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Here the best fit with theory yields an equili-
brium distribution coefficient of 0·13 for small
amounts of tin in bismuth.

With the viscosity value of liquid bismuth
cited in[1], the diffusion coefficient of tin in
liquid bismuth at about 275°C is calculated
to be $1·6 \times 10^{-5}$ cm²/sec. Niwa *et al.*[5]
measured this diffusion coefficient in the
temperature range 450°–600°C. The extra-
polation of their data to 275°C results in a
value of $2·8 \times 10^{-5}$ cm²/sec.

J. M. NOOTHOVEN VAN GOOR
H. M. G. J. TRUM

*Philips Research Laboratories,
N. V. Philips Gloeilampenfabrieken,
Eindhoven,
The Netherlands*

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Elastic Grüneisen parameters in crystals of low symmetry*

THE GRÜNEISEN parameters play an impor-
tant role in the theory of anharmonic effects
in solids, and their properties and behavior

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in cubic crystals have been extensively
investigated[1–5]. Recently, Brugger[6] has
formulated a generalized scheme of Grun-
eisen mode parameters in crystals of any
symmetry. In the present note, the relations
between the mode Gruneisen parameters
and the pressure derivatives of the elastic
moduli in several crystal classes of lower
symmetry than cubic will be derived. The
results will be applied to some materials where
experimental data are available.

An anisotropic continuum model, neglect-
ing dispersion, will be assumed. In addition,
the discussion will be limited to crystal
structures where the linear thermal expansion
tensor α_{ij} referred to crystalline axes is
diagonal, and the elastic compliance moduli
s_{ij} obey the relation:

$$s_{ij} = 0; \quad i = 1, 2, 3; \quad j = 4, 5, 6. \tag{1}$$

These assumptions limit the treatment to
cubic, tetragonal, hexagonal and ortho-
rhombic crystals.

The general mode Grüneisen parameter for
a mode of wave vector $\mathbf{q}$ and polarization
index p is defined as[7]:

$$\gamma_{jk}^p = -[\partial \ln \omega_p(\mathbf{q})/\partial \eta_{jk}]_T; \quad j, k = 1, 2, 3 \tag{2}$$

where η_{ij} are the Lagrangian strains, $\omega_p(\mathbf{q})$
the frequency of the mode $\mathbf{q}, p$. Confining the
strain to hysrostatic pressure P, we have the
relation[6]:

$$[\partial \ln \omega_p(\mathbf{q})/\partial P]_T = -s_{iijk}^T [\partial \ln \omega_p(\mathbf{q})/\partial \eta_{jk}]_T \tag{3}$$

where summation over repeated indices is
implied. In our case, $\eta_{ij} = 0$ for $i \neq j$, and as
a result of equation (1) we have:

$$[\partial \ln \omega_p(q)/\partial P]_T = \sum_{i,j=1}^{3} s_{ij}^T \gamma_j^p(q) \tag{4}$$

the mode gamma tensor being diagonal. Now,
as we neglect dispersion, $\omega_p(q)$ is given by:

$$\omega_p(q) = qs_p(\theta, \phi). \tag{5}$$

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eing diagonal. Now,
$\omega_p(q)$ is given by:

$$_p(\theta, \phi). \qquad (5)$$

But,

$$q \propto (L_1^2 + L_2^2 + L_3^2)^{-1/2} \qquad (6)$$

where L_1, L_2 and L_3 are the lengths of the crystal parallel to the x, y and z axes, and $s_p(\theta, \phi)$ is the sound velocity for the mode q, p. Hence, one obtains the relation:

$$[\partial \ln \omega_p(\mathbf{q})/\partial P]_T = (l^2 K_1^T + m^2 K_2^T + n^2 K_3^T)$$
$$+ [\partial \ln s_p(\theta, \phi)/\partial P]_T \qquad (7)$$

where K_1^T, K_2^T and K_3^T are the isothermal linear compressibilities in the directions of the crystalline axes, and l, m, n, are the *direction cosines of* q. Denoting the elastic stiffness modulus associated with the mode q, p by c_p, one obtains:

$$(\partial \ln \omega_p(\mathbf{q})/\partial P) = l^2 K_1^T + m^2 K_2^T + n^2 K_3^T$$
$$- 0{\cdot}5\, K_V^T + 0{\cdot}5(\partial \ln c_p/\partial P)_T \qquad (8)$$

where K_V^T is the isothermal volume compressibility. Thus, we have

$$\sum_{i,j=1}^{3} s_{ij}\gamma_j^p(\mathbf{q}) = l^2 K_1^T + m^2 K_2^T + n^2 K_3^T$$
$$- 0{\cdot}5 K_V^T + 0{\cdot}5(\partial \ln c_p/\partial P)_T. \qquad (9)$$

Defining now an averaged mode gamma

$$\gamma^p(\mathbf{q}) = \left(\sum_{i,j=1}^{3} s_{ij}\right)^{-1} \times \left[\sum_{i,j=1}^{3} s_{ij}\gamma_j^p(\mathbf{q})\right] \qquad (10)$$

one obtains

$$\gamma^p(\mathbf{q}) = [l^2 K_1^T + m^2 K_2^T + n^2 K_3^T - 0{\cdot}5 K_V^T$$
$$+ 0{\cdot}5(\partial \ln c_p/\partial P)_T]\Big/\left(\sum_{i,j=1}^{3} s_{ij}\right). \qquad (11)$$

As can be seen the individual mode gammas $\gamma_i^p(\mathbf{q})$ cannot be deduced from the pressure derivatives of the elastic moduli alone, but only their weighted average. In order to determine the individual $\gamma_i^p(\mathbf{q})$, uniaxial as well as hysrostatic pressure derivatives of the elastic moduli are required.

