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

$$d\mathcal{G}_2 = -D_n\,\mathrm{d}E_n + T_{ij}\,\mathrm{d}S_{ij} - \sigma\,\mathrm{d}\Theta.$$

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):

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

where the components $\left(c_{ijkl}\right)^{E,\Theta}$ 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,

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

from which it follows that

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

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

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

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

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

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

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

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:

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

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
$t_{i_1 \ldots i_p}^{j_1 \ldots j_q}$	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
$\bigwedge$	outer product
$\wedge$	vector product
∂_i	partial derivative with respect to x_i
δ_i^j	Kronecker symbol
ε_{ijk}	permutation tensor
V	volume