The magnitude of the $\Delta\mathbf{r}_j$ for a particular system will depend on the anharmonicity present and on the symmetry at the atomic sites concerned. For example, in CdS, which has the rather highly symmetric wurtzite structure, the sum of the $\Delta\mathbf{r}_j$ for adjacent Cd and S atoms, as measured by the change in the structural parameter for the equilibrium and minimum energy configurations, is 0·0019 Å at room temperature (Barnea & Stevenson, 1980). This represents a significant change in the structural parameter, of magnitude three times its standard deviation. In a less highly symmetric system undergoing large thermal vibrations the $\Delta\mathbf{r}_j$ will be correspondingly higher.

An important consequence of the measurability of $\mathbf{r}_j^{(e)}$ for ionic crystals is that a series of measurements as a function of temperature will provide the temperature-dependence of the rigid-ion contribution to the primary pyro-electric coefficient, $\mathbf{p}^{(1)}$ (see, for example, Mair & Barnea, 1975), which is given by

$$p_\alpha^{(1)} = \frac{1}{V}\sum_{\kappa=1}^{5} q_\kappa \frac{\partial r_{\kappa\alpha}^{(e)}}{\partial T} - p_\alpha^{(2)}. \qquad (11)$$

Here q_κ is the charge associated with the κth ion (assumed to be independent of T), V is the volume of the unit cell, and $p_\alpha^{(2)}$ is the secondary pyro-electric coefficient, which can be calculated from thermal expansion data.

We conclude that, if the full Debye–Waller factor is used, the reference positions obtained from an X-ray or neutron diffraction analysis are the positions $\mathbf{r}_j^{(m)}$ defining the minimum of the potential energy in the deformed lattice. If no Debye–Waller factor, or a conventional harmonic Debye–Waller factor, is used, one might expect the positions obtained to correspond closely to the equilibrium or mean positions of the atoms, $\langle\mathbf{r}_j\rangle = \mathbf{r}_j^{(e)}$. For sites fully determined by symmetry, we have the further condition that $\mathbf{r}_j^{(m)} = \mathbf{r}_j^{(e)}$.

If a refinement with the full Debye–Waller factor is made, both $\mathbf{r}_j^{(m)}$ and $\mathbf{r}_j^{(e)}$ can be obtained, and the linear and higher-order coefficients of the one-particle potentials, expanded about the equilibrium positions, may then be deduced. If the crystal is ionic, measurements of $\mathbf{r}_j^{(m)}$ and $\mathbf{r}_j^{(e)}$ against temperature enable one to obtain the pyro-electric coefficient in the rigid-ion approximation.

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References

BARNEA, Z. & STEVENSON, A. (1980). Private communication.

BORN, M. (1942–3). *Rep. Prog. Phys.* **9**, 294–333.

BORN, M. & HUANG, K. (1954). *Dynamical Theory of Crystal Lattices*, p. 302. Oxford: Clarendon Press.

DAWSON, B., HURLEY, A. C. & MASLEN, V. W. (1967). *Proc. R. Soc. London Ser. A*, **298**, 289–306.

FREESE, H. & DÖRING, W. (1979). *Z. Phys.* B**34**, 135–140.

International Tables for X-ray Crystallography (1952). Vol. 1. Birmingham: Kynoch Press.

LAX, M. (1974). *Symmetry Principles in Solid State and Molecular Physics*, p. 113. New York: Wiley.

LIEBFRIED, S. & LUDWIG, W. (1961). *Solid State Physics*, Vol. 12, edited by F. SEITZ & D. TURNBULL. New York: Academic Press.

MAIR, S. L. (1980). *J. Phys. C*, **13**, 1419–1425, 2857–2868.

MAIR, S. L. & BARNEA, Z. (1975). *Acta Cryst.* A**31**, 201–207.

SEGMÜLLER, A. (1964). *Phys. Kondens. Mater.* **3**, 18–28.

STEWART, R. F. (1976). *Acta Cryst.* A**32**, 565–574.

WHITELEY, B., MOSS, G. & BARNEA, Z. (1978). *Acta Cryst.* A**34**, 130–136.

Acta Cryst. (1981). A**37**, 266

A new structural principle in anion-excess fluorite-related superlattices: erratum.

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Abstract

Fig. 1 of Bevan, Greis & Strähle [*Acta Cryst.* (1980), A**36**, 889–890] has been printed upside-down. The legend is correct.

All information is given in the *Abstract*.

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