The Grüneisen parameter, defined by

$$\gamma = \beta V \Big/\left(C_V \sum_{i,j=1}^{3} s_{ij}\right) \qquad (12)$$

where β is the volume expansion thermal expansion coefficient ($\beta = \alpha_1 + \alpha_2 + \alpha_3$), C_V the specific heat at constant volume V, is given by[7]

$$\gamma = \left[\sum_{q,p} C_p(\mathbf{q})\gamma^p(\mathbf{q})\right]\Big/\left[\sum_{q,p} C_p(\mathbf{q})\right] \qquad (13)$$

where $C_p(\mathbf{q})$ is the specific heat associated with the mode q.p. The low and high temperature limits of the Grüneisen parameter, γ_L and γ_H may be easily calculated, as at the low temperature limit $C_p(\mathbf{q}) \propto c_p^{-3/2}$, while in the high temperature limit $C_p(\mathbf{q}) = kT$. Hence, in these two limiting cases the sum in equation (13) may be evaluated in a straight forward manner.

A computer program for the CDC 3600 computer which evaluates the averaged mode gammas $\gamma^p(\mathbf{q})$, as well as γ_L and γ_H in crystals of cubic, hexagonal, tetragonal and orthorhombic symmetry has been written. The input data to the program are the room temperature elastic moduli, their pressure derivatives, and the low temperature elastic moduli. The program computes the sound velocity in any direction by calculating the eigenvalues of the Christoffel determinant[8], as well as the pressure derivatives in any direction. From the latter quantities the $\gamma^p(\mathbf{q})$ as function of direction are determined. γ_L and γ_H are evaluated by numerical quadrature.*

The above program has been applied to three materials of hexagonal symmetry, where the values of the elastic moduli and their pressure derivatives are available, i.e. magnesium[9, 10], cadmium[11, 12] and cadmium sulfide[13, 14]. Since the hexagonal structure has transverse symmetry, the $\gamma^p(q)$ need only be evaluated as a function of the latitude angle θ. The results of the computation are shown in Figs. 1–3, where $p = 1$ is the longitudinal mode, $p = 2$ the fast shear mode, and

