

1. TENSORIAL ASPECTS OF PHYSICAL PROPERTIES

1.1.5.2. Other forms of the piezoelectric constants

We use here another Gibbs function, the electric Gibbs function, \mathcal{G}_2 , defined by

$$\mathcal{G}_2 = \mathcal{U} - E_n D_n - \Theta \sigma.$$

Differentiation of \mathcal{G} gives

$$d\mathcal{G}_2 = -D_n dE_n + T_{ij} dS_{ij} - \sigma d\Theta.$$

It follows that

$$T_{ij} = \frac{\partial \mathcal{G}_2}{\partial S_{ij}}; \quad D_n = -\frac{\partial \mathcal{G}_2}{\partial E_n}; \quad \sigma = -\frac{\partial \mathcal{G}_2}{\partial \Theta}$$

and a set of relations analogous to (1.1.5.1):

$$\left. \begin{aligned} T_{ij} &= (c_{ijkl})^{E,\Theta} S_{kl} - (e_{ijn})^{S,\Theta} E_n - (\lambda_{ij})^{E,S} \delta\Theta \\ D_n &= (e_{nij})^{E,\Theta} S_{ij} + (\varepsilon_{nm})^{S,\Theta} E_m + (p_n)^S \delta\Theta \\ \delta\sigma &= (\lambda_{ij})^E S_{ij} + (p_n)^S E_n + \rho C^{E,S} \delta\Theta/\Theta, \end{aligned} \right\} \quad (1.1.5.2)$$

where the components $(c_{ijkl})^{E,\Theta}$ are the isothermal elastic stiffnesses at constant field and constant temperature,

$$e_{ijn} = -\frac{\partial T_{ij}}{\partial E_n} = -\frac{\partial^2 \mathcal{G}_2}{\partial E_n \partial S_{ij}} = -\frac{\partial^2 \mathcal{G}_2}{\partial S_{ij} \partial E_n} = \frac{\partial D_n}{\partial S_{ij}} = e_{nij}$$

are the piezoelectric stress coefficients at constant strain and constant temperature,

$$\lambda_{ij} = -\frac{\partial T_{ij}}{\partial \Theta} = -\frac{\partial^2 \mathcal{G}_2}{\partial \Theta \partial S_{ij}} = -\frac{\partial^2 \mathcal{G}_2}{\partial S_{ij} \partial \Theta} = \frac{\partial \delta\sigma}{\partial S_{ij}}$$

are the temperature-stress constants and

$$p_n = \frac{\partial D_n}{\partial \Theta} = -\frac{\partial^2 \mathcal{G}_2}{\partial \Theta \partial E_n} = -\frac{\partial^2 \mathcal{G}_2}{\partial E_n \partial \Theta} = \frac{\partial \delta\sigma}{\partial D_n}$$

are the components of the pyroelectric effect at constant strain.

The relations between these coefficients and the usual coefficients d_{kln} are easily obtained:

(i) At constant temperature and strain: if one puts $\delta\Theta = 0$ and $S_{kl} = 0$ in the first equation of (1.1.5.1) and (1.1.5.2), one obtains, respectively,

$$\begin{aligned} 0 &= s_{klj} T_{ij} + d_{kln} E_n \\ T_{ij} &= -e_{ijn} E_n, \end{aligned}$$

from which it follows that

$$d_{kln} = s_{klj} e_{ijn}$$

at constant temperature and strain.

(ii) At constant temperature and stress: if one puts $\delta\Theta = 0$ and $T_{ij} = 0$, one obtains in a similar way

$$\begin{aligned} S_{kl} &= d_{kln} E_n \\ 0 &= c_{ijkl} S_{kl} - e_{ijn} E_n, \end{aligned}$$

from which it follows that

$$e_{ijn} = c_{ijkl} d_{kln}$$

at constant temperature and stress.

1.1.5.3. Relation between the pyroelectric coefficients at constant stress and at constant strain

By combining relations (1.1.5.1) and (1.1.5.2), it is possible to obtain relations between the pyroelectric coefficients at constant stress, p_n^T , and the pyroelectric coefficients at constant strain, p_n^S , also called *real* pyroelectric coefficients, p_n^S . Let us put $T_{ij} = 0$ and

$E_n = 0$ in the first equation of (1.1.5.1). For a given variation of temperature, $\delta\Theta$, the observed strain is

$$S_{kl} = [\alpha_{kl}]^{E,T} \delta\Theta.$$

From the second equations of (1.1.5.1) and (1.1.5.2), it follows that

$$\begin{aligned} D_n &= p_n^T \delta\Theta \\ D_n &= e_{nkl} S_{kl} + p_n^S \delta\Theta. \end{aligned}$$

Substituting the expression S_{kl} and eliminating D_n , it follows that

$$p_n^T = e_{nkl} [\alpha_{kl}]^{E,T} + p_n^S. \quad (1.1.5.3)$$

This relation shows that part of the pyroelectric effect is actually due to the piezoelectric effect.

