UPPER BOUNDS FOR MATERIAL COEFFICIENTS

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Upper bounds for the piezo-electric, piezomagnetic, pyro-electric, pyromagnetic and two other coefficients are derived from the requirement of thermodynamic stability.

Brown et al. [1] have shown that there exists an upper bound for the magneto-electric coefficient of a crystal. This upper bound is given by an inequality expressing a necessary condition of thermodynamic stability of the crystal [2]. The same condition yields, upon choice of the appropriate intensive variables, upper bounds for other material coefficients.

Take for definiteness a density of (stored) free enthalpy $g(T, E, H, p)$ as function of temperature T, electric field E, magnetic field H and stress p. The condition of stability of a phase described by such a free enthalpy is that the Hessian

$$\partial^2 g(T,E,H,p) = \begin{pmatrix} -c_{EHp}/T & -\pi^i_{Hp} & -\mu^i_{Ep} & -a^\alpha_{EH} \\ -\tilde{\pi}^i_{Hp} & -\kappa^{ik}_{THp} & -\alpha^{ik}_{Tp} & -d^{i\alpha}_{TH} \\ -\tilde{\mu}^i_{Ep} & -\tilde{\alpha}^{ik}_{Tp} & -\chi^{ik}_{TEp} & -b^{i\alpha}_{TE} \\ -\tilde{a}^\alpha_{EH} & -\tilde{d}^{i\alpha}_{TH} & -\tilde{b}^{i\alpha}_{TE} & -l^{\alpha\beta}_{TEH} \end{pmatrix}$$

be negative definite. Here c is the specific heat, κ the electric susceptibility, χ the magnetic susceptibility, l the elastic compliance, π the pyro-electric coefficient, μ the pyromagnetic coefficient, α the magneto-electric susceptibility, d the piezo-electric coefficient, b the piezomagneti coefficient and a the derivative if strain with respect to temperature. Subscripts denote the intensive variables which are held constant. The superscripts i and k, running from 1 to 3, denote vector components; the superscripts α and β, running from 1 to 6, denote the components of a symmetric tensor, and the tilda indicates transposition. A necessary condition for the negative definiteness of a matrix is that the principal minors of even order be positive [3]. This condition applied to the principal minors of order two gives the following upper bounds for the magneto-electric susceptibility, the piezo-electric and piezomagnetic coefficients, the pyro-electric and pyromagnetic coefficients and for a:

$$(\alpha^{ik}_{Tp})^2 < \kappa^{ii}_{THp}\,\chi^{kk}_{TEp}\,, \qquad (d^{i\alpha}_{TH})^2 < \kappa^{ii}_{THp}\,l^{\alpha\alpha}_{TEH}\,,$$

$$(b^{i\alpha}_{TE})^2 < \chi^{ii}_{TEp}\,l^{\alpha\alpha}_{TEH}\,, \qquad (\pi^i_{Hp})^2 < T^{-1}\,c_{EHp}\,\kappa^{ii}\,,$$

$$(\mu^i_{Ep})^2 < T^{-1}\,c_{EHp}\,\chi^{ii} \qquad (a^\alpha_{EH})^2 < T^{-1}\,c_{EHp}\,l^{\alpha\alpha}_{TEH}\,.$$

These inequalities are useful in material science; in particular they permit simplifications of various figures of merit of devices based on the effects described by the various coefficients. They play however an important rôle also in the theory of phase transitions, as will be shown in a forthcoming paper.

References

[1] W.F. Brown Jr., R.M. Hornreich and S. Shtrikman, Phys. Rev. 168 (1968) 574.
[2] E. Ascher and P.B. Scheurer, Helv. Phys. Acta (to appear).
[3] F.R. Gantmacher, Matrix theory (Chelsea Publishing Co., New York, 1959).