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*A write-up of the program may be obtained from the author upon request.
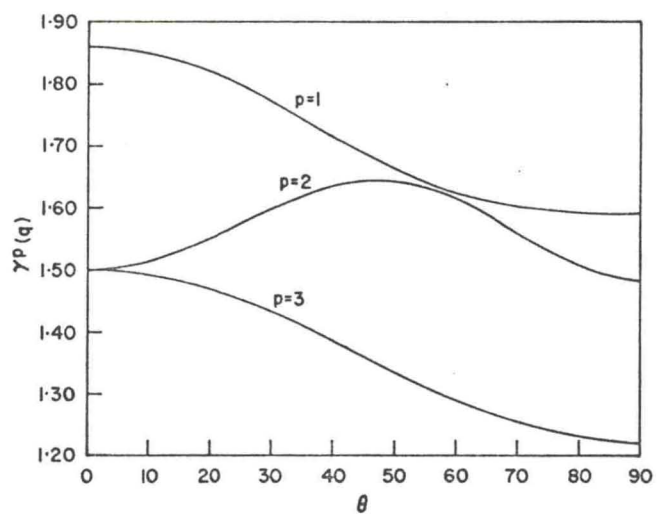
Fig. 1. $\gamma^p(q)$ as a function of θ for Mg.
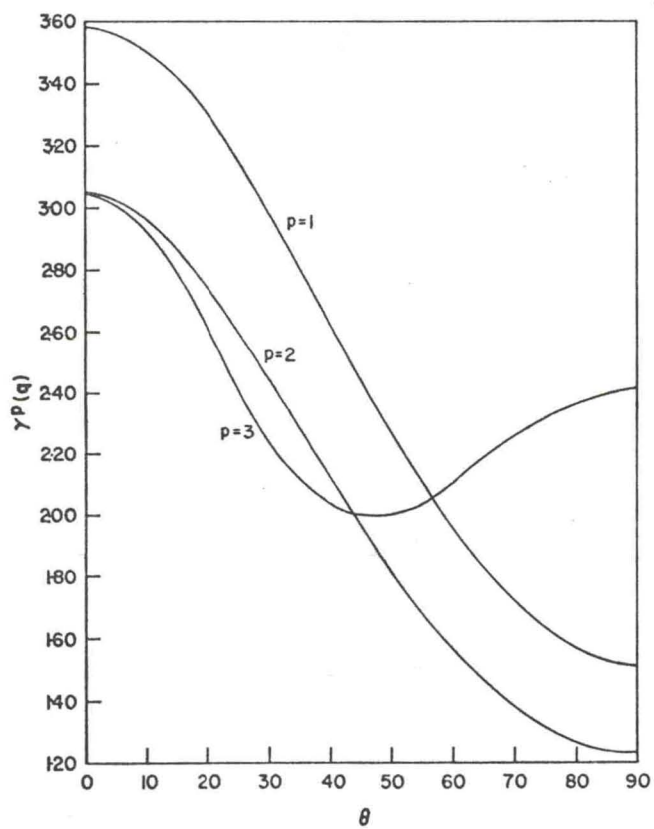
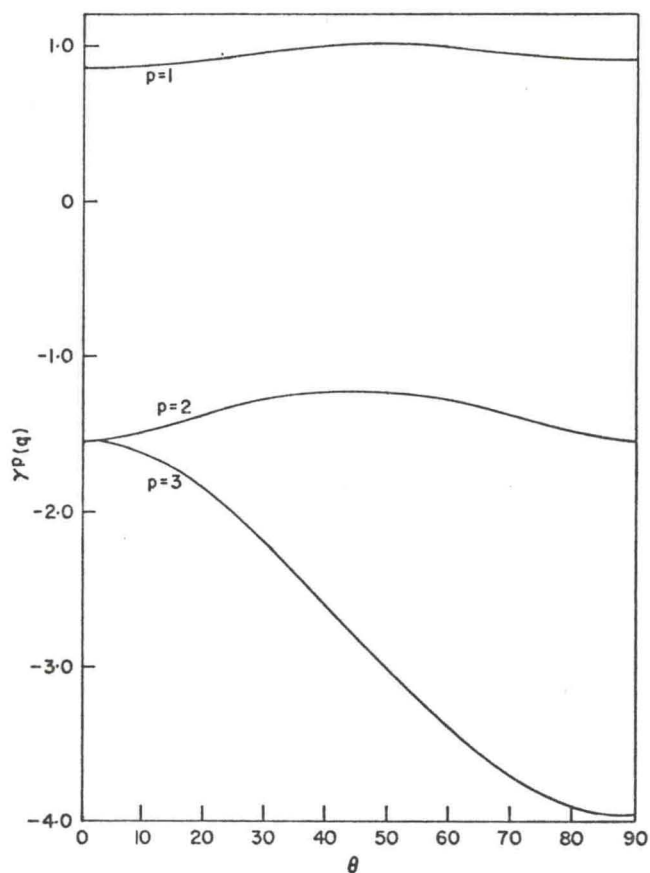Fig. 2. $\gamma^p(q)$ as a function of θ for Cd.

Fig. 3. $\gamma^p(\mathbf{q})$ as a function of θ for CdS.

Table 1. *The values of* γ_L *and* γ_H *for* Mg, Cd *and* CdS, *as obtained from elastic and thermal expansion data*

| | Elastic data | | Thermal expansion data | |
	γ_L	γ_H	γ_L	γ_H
Mg	1·45	1·52	1·40(10°K) [7]	1·50(300°K) [7]
Cd	2·16	2·06	2·10(20°K) [16, 18]	1·86(300°K) [16, 18]
CdS	−2·19	−1·19	−2·34(20°K) [15, 18]	0·45(300°K) [15, 18]

$p = 3$ the slow shear mode. In Table 1 the values of γ_L and γ_H as obtained from elastic data, are compared with the similar quantities derived from thermal expansion data. As can be seen, the agreement between the two sets of data is very good for magnesium and cadmium, while in the case of cadmium sulfide, there are large discrepancies between the thermal expansion and elastic γ_H. This is not surprising, as such discrepancies are expected when optical phonons contribute appreciably to the lattice vibration spectrum [4], which is the case for cadmium sulfide. The thermal expansion value of γ_L contains probably some error, as the values of the low temperature thermal expansion coefficient were determined from data of the lattice parameter as a function of temperature[15].

It is interesting to note that the negative thermal expansion coefficient of cadmium at low temperatures[16, 17] is not reflected in $\gamma^p(\mathbf{q})$ becoming negative. This is probably due to the dominance of the modes with positive values of $\gamma^p(\mathbf{q})$ in the averaging process. On the other hand, in the case of cadmium sulfide, the $\gamma^p(\mathbf{q})$ for the shear modes are both negative throughout, as well as γ_L. This is in agreement with the fact that both thermal expansion coefficients of cadmium sulfide become negative at low temperatures.

Argonne National Laboratory,   D. GERLICH†
Argonne, Ill. 60439,
U.S.A.

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Antiferromagnetic structures of USb and UBi*

THE URANIUM compounds with group VA elements (N, P, As, Sb, and Bi, denoted by v) that have the NaCl-type structure are antiferromagnetic. The values of the Néel temperature (T_N), the paramagnetic Curie temperature (θ), and the paramagnetic moment (n_p) increase along the series from UN to UBi. These properties and the high electrical conductivity were considered in a