1.1.5.4. Adiabatic study

Piezoelectric resonators usually operate at a high frequency where there are no heat exchanges, and therefore in an adiabatic regime ($\Theta\delta\sigma = 0$). From the third equation of (1.1.5.1), we obtain a relation between the temperature variation, the applied stress and the electric field:

$$(\alpha_{ij})^E T_{ij} + (p_m)^T E_m + \frac{\rho C^{T,E}}{\Theta} \delta\Theta = 0.$$

If we substitute this relation in the two other relations of (1.1.5.1), we obtain two equivalent relations, but in the *adiabatic* regime:

$$\begin{aligned} S_{kl} &= (s_{klj})^{E,\sigma} T_{ij} + (d_{klm})^{T,\sigma} E_m \\ D_n &= (d_{nij})^{E,\sigma} T_{ij} + (\varepsilon_{nm})^{T,\sigma} E_m. \end{aligned}$$

By comparing these expressions with (1.1.5.1), we obtain the following relations between the adiabatic and the isothermal coefficients:

$$\begin{aligned} (s_{ijkl})^{E,\sigma} &= (s_{ijkl})^{E,\theta} - \frac{(\alpha_{ij})^E (\alpha_{kl})^E \Theta}{\rho C^{T,E}} \\ (d_{nij})^{E,\sigma} &= (d_{nij})^{E,\theta} - \frac{(p_n)^T (\alpha_{kl})^E \Theta}{\rho C^{T,E}} \\ (\varepsilon_{mn})^{T,\sigma} &= (\varepsilon_{mn})^{T,\theta} - \frac{(p_n)^T (p_m)^T \Theta}{\rho C^{T,E}}. \end{aligned}$$

1.1.6. Glossary

\mathbf{e}_i	basis vectors in direct space (covariant)
\mathbf{e}^i	basis vectors in reciprocal space (contravariant)
x^i	components of a vector in direct space (contravariant)
x_i	components of a vector in reciprocal space (covariant)
g_{ij}	components of the metric tensor
$\overset{j_1 \dots j_q}{i_1 \dots i_p}$	components of a tensor of rank n , p times covariant and q times contravariant ($n = p + q$)
A^T	transpose of matrix A
\otimes	tensor product
\wedge	outer product
\wedge	vector product
∂_i	partial derivative with respect to x_i
δ_i^j	Kronecker symbol
ε_{ijk}	permutation tensor
V	volume

1.1. INTRODUCTION TO THE PROPERTIES OF TENSORS

p	pressure
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
s_{ijkl}	elastic compliances
$s_{\alpha\beta}$	reduced elastic compliances
$(s_{ijkl})^\sigma$	adiabatic elastic compliances
c_{ijkl}	elastic stiffnesses
$c_{\alpha\beta}$	reduced elastic stiffnesses
ν	Poisson's ratio
E	Young's modulus
Θ	temperature
σ	entropy
α_{ij}	thermal expansion
λ_{ij}	temperature-stress constant
\mathcal{U}	internal energy
\mathcal{G}	Gibbs free energy
$C^{E,T}$	specific heat at constant stress and applied electric field
E	electric field
D	electric displacement
H	magnetic field
B	magnetic induction
ϵ_0	permittivity of vacuum
ϵ	dielectric constant
ϵ_{ij}	dielectric tensor
$(\epsilon_{ij})^\sigma$	adiabatic dielectric tensor
χ_e	dielectric susceptibility
η_{ij}	dielectric impermeability
p_i	pyroelectric tensor
d_{ijk}	piezoelectric tensor
$d_{i\alpha}$	reduced piezoelectric tensor
$d_{\alpha i}$	reduced inverse piezoelectric tensor
$(d_{ijk})^\sigma$	adiabatic piezoelectric tensor
e_{ijk}	piezoelectric tensor at constant strain
Q_{ijkl}	electrostriction tensor
$Q_{\alpha\beta}$	reduced electrostriction tensor
π_{ijkl}	piezo-optic tensor
$\pi_{\alpha\beta}$	reduced piezo-optic tensor
p_{ijkl}	elasto-optic tensor
$p_{\alpha\beta}$	reduced elasto-optic tensor
$R_{H\ ij k}$	Hall constant

