

1.3. ELASTIC PROPERTIES

Table 1.3.7.1. Relationships between ρW^2 , its pressure derivatives and the second- and third-order elastic constants

Propagation	Polarization	$(\bar{\rho}_0 W^2)_0$	$\partial(\bar{\rho}_0 W^2)_0/\partial p$
[100]	[100]	\bar{c}_{11}	$-1 - (2\bar{c}_{11} + \Gamma_{1111})/3\bar{\kappa}$
[100]	[010]	\bar{c}_{44}	$-1 - (2\bar{c}_{44} + \Gamma_{2323})/3\bar{\kappa}$
[110]	[110]	$(\bar{c}_{11} + \bar{c}_{12} + 2\bar{c}_{44})/2$	$-1 - (\bar{c}_{11} + \bar{c}_{12} + 2\bar{c}_{44} + 0.5[\Gamma_{1111} + \Gamma_{1122} + \Gamma_{2323}])/3\bar{\kappa}$
[110]	[110]	$(\bar{c}_{11} - \bar{c}_{12} + \bar{c}_{44})/3$	$-1 - (\bar{c}_{11} - \bar{c}_{12} + 0.5[\Gamma_{1111} - \Gamma_{1122}])/3\bar{\kappa}$
[110]	[001]	\bar{c}_{44}	$-1 - (2\bar{c}_{44} + \Gamma_{2323})/3\bar{\kappa}$
[111]	[111]	$(\bar{c}_{11} + 2\bar{c}_{12} + 4\bar{c}_{44})/3$	$-1 - (2\bar{c}_{11} + 4\bar{c}_{12} + 8\bar{c}_{44} + [\Gamma_{1111} + 2\Gamma_{1122} + 4\Gamma_{2323}])/9\bar{\kappa}$
[111]	[110]	$(\bar{c}_{11} - \bar{c}_{12} + \bar{c}_{44})/3$	$-1 - (2\bar{c}_{11} - 2\bar{c}_{12} + 2\bar{c}_{44} + [\Gamma_{1111} - \Gamma_{1122} + \Gamma_{2323}])/9\bar{\kappa}$

or

$$\rho_0 \omega^2 A_j = \Delta_{jk} A_k$$

with $\Delta_{jk} = D_{ijkl} k_j k_l$.

The quantities $\rho_0 \omega^2 A_j$ and A are, respectively, the *eigenvalues* and *eigenvectors of the matrix* Δ_{jk} . Since Δ_{jk} is a real symmetric matrix, the eigenvalues are real and the eigenvectors are orthogonal.

1.3.7.6. Experimental determination of third- and higher-order elastic constants

The main experimental procedures for determining the third- and higher-order elastic constants are based on the measurement of stress derivatives of ultrasonic velocities and on harmonic generation experiments. Hydrostatic pressure, which can be accurately measured, has been widely used; however, the measurement of ultrasonic velocities in a solid under hydrostatic pressure cannot lead to the whole set of third-order elastic constants, so uniaxial stress measurements or harmonic generation experiments are then necessary.

In order to interpret wave-propagation measurements in stressed crystals, Thurston (1964) and Brugger (1964) introduced the concept of natural velocity with the following comments:

‘According to equation of motion, the wave front is a material plane which has unit normal \mathbf{k} in the natural state; a wave front moves from the plane $\mathbf{k} \cdot \mathbf{a} = \mathbf{0}$ to the plane $\mathbf{k} \cdot \mathbf{a} = \mathbf{L}_0$ in the time L_0/W . Thus W , the *natural velocity*, is the wave speed referred to natural dimensions for propagation normal to a plane of natural normal \mathbf{k} .

In a typical ultrasonic experiment, plane waves are reflected between opposite parallel faces of a specimen, the wave fronts being parallel to these faces. One ordinarily measures a repetition frequency F , which is the inverse of the time required for a round trip between the opposite faces.’

Hence

$$W = 2L_0 F.$$

In most experiments, the third-order elastic constants and higher-order elastic constants are deduced from the stress derivatives of $\bar{\rho}_0 W^2$. For instance, Table 1.3.7.1 gives the expressions for $(\bar{\rho}_0 W^2)_0$ and $\partial(\bar{\rho}_0 W^2)_0/\partial p$ for a cubic crystal. These quantities refer to the natural state free of stress. In this table, p denotes the hydrostatic pressure and the Γ_{ijkl} ’s are the following linear combinations of third-order elastic constants:

$$\Gamma_{1111} = \bar{c}_{111} + 2\bar{c}_{111}$$

$$\Gamma_{1122} = 2\bar{c}_{112} + \bar{c}_{123}$$

$$\Gamma_{2323} = \bar{c}_{144} + 2\bar{c}_{166}$$

1.3.8. Glossary

\mathbf{e}_i	covariant basis vector
A^T	transpose of matrix A
u_i	components of the displacement vector
S_{ij}	components of the strain tensor
S_α	components of the strain Voigt matrix
T_{ij}	components of the stress tensor
T_α	components of the stress Voigt matrix
p	pressure
ν	normal stress
τ	shear stress
s_{ijkl}	second-order elastic compliances
$s_{\alpha\beta}$	reduced second-order elastic compliances
$(s_{ijkl})^\sigma$	adiabatic second-order elastic compliances
s_{ijklmn}	third-order elastic compliances
c_{ijkl}	second-order elastic stiffnesses
$(c_{ijkl})^\sigma$	adiabatic second-order elastic stiffnesses
$c_{\alpha\beta}$	reduced second-order elastic stiffnesses
c_{ijklmn}	third-order elastic stiffnesses
ν	Poisson’s ratio
E	Young’s modulus
κ	bulk modulus (volume compressibility)
λ, μ	Lamé constants
Θ	temperature
c^S	specific heat at constant strain
ρ	volumic mass
Θ_D	Debye temperature
k_B	Boltzmann constant
U	internal energy
F	free energy

