(q_3)$. Since $N_1(\vec{q};z,t)$ is essentially the square of the Fourier transformation of particle momentum and particle displacement[47] we thus see that a lack of symmetry in particle velocity implies the existence of a phonon drift velocity. In general a gradient in particle velocity implies a lack of symmetry in p(z) and in turn a phonon drift velocity. This conclusion is in agreement with the linearized result (Appendix B)

$$\lambda_3 = \hbar c^2 \gamma \tau_u \frac{\partial \eta}{\partial z}, \qquad \text{Eq. (5-3)}$$

where $\frac{\partial \eta}{\partial z} = i\Omega_p C^{-1} \eta$ has been used along with $(\Omega_p \tau_u) \longrightarrow 0$. These considerations must mean that a shock front can be thought of as a cloud of drifting phonons. Thus, in the presence of a strong phonon drag[48] effect we have a mechanism which makes it valid to also think of a shock front as a cloud of drifting electrons*.

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*This is not to imply that the phonon drag effect is the only source of a propagating charge cloud in a shocked medium. Duvall and Thomson consider the gradient in Fermi energy generated by a shock front. A gradient in Fermi energy is a nonequilibrium situation and will give rise to an electric current. See G. E. Duvall and R. M. Thomson, Physics of Solids at High Pressures (Academic Press, New York, 1965), C. T. Tomizuka and R. M. Emrick editors.

It must be mentioned that equation such as Eq. (5-3) relate internal parameters (e.g. λ_s) to the external parameters (e.g. $\frac{\partial \eta}{\partial z}$) and in general result from solving conservation equations. For example, neglecting the zero point energy, and letting the instantaneous total energy density be E

$$E(z,t) = \hbar \sum_{\vec{q}} N(\vec{q}, z, t)\,\omega(\vec{q}, z, t) + U(\eta) + \frac{\rho}{2} u_p^2 , \qquad \text{Eq. (5-4)}$$

where $U(\eta)$ is the purely volume dependent part of the strain energy and u_p is the particle velocity. If W_a is the energy density of the perturbed unequilibrated state, and W_b is the energy density of the perturbed (same strain) but equilibrated state, then since $W_a = W_b$

$$\frac{\rho}{2}\left[u_p^2(b) - u_p^2(a)\right] = \hbar \sum_{\vec{q}} \left[N_b(\vec{q}, z, t) - N_a(\vec{q}, z, t)\right] \omega(\vec{q}, z, t) . \qquad \text{Eq. (5-5)}$$

We note that Eq. (5-5) can be put in a more appropriate form via

$$\frac{\partial u_p(b)}{\partial t} = \int_0^z \left(\frac{\partial \epsilon}{\partial t}\right)_b \frac{dz}{(1+2\epsilon)^{\frac{1}{2}}} + u_p(0, t_b) , \qquad \text{Eq. (5-6)}$$

where Eq. (4-6) has been used. The point is that Eq. (5-5) due to its quadratic nature has been too difficult to solve, but will have to be considered further in the process of learning more about the phonon drift in the presence of a large amplitude shock.

D. Translational Invariance

Lastly we should like to mention that the region of a shock front is a region of translational invariance in the direction parallel to the propagation direction. If q_n denotes the component of q perpendicular to the shock front, then the lack of translational invariance means that q_n is not a good quantum number. If q_n is not a good quantum number then the conservation relations are fuzzy and the scattering probability increases. This effect is important as it allows longitudinal phonon-longitudinal phonon interactions even in the presence of dispersion (such transitions would otherwise be relatively forbidden[3,49]).

APPENDIX A*

DERIVATION OF THE BOLTZMANN EQUATION

Let N be the density of phonons in some six dimensional space $(\chi_1, \chi_2, \chi_3; \mu_1, \mu_2, \mu_3)$ and Σ the rate of phonon creation in that space. Then if V_0 denotes an arbitrary element of our six dimensional volume bounded by the surface s_0

$$\int_{V_0}\left(\frac{\partial N}{\partial t}\right)dV + \int_{S_0} d\vec{S}\cdot(\vec{v}N) = \int_{V_0}\Sigma\, dV \qquad \text{Eq. (A-1)}$$

where $\vec{v} \equiv (\dot{\chi}_1, \ldots, \dot{\mu}_3)$. Or, upon using the divergence theorem,

$$\frac{\partial N}{\partial t} + \left[\dot{\chi}_1\frac{\partial N}{\partial \chi_1} + \cdots + \dot{\mu}_3\frac{\partial N}{\partial \mu_3}\right] + N\left[\frac{\partial \dot{\chi}_1}{\partial \chi_1} + \cdots + \frac{\partial \dot{\mu}_3}{\partial \mu_3}\right] = \Sigma \qquad \text{Eq. (A-2)}$$

