

ing letter. In general, when more than one sublattice has appreciable ionic polarization, considerations similar to those used to obtain the local field must be used to obtain the elastic restoring forces on an ion. The ionic polarization equations should be

$$\mathbf{E}_k = \sum_i \beta_{ki} \mathbf{P}_i, \quad (5)$$

where the local field \mathbf{E}_k includes the electronic contribution and where the β_{ki} are related to the noncoulomb forces within the crystal.

* This research has been assisted in part by the ONR.

Ferroelectricity versus Antiferroelectricity in Barium Titanate*

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(Received August 21, 1951)

SLATER'S recent treatment of BaTiO_3 ¹ has shown that the probable origin of the ferroelectricity of BaTiO_3 and similar substances of perovskite structure is the strong dipole-dipole interaction within lines of O and Ti ions parallel to the spontaneous polarization. Slater found that the value of the ionic polarizability necessary for spontaneous polarization of the Ti ion alone is 0.947×10^{-24} cc. This value was checked here (see row 1, Table I).

Qualitative considerations suggest that the dipole-dipole interactions in BaTiO_3 might be stronger in an antiferroelectric state² than in the observed ferroelectric state, just as in the simple cubic structure. Consequently a treatment of BaTiO_3 similar to that of Slater was carried out for an antiferroelectric state to determine the ionic polarizability necessary for spontaneous antiparallel polarization.

The O ion on the y - z face of the unit cell will be designated as O_x and similarly for O_y and O_z as shown in Fig. 1(A). The antiferroelectric state considered is one with polarization in a Z_4 array (in the notation of Luttinger and Tisza³), Fig. 1(B), on the Ti and O_x sublattices, and with no polarization on the O_y , O_z , and Ba sublattices. For convenience, the Ti and O_x ions will be referred to as 1 and 2, respectively. The only nonzero field constants for this arrangement are $f_{11} = f_{22} = 5.351$ and $f_{12} = 33.118$. The value of f_{12} was calculated by the Ewald method. The electronic polarizabilities used were those given by Slater.¹ The edge of the unit cell was taken as 4.00 Å.

Calculations were made assuming that Ti or O_x alone contributes ionic polarization. The local fields at the original lattice points were used, as has been customary. However, as pointed out elsewhere in this issue,⁴ the local fields at the displaced lattice points should have been used. The calculations were repeated using the local fields given by Eqs. (4) and (5) of reference 4. For the ferroelectric arrangement $g_2 = 47.013$, enhancing the local field at the O_x ion considerably. On the other hand, $g_1 = f_{11} = 4\pi/3$. Hence the calculated polarizability is the same for Ti with both methods. For the antiferroelectric arrangements $g_2 = 66.236$ and $g_1 = 16.559$, enhancing the local field at both ions. The results of the calculations are given in Table I.

In general, the greater the local field and the greater the elec-

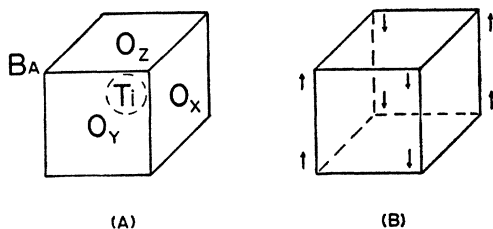


FIG. 1. (A) Unit cell of BaTiO_3 . (B) Z_4 array.

TABLE I. Ionic polarizability required for spontaneous polarization.

Type of array	Local field	Ion displaced	Polarizability cc
1. ferroelectric (f.e.)	at original position	Ti	0.947×10^{-24}
2. antiferroelectric (a.f.e.)	at original position	Ti	0.947
3. f.e.	at original position	O_x	3.01
4. a.f.e.	at original position	O_x	5.06
5. f.e.	at displaced position	Ti	0.947
6. a.f.e.	at displaced position	Ti	0.787
7. f.e.	at displaced position	O_x	0.646
8. a.f.e.	at displaced position	O_x	0.626

tronic polarizability of the ion contributing most to the local field, the smaller the ionic polarizability required for spontaneous polarization. When the local fields at the original lattice points are used, the results for ferro- and antiferroelectricity are the same for Ti. For O_x less ionic polarizability is required for antiferroelectricity and hence antiferroelectricity is favored. In the actual crystal, however, both ions may contribute ionic polarization.⁵ Since Ti requires less polarizability than O_x in both arrangements, one would expect the Ti ion to contribute most of the ionic polarization. Hence, one cannot interpret decisively the favoring of ferroelectricity in BaTiO_3 with simple dipole-dipole interactions alone if the local fields are taken at the original lattice points. When the local fields at the actual lattice points of the ions are used, antiferroelectricity is favored for the Ti and the O_x ions both. Thus even if one uses local fields at the actual lattice points, one still cannot explain the favoring of ferroelectricity in BaTiO_3 with the simple dipole-dipole interaction model.

I wish to thank Professor Charles Kittel for having suggested this problem and for many informative and stimulating discussions.

* This research has been assisted in part by the ONR.

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² C. Kittel, Phys. Rev. **82**, 729 (1951).

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⁴ M. H. Cohen, Phys. Rev. **84**, 373 (1951).

⁵ W. Kaenzig, Phys. Rev. **80**, 94 (1950); Helv. Phys. Acta. **24**, 175 (1951); H. T. Evans and R. A. Hutner, Phys. Rev. **83**, 879 (1951).

Angular Correlation in Magnetic Fields

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(Received September 4, 1951)

THE angular correlation of two successively emitted nuclear particles can be influenced by magnetic fields (e.g., from the electron shell, from neighboring atoms, or from an external source). In order to calculate a general expression, we start with the formula of Goertzel¹ for the emission probability W of two particles with directional vectors \mathbf{k}_1 and \mathbf{k}_2 .

$$W(\mathbf{k}_1, \mathbf{k}_2) = S_1 S_2 \sum_{l m m' p} (A_l | H_1 | B_m) (B_m | H_2 | C_p)^* \times (A_l | H_1 | B_{m'})^* (B_{m'} | H_2 | C_p) \frac{1}{1 - i\omega_{BB'}\tau}. \quad (1)$$

A_1, B_m, C_p are the wave functions of the atom (nucleus+shell) for the 3 states of the cascade. H_1, H_2 designate the hamiltonians responsible for the emission of the first and second particles, respectively. $\omega_{BB'}$ is the energy splitting of the two levels $B_m, B_{m'}$, divided by \hbar . τ is the mean life of the intermediate state. We can now modify Goertzel's expression (1) by choosing an arbitrary z -axis. Introducing solid harmonics $Y_k^r(\mathbf{k})$ we get instead of (1)

$$W(\mathbf{k}_1, \mathbf{k}_2) = \sum_{r, k} G_k^r A_k \frac{1}{2k+1} Y_k^r(\mathbf{k}_1) Y_k^r(\mathbf{k}_2)^*. \quad (2)$$

As is seen later, the coefficients a_k are independent of the magnetic field. The whole influence of the magnetic field is in fact contained in the attenuation factor G_k^r . This attenuation factor can be calculated for the two special cases of a weak and strong field.