References

Breazeale, M. A. (1984). *Determination of third-order elastic constants from ultrasonic harmonic generation. Physical acoustics*, Vol. 17, edited by R. N. Thurston, pp. 2–75. New York: Academic Press.

Brillouin, L. (1932). *Propagation des ondes électromagnétiques dans les milieux matériels. Congrès International d’Électricité*, Vol. 2, Section 1, pp. 739–788. Paris: Gauthier-Villars.

Brugger, K. (1964). *Thermodynamic definition of higher-order elastic coefficients. Phys. Rev.* **133**, 1611–1612.

De Launay, J. (1956). *The theory of specific heats and lattice vibrations. Solid state physics*, Vol. 2, edited by F. Seitz & D. Turnbull, pp. 219–303. New York: Academic Press.

Fischer, M. (1982). *Third- and fourth-order elastic constants of fluoperovskites CsCdF₃, TICdF₃, RbCdF₃, RbCaF₃. J. Phys. Chem. Solids*, **43**, 673–682.

Fischer, M., Zarembowitch, A. & Breazeale, M. A. (1980). *Nonlinear elastic behavior and instabilities in crystals. Ultrasonics Symposium Proc. IEEE*, pp. 999–1002.

Fumi, F. G. (1951). *Third-order elastic coefficients of crystals. Phys. Rev.* **83**, 1274–1275.

Fumi, F. G. (1952). *Third-order elastic coefficients in trigonal and hexagonal crystals. Phys. Rev.* **86**, 561.

Fumi, F. G. (1987). *Tables for the third-order elastic tensors in crystals. Acta Cryst.* **A43**, 587–588.

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- Green, R. E. (1973). *Treatise on material science and technology*, Vol. 3. New York: Academic Press.
- Landolt-Börnstein (1979). Group III. *Crystal and solid state physics*. Berlin: Springer-Verlag.
- McSkimmin, H. J. (1964). *Ultrasonic methods for measuring the mechanical properties of solids and fluids*. *Physical acoustics*, Vol. 1A, edited by W. P. Mason, pp. 271–334. New York: Academic Press.
- Melcher, R. L. & Scott, B. A. (1972). *Soft acoustic modes at the cooperative Jahn–Teller transition in DyVO₄*. *Phys. Rev. Lett.* **28**, 607–610.
- Michard, F., Zarembowitch, A., Vacher, R. & Boyer, L. (1971). *Premier son et son zéro dans les nitrates de strontium, barium et plomb. Phonons*, edited by M. A. Nusimovici, pp. 321–325. Paris: Flammarion.
- Murnaghan, F. D. (1951). *Finite deformation in an elastic solid*. New York: John Wiley and Sons.
- Nouet, J., Zarembowitch, A., Pisarev, R. V., Ferré, J. & Lecomte, M. (1972). *Determination of T_N for KNiF₃ through elastic, magneto-optical and heat capacity measurements*. *Appl. Phys. Lett.* **21**, 161–162.
- Rousseau, M., Gesland, J. Y., Julliard, J., Nouet, J., Zarembowitch, J. & Zarembowitch, A. (1975). *Crystallographic, elastic and Raman scattering investigations of structural phase transitions in RbCdF₃ and TlCdF₃*. *Phys. Rev.* **12**, 1579–1590.
- Salje, E. K. H. (1990). *Phase transitions in ferroelastic and co-elastic crystals*. Cambridge University Press.
- Thurston, R. N. (1964). *Wave propagation in fluids and normal solids*. *Physical acoustics*, Vol. 1A, edited by W. P. Mason, pp. 1–109. New York: Academic Press.
- Truesdell, C. & Toupin, R. (1960). *The classical field theories*. *Handbuch der Physik*, Vol. III/1, edited by S. Flügge. Berlin, Göttingen, Heidelberg: Springer-Verlag.
- Voigt, W. (1910). *Lehrbuch der Kristallphysik*. 2nd ed. (1929). Leipzig: Teubner. Photoreproduction (1966). New York: Johnson Reprint Corp.
- Wallace, D. C. (1970). *Thermoelastic theory of stressed crystals and higher-order elastic constants*. *Solid state physics*, Vol. 25. New York: Academic Press.
- Wallace, D. C. (1972). *Thermodynamics of crystals*. New York: John Wiley and Sons.
- Zarembowitch, A. (1965). *Etude théorique et détermination optique des constantes élastiques de monocristaux*. *Bull. Soc. Fr. Minéral. Cristallogr.* **28**, 17–49.