We now let (χ_i, μ_i) be chosen such that if K is some Hamiltonian

$$\dot{\chi}_i = \frac{\partial K_0}{\partial \mu_i}, \quad \text{and} \quad \dot{\mu}_i = -\frac{\partial K_0}{\partial \chi_i}, \qquad \text{Eq. (A-3)}$$

where $K = K_0 + K_1$; i.e., we require that (χ_i, μ_i) form a set of canonically conjugate variables with respect to a piece K_0 of the complete Hamiltonian. We do not require that (χ_i, μ_i) be physically obvious variables. Substituting K_0 and its derivatives into Eq. (A-3) yields

$$\frac{\partial N}{\partial t} + \left[\frac{\partial N}{\partial \chi_1}\frac{\partial K_0}{\partial \mu_1} + \cdots - \frac{\partial N}{\partial \mu_3}\frac{\partial K_0}{\partial \chi_3}\right] = \Sigma. \qquad \text{Eq. (A-4)}$$

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*The author is indebted to Dr. R. F. Greene for outlining the method of attack used in this section.

If we restrict our physics to the interior of a crystal then the only source of phonon creation is thermalization so that $\Sigma = \frac{\partial N}{\partial t}\Big|_{coll.}$. The remaining task is to subdivide K so that K_0 does not contain any collision terms. The physical interpretation of the variables (χ_i, u_i) depends upon the physics contained in K_0.

It is understood that we have a Lagrangian[31] coordinate system, $(x_1, x_2, x_3) \equiv (x, y, z)$, for reference. We assume that at any instant u_i may be decomposed

$$u_i = \bar{u}_i + \tilde{u}_i \, , \qquad i = 1, 2, 3 \qquad \text{Eq. (A-5)}$$

where $\bar{u_i}$ is a purely volume depent (low frequency) term, and $\tilde{u_i}$ denotes the purely thermal (high frequency) fluctuations. Such a decomposition is always possible if the relaxation time for the thermal vibrations is small compared to the period associated with the impressed volume changes.

If the subdivision contained in Eq. (A-5) then the complete Hamiltonian may be similarly subdivided

$$K = \bar{K} + \tilde{K} \, . \qquad \text{Eq. (A-6)}$$

It is understood that the thermal term in Eq. (A-6) can have coefficients which are modulated by a strain dependence. Indeed in the limit of third order elasticity $\tilde{K}_2$ must be derivable from a Hamiltonian given by

$$\frac{1}{2}\left[C_{ijkl} + C_{ijklmn}\bar{u}_{mn}\right]\tilde{u}_{ij}\,\tilde{u}_{kl} \, , \qquad \text{Eq. (A-7)}$$

where $C_{ijk\ell}$ and $C_{ijk\ell mn}$ are second and third order elastic constants[a] respectively. Because of our condition $\Omega_p\tau<1$ we can consider N to be a constant of the motion for time intervals of the order of a few relaxation times (i.e., until changes in $\bar{u}_{mn}$ in Eq. (A-7) become important). But if N is a constant of the motion it is valid to consider the Hamiltonian of a single phonon, $\tilde{m}(\vec{q})$, $\vec{q}$ being an allowed value[a] of the phonon wave number (polarization and branches included). Let us identify K_0 of Eq. (A-3) with $\tilde{m}(\vec{q})$ and u_i with q_i. Since, neglecting dispersion

$$K_0 \equiv \tilde{m}(\vec{q}) = \hbar\omega(\vec{q}, z,t) = \hbar c(z,t) q \, , \qquad \text{Eq. (A-8)}$$

where a similar equation holds for each polarization.

$$\frac{\partial K_0}{\partial q_i} = \hbar C(z,t)\frac{\partial q}{\partial q_i} \, . \qquad \text{Eq. (A-9)}$$

If we now consider only the question of one dimensional strain, such that $\bar{u}_{33}$ is the only nonvanishing element of strain with the shock propagating in the z direction, then

$$\frac{\partial K_0}{\partial q_3} = \hbar c(z,t)\cos\theta = \hbar C_3(z,t) \, , \qquad \text{Eq. (A-10)}$$

where θ is the angle that $\vec{q}$ makes with the positive z axis, and $C_3 = C\cos\theta$. Thus, aside from a factor of $\hbar$, we must show that it is consistent to identify $\dot{\chi}_3$ as the z component of the phonon group velocity in the deforming media. Upon integrating $\dot{\chi}_3 = C_3(z,t)$ we find

$$\chi_3 = \int_{t_0}^{t} C_3(z,t')\,dt' + g(z), \qquad \text{Eq. (A-11)}$$

where t_0 is some constant, and $g(z)$ is an arbitrary function of z. Thus χ_3 cannot be identified as being simply proportional to z. χ_3 is a variable which is canonically conjugate to the internal[†] variable q_3, and thus must be an internal variable itself.