References

- Bhagavantam, S. (1966). *Crystal symmetry and physical properties*. London: Academic Press.
- Billings, A. (1969). *Tensor properties of materials*. London/New York: Wiley Interscience.
- Brillouin, L. (1949). *Les tenseurs en mécanique et en élasticité*. Paris: Masson & Cie.
- Cady, W. G. (1964). *Piezoelectricity*. New York: Dover.
- Curie, J. & Curie, P. (1880). *Développement par pression de l'électricité polaire dans les cristaux hémédres à faces inclinées*. *C. R. Acad. Sci.* **91**, 294–295.
- Curie, J. & Curie, P. (1881). *Contractions et dilatations produites par des tensions électriques dans les cristaux hémédres à faces inclinées*. *C. R. Acad. Sci.* **93**, 1137–1140.
- Curie, P. (1884). *Sur les questions d'ordre: répétitions*. *Bull. Soc. Fr. Minéral.* **7**, 89–110.
- Curie, P. (1894). *Sur la symétrie dans les phénomènes physiques, symétrie d'un champ électrique et d'un champ magnétique*. *J. Phys. (Paris)*, **3**, 393–415.
- Fumi, F. G. (1951). *Third-order elastic coefficients of crystals*. *Phys. Rev.* **83**, 1274–1275.
- Fumi, F. G. (1952a). *Physical properties of crystals: the direct inspection method*. *Acta Cryst.* **5**, 44–48.
- Fumi, F. G. (1952b). *The direct-inspection method in systems with a principal axis of symmetry*. *Acta Cryst.* **5**, 691–694.
- Fumi, F. G. (1952c). *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.
- Fumi, F. G. & Ripamonti, C. (1980a). *Tensor properties and rotational symmetry of crystals. I. A new method for group $3(3_2)$ and its application to general tensors up to rank 8*. *Acta Cryst.* **A36**, 535–551.
- Fumi, F. G. & Ripamonti, C. (1980b). *Tensor properties and rotational symmetry of crystals. II. Groups with 1-, 2- and 4-fold principal symmetry and trigonal and hexagonal groups different from group 3*. *Acta Cryst.* **A36**, 551–558.
- Ikeda, T. (1990). *Fundamentals of piezoelectricity*. Oxford University Press.
- International Tables for Crystallography* (2000). Vol. B. *Reciprocal space*, edited by U. Shmueli. Dordrecht: Kluwer Academic Publishers.
- International Tables for Crystallography* (2002). Vol. A. *Space-group symmetry*, edited by Th. Hahn. Dordrecht: Kluwer Academic Publishers.
- Kumaraswamy, K. & Krishnamurthy, N. (1980). *The acoustic gyrotropic tensor in crystals*. *Acta Cryst.* **A36**, 760–762.
- Lichnerowicz, A. (1947). *Algèbre et analyse linéaires*. Paris: Masson.
- Mason, W. P. (1966). *Crystal physics of interaction processes*. London: Academic Press.
- Neumann, F. (1885). *Vorlesungen über die Theorie der Elastizität der festen Körper und des Lichtäthers*, edited by O. E. Meyer. Leipzig: B. G. Teubner-Verlag.
- Nowick, A. S. (1995). *Crystal properties via group theory*. Cambridge University Press.
- Nye, J. F. (1957). *Physical properties of crystals*, 1st ed. Oxford: Clarendon Press.
- Nye, J. F. (1985). *Physical properties of crystals*, revised ed. Oxford University Press.
- Onsager, L. (1931a). *Reciprocal relations in irreversible processes. I*. *Phys. Rev.* **37**, 405–426.
- Onsager, L. (1931b). *Reciprocal relations in irreversible processes. II*. *Phys. Rev.* **38**, 2265–2279.
- Pasteur, L. (1848a). *Recherches sur les relations qui peuvent exister entre la forme cristalline, la composition chimique et le sens de la polarisation rotatoire*. *Ann. Chim. (Paris)*, **24**, 442–459.
- Pasteur, L. (1848b). *Mémoire sur la relation entre la forme cristalline et la composition chimique, et sur la cause de la polarisation rotatoire*. *C. R. Acad. Sci.* **26**, 535–538.
- Pauffer, P. (1986). *Physikalische Kristallographie*. Berlin: Akademie-Verlag.
- Sands, D. E. (1995). *Vectors and tensors in crystallography*. New York: Dover.
- Schwartz, L. (1975). *Les tenseurs*. Paris: Hermann.
- Shuvalov, L. A. (1988). *Modern crystallography IV (physical properties of crystals)*. Berlin: Springer-Verlag.
- Sirotnin, Y. I. & Shaskol'skaya, M. P. (1982). *Fundamentals of crystal physics*. Moscow: Mir.
- Voigt, W. (1910). *Lehrbuch der Kristallphysik*. Leipzig: Teubner. 2nd ed. (1929); photorep. (1966). New York: Johnson Reprint Corp. and Leipzig: Teubner.
- Wooster, W. A. (1973). *Tensors and group theory for the physical properties of crystals*. Oxford: Clarendon Press.
- Zheludev, I. S. (1986). *Space and time inversion in physical crystallography*. *Acta Cryst.* **A42**, 122–127.