

1. TENSORIAL ASPECTS OF PHYSICAL 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}	$-1 - (2\bar{c}_{11} + \Gamma_{1111})/3\bar{k}$
[100]	[010]	\bar{c}_{44}	$-1 - (2\bar{c}_{44} + \Gamma_{2323})/3\bar{k}$
[110]	[110]	$(\bar{c}_{11} + \bar{c}_{12} + 2\bar{c}_{44})/2$	$-1 - (\bar{c}_{11} + \bar{c}_{12} + 2\bar{c}_{44} + 0.5[\Gamma_{1111} + \Gamma_{1122} + \Gamma_{2323}])/3\bar{k}$
[110]	[110]	$(\bar{c}_{11} - \bar{c}_{12} + \bar{c}_{44})/3$	$-1 - (\bar{c}_{11} - \bar{c}_{12} + 0.5[\Gamma_{1111} - \Gamma_{1122}])/3\bar{k}$
[110]	[001]	\bar{c}_{44}	$-1 - (2\bar{c}_{44} + \Gamma_{2323})/3\bar{k}$
[111]	[111]	$(\bar{c}_{11} + 2\bar{c}_{12} + 4\bar{c}_{44})/3$	$-1 - (2\bar{c}_{11} + 4\bar{c}_{12} + 8\bar{c}_{44} + [\Gamma_{1111} + 2\Gamma_{1122} + 4\Gamma_{2323}])/9\bar{k}$
[111]	[110]	$(\bar{c}_{11} - \bar{c}_{12} + \bar{c}_{44})/3$	$-1 - (2\bar{c}_{11} - 2\bar{c}_{12} + 2\bar{c}_{44} + [\Gamma_{1111} - \Gamma_{1122} + \Gamma_{2323}])/9\bar{k}$

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 $\mathbf{k} \cdot \mathbf{a} = 0$ 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

$$W = 2L_0F.$$

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:

$$\begin{aligned} \Gamma_{1111} &= \bar{c}_{111} + 2\bar{c}_{111} \\ \Gamma_{1122} &= 2\bar{c}_{112} + \bar{c}_{123} \\ \Gamma_{2323} &= \bar{c}_{144} + 2\bar{c}_{166}. \end{aligned}$$

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
\mathbf{v}	normal stress
$\boldsymbol{\tau}$	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.

Every, A. G. & McCurdy, A. K. (1992). *Second and higher order elastic constants*. In Landolt-Börnstein, Group III, *Condensed Matter*, Volume 29, Subvolume A. Berlin/Heidelberg/New York: Springer.

Fischer, M. (1982). *Third- and fourth-order elastic constants of fluoperovskites CsCdF₃, TlCdF₃, 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.

Green, R. E. (1973). *Treatise on Material Science and Technology*, Vol. 3. New York: Academic Press.

McSkimmin, H. J. (1964). *Ultrasonic methods for measuring the mechanical properties of solids and fluids*. *Physical Acoustics*, Vol. IA, 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.