As the variable conjugate to q_3 must be coordinate-like let $\chi_3 \equiv z_1$. Thus

$$\frac{\partial K_0}{\partial z_1} = \hbar c(z,t)\frac{\partial q}{\partial z_1}, \qquad \text{Eq. (A-12)}$$

where in the absence of dispersion we have assumed that the phase velocity is independent of the internal parameter z_1. Since we are doing a one dimensional problem $\frac{\partial q_1}{\partial z_1} = \frac{\partial q_2}{\partial z_1} = 0$ so that

$$\frac{\partial K_0}{\partial z_1} = \hbar C_3(z,t)\frac{\partial q_3}{\partial z_1}. \qquad \text{Eq. (A-13)}$$

If, in Eq. (A-13), we now make the substitution

$$\frac{\partial}{\partial z_1} = -\frac{1}{C_3(z,t)}\frac{\partial}{\partial t}, \qquad \text{Eq. (A-14)}$$

then

$$\frac{\partial K_0}{\partial z_1} = -\hbar\frac{\partial q_3}{\partial t}, \qquad \text{Eq. (A-15)}$$

as desired. Eq. (A-14) says that the phonons propagate as plane waves in the internal space.

[†] q_3 is an internal variable in the sense that it describes momentum with respect to the center of mass of the system.

Utilizing all of the above considerations in Eq. (A-4) gives

$$\frac{\partial N}{\partial t} + \frac{1}{\hbar}\left[\frac{\partial N}{\partial z_1}\frac{\partial k_0}{\partial q_3} - \frac{\partial N}{\partial q_3}\frac{\partial k_0}{\partial z_1}\right] = \left.\frac{\partial N}{\partial t}\right|_{\text{Coll.}} . \qquad \text{Eq. (A-16)}$$

Thus we have shown that the Boltzmann equation is valid, regardless of the strain amplitude, providing only that $\Omega_p \tau < 1$ and that we are careful about the physical identification of the conjugate variables.

APPENDIX B

SOME LINEAR THEORY

From the conservation of "crystal" momentum and energy, Woodruff and Ehrenreich[1] derive their Eqs. (4-3) and (4-4) which we rewrite as Eqs. (A-1) and (A-2) respectively.

$$i\Omega_p I_{11}\left(\frac{\Delta T}{T_0}\right) - \frac{I_{20}}{\tau_u}\left(\frac{\Lambda}{\hbar c}\right) + i\Omega_p I_{21}\left(\frac{\Lambda}{\hbar c}\right) = -i\Omega_p I_{10}\gamma\eta, \qquad \text{Eq. (B-1)}$$

$$i\Omega_p I_{01}\left(\frac{\Delta T'}{T_0}\right) + \frac{I_{10}}{\tau_n}\left(\frac{\Lambda}{\hbar c}\right) = -i\Omega_p I_{00}\gamma\eta, \qquad \text{Eq. (B-2)}$$

where Λ is the modulus of a running wave λ_s, and η and (ΔT) are the modulii of similar quantities. The I_{mn} are integrals which sum over phonon propagation directions

$$I_{mn}(\Omega_p\tau) = \int_{-1}^{1} \frac{\mu^m(1-\mu)^n}{1 - i\Omega_p\tau(1-\mu)}\, d\mu, \qquad \text{Eq. (B-3)}$$

and are easily evaluated in the limit $(\Omega_p\tau) \to 0$. Some representative values for use in Eqs. (B-1) and (B-2) are

$$I_{00} = 2, \qquad I_{11} = -2/3,$$
$$I_{01} = 2, \qquad I_{20} = 2/3, \qquad \text{Eq. (B-4)}$$
$$I_{10} = 0, \qquad I_{21} = 2/3\ .$$

Solving Eqs. (B-1) and (B-2) simultaneously for $\left(\frac{\Lambda}{\hbar c}\right)$ and then using Eqs. (B-4) gives

$$\left(\frac{\Lambda}{\hbar c}\right) = - \frac{i\Upsilon(\Omega_p \tau_u)\eta}{i(\Omega_p \tau_u) - 1} , \qquad \text{Eq. (B-5)}$$

while substituting I_{10} from Eq. (B-4) directly into Eq. (B-2) gives

$$\left(\frac{\Delta T}{T_0}\right) = - \Upsilon\eta . \qquad \text{Eq. (B-6)}$$

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A Boltzmann equation approach is used to investigate the phonon distribution in a solid undergoing finite amplitude shock loading. Phonon-phonon interactions, via the anharmonic content of the crystal, lead to a collision term in the spirit of the Callaway thermal conductivity model. The theory is used to consider the phonon-phonon attenuation of a shock wave. In order to complement the microscopic theory, some macroscopic theory is considered.

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