The mechanism of dislocation relaxation proposed by Seeger[5] does not seem to offer an explanation for the apparent absence of peaks in bcc metals. A principal difference between dislocations in fcc and bcc metals is that for the latter a dissociation of complete dislocations into symmetric partials is not possible. The insensitivity of the peaks to impurity content indicates that intrinsic point defects such as vacancies may be important. These facts suggest a new mechanism based upon the thermally activated motion of symmetric paired partial dislocations between vacancy-pinning points; minimum energy configurations are those for which the vacancy is immediately above either partial. It is in these positions that its interaction with the dilatational stress field of the partial will be strongest. The activation energy is determined by the energy required for the transition (by glide of the dislocation pair) between the two stable states. This model will be discussed in detail in a forthcoming publication.[6]

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CRYSTAL STABILITY AND THE THEORY OF FERROELECTRICITY

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The condition that a crystal should be stable for all small deformations is that all the normal modes should have real frequencies.[1] The limit of stability against a particular mode of vibration is approached as the corresponding frequency approaches zero. In what follows we show that there is reason to believe that a ferroelectric transition, at least in certain crystals, is associated with such an instability or near-instability. The condition for a ferroelectric transition is therefore a problem in lattice dynamics, and when it is treated as such new insight into the problem is obtained. We illustrate this by means of a simple example, in which it is shown that it is possible for a diatomic cubic crystal to exhibit properties which are remarkably similar to those of barium titanate.

A shell model for the ions in an alkali halide crystal, proposed by Dick and Overhauser,[2] has been found to give a satisfactory explanation of the dielectric properties of alkali halides[3,4] and of the lattice dynamics of sodium iodide.[5] A similar model accounts quite well for the observed relation between frequency ω $(=2\pi\nu)$ and wave vector $\vec{q}$ $(q=2\pi/\lambda)$ of certain of the normal modes of germanium.[6] The theory of Woods, Cochran, and Brockhouse,[5] based on this model, gives the following expressions for the frequencies of the transverse optic (T.O.) and longitudinal optic (L.O.) modes of wave vector zero in a diatomic cubic crystal:

$$\mu\omega_T^2 = R_0' - 4\pi(\epsilon+2)(Z'e)^2/9v, \qquad (1)$$

$$\mu\omega_L^2 = R_0' + 8\pi(\epsilon+2)(Z'e)^2/9v\epsilon. \qquad (2)$$

Here μ is the reduced mass of the ions, ϵ the high-frequency dielectric constant (the square of the optical refractive index), and v the volume of the unit cell. $Z'e$ is the effective ionic charge, while $R_0'\vec{u}$ is the restoring "short-range" force on any one atom when the two lattices carrying the nuclei of different type are displaced a small relative distance $\vec{u}$. Primed quantities depend explicitly on the parameters of the shell model. In a crystal such as sodium iodide the two quantities on the right of Eq. (1) are of the same order of magnitude, but the term R_0' which arises from the short-range interaction is about twice as great as the other, which arises from the Coulomb interaction. Let us consider the situation that would arise if their difference approached zero.

It is found from the theory[5] that ω_T may approach zero without the crystal necessarily becoming unstable against other vibration modes; indeed all transverse optic modes for which $\vec{q}$ is not close to zero may retain quite usual frequencies. The quantities which appear on the right of Eq. (1) may be temperature dependent, as the lattice vibrations are in practice not completely harmonic, so that near $T = T_c$ we may postulate

$$\frac{\mu\omega_T^2}{R_0'} = 1 - \frac{4\pi(\epsilon+2)(Z'e)^2}{9vR_0'} = \gamma(T - T_c), \tag{3}$$

where γ is a temperature coefficient and T_c is the temperature at which the crystal would become unstable. It has been shown by Lyddane, Sachs, and Teller[7] that

$$\omega_L^2/\omega_T^2 = \epsilon_0/\epsilon, \tag{4}$$

where ϵ_0 is the static dielectric constant. Combining these equations, one finds

$$\frac{\epsilon_0 - 1}{4\pi} \simeq \frac{\epsilon_0 - \epsilon}{4\pi} = \frac{(\epsilon+2)^2(Z'e)^2}{9vR_0'\gamma(T - T_c)}, \tag{5}$$

so that a Curie-Weiss law is followed with a Curie constant

$$C = (\epsilon+2)^2(Z'e)^2/9vR_0'\gamma \simeq (\epsilon+2)/4\pi\gamma. \tag{6}$$

The condition $\epsilon_0 \to \infty$ is thus $\omega_T^2 \to 0$. The ionic polarizability of one unit cell is found to be given by

$$\alpha_i = (Z'e)^2/R_0', \tag{7}$$

while the electronic polarizability is as usual given by

$$4\pi\alpha_e/3v = (\epsilon - 1)/(\epsilon + 2). \tag{8}$$

The condition $\omega_T^2 = 0$ is therefore the same as

$$(4\pi/3v)(\alpha_i + \alpha_e) = 1, \tag{9}$$

so that the terms "instability" and "polarizability catastrophe" are synonymous in this instance.

If one now postulates that the short-range potential between the two Bravais lattices is neither precisely harmonic nor precisely isotropic for comparatively large displacements, it can be shown that the crystal may become spontaneously polarized without becoming completely unstable. Instead it makes a transition to another phase. When the short-range potential is given explicitly by

$$\begin{aligned} V_R = {} & \tfrac{1}{2}R_0'(u_x^2 + u_y^2 + u_z^2) + \tfrac{1}{4}B(u_x^4 + u_y^4 + u_z^4) \\ & + \tfrac{1}{6}B'(u_x^6 + u_y^6 + u_z^6) \\ & + \tfrac{1}{2}B''(u_x^2u_y^2 + u_y^2u_z^2 + u_z^2u_x^2), \end{aligned} \tag{10}$$

with $B < 0$, B' and $B'' > 0$, the crystal makes a first-order transition to a tetragonal phase at a temperature exceeding T_c. Equation (10) refers to the "free" crystal; the potential V_R cannot therefore be used as it stands to give ω_T in a noncubic phase, since, for the lattice vibrations, the crystal is "clamped" by its inertia. At the cubic-tetragonal transition the atoms become displaced a relative amount

$$u_0 = (3|B|/4B')^{1/2},$$

along a crystallographic axis, say [001]. The minimum T.O. frequency is reached just before the transition, and is given by

$$\mu(\omega_T^2)_{\min} = 3B^2/16B'.$$

Expressions for the spontaneous polarization as a function of temperature, etc., are also obtained in terms of the above atomic parameters. As the temperature decreases still further the crystal makes a second transition in which the atoms become relatively displaced along [011], followed by a third which leaves them displaced along [111]. These results will be understood when it is pointed out that Eqs. (3) and (10) lead eventually to an expression for the free energy G_1 of the unstressed crystal which is almost identical with that postulated by Devonshire.[8]

The theory has been extended to apply to antiferroelectric transitions in diatomic crystals, and to ferroelectric transitions in other cubic crystals, including barium titanate. The equations which apply to the latter are greatly simplified by assuming that in the T.O. mode of lowest frequency (there are three T.O. modes in all), or in a static field, the framework of oxygen atoms is not distorted. The crystal structure analyses[9,10] of tetragonal barium titanate and lead titanate support this assumption. The dielectric properties of barium titanate, and the movements of barium and titanium atoms relative to the oxygen octahedron, may be accounted for by assuming a temperature dependence of certain atomic parameters analogous to that given by Eq. (3), and a short-range potential for relative movement of titanium and oxygen atoms given by Eq. (10). A very small departure from a harmonic potential is found to be sufficient to account for the dielectric properties, and the numerical values required for other atomic parameters are physically reasonable.

The equation corresponding to Eq. (4), applicable to a perovskite-type crystal, is found to be

$$(\omega_2\omega_3\omega_4)_L{}^2/(\omega_2\omega_3\omega_4)_T{}^2=\epsilon_0/\epsilon. \qquad (11)$$

(This result does not depend on the assumption of an undistorted oxygen framework.) The infrared absorption frequencies $(\omega_3)_T$ and $(\omega_4)_T$ have been measured by Last,[11] and are in no way unusual. It follows from the theory that $(\omega_2)_T{}^2$ should be proportional to $(T - T_c)$ in the cubic phase, and should reach an abnormally low value estimated as $\nu = 2$ or 3×10^{11} cps just before the first transition. This frequency should split appreciably in the tetragonal phase, and each frequency in this phase should vary inversely as the square root of the corresponding "clamped" dielectric constant. Although relaxation of the dielectric constant of barium titanate has been reported for frequencies of the order 10^{10} cps, Benedict and Durand[12] found that when a single crystal is used, the dielectric constant of the cubic phase is the same as the static value up to $\nu = 2.4\times10^{10}$ cps, the limit of their experiment. The resonance frequency predicted here lies in the millimeter wavelength range. A study of the properties of barium titanate in this difficult frequency range should yield interesting results.

The statement that the problem of the onset of ferroelectric properties in any crystal is a problem in lattice dynamics is probably correct, but at present there is little prospect of detailed application of the theory of lattice dynamics to low-symmetry or disordered crystals.

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NEW MECHANISM OF ANTIFERROMAGNETISM

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The well-known anomalous properties of dilute Cu-Mn alloys suggest an antiferromagnetic mechanism that requires neither two-body interactions between paramagnetic solute spins, nor a sublattice structure. Such a mechanism may be recognized by considering a new-type excited state of the conduction electron gas. This state will have the following properties. The expectation value $\hbar\vec{s}$ of the total conduction electron spin density operator, relative to an axis of quantization $\vec{\epsilon}$, will vary with position $\vec{R}$ as follows:

$$\vec{s} = bN\vec{\epsilon}\cos(\vec{q}\cdot\vec{R}), \qquad (1)$$

where b is a dimensionless amplitude and N is the number of atoms per cc. This static spin density wave will allow the total charge density of the gas to remain spatially uniform. Such a collective excited state may be visualized as the sum of two charge density waves, one of electrons with spin parallel to $\vec{\epsilon}$ and the other of antiparallel spin, which are equal in magnitude but opposite in phase. This state must be dynamically self sustaining, which is to say that it should be an eigenfunction of the Hartree-Fock equations. The possibility of such a self-con-