is about 36 (kc/sec)², about 1.6 times as large as the theoretical value for dipole-dipole interaction alone.

V. CONCLUSIONS

The work reported here indicates agreement between theory and experiment for a number of the satellite lines in lithium metal. The method appears to be applicable to a number of problems, including some of those involving quadrupole interactions in alloys.

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Far-Infrared Ferroelectric Vibration Mode in SrTiO₃†

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The real and imaginary parts of the dielectric constant of SrTiO₃ have been obtained for the region 2.5 to 3000 cm⁻¹ from an analysis of the reflectivity. The imaginary part exhibits a very strong peak at 100 cm⁻¹ at room temperature which shifts to 40 cm⁻¹ at 93°K. This mode is of sufficient strength to account for more than 90% of the low-frequency dielectric constant. The accompanying dispersion of the real part of the dielectric constant is of resonant form. The connection of this mode with Cochran's theory of ferroelectricity is discussed.

I. INTRODUCTION

THE low-frequency dielectric constant of ferro-electric crystals is well known to obey a Curie law $\epsilon' = C/(T - T_c)$ for temperatures above a certain critical temperature which is usually very close to T_c. Values of ϵ' can be as large as 10^6. One of the Kramers-Kronig relations provides a connection between the behavior of the imaginary part of the dielectric constant and the low-frequency real part:

$$\epsilon'(0,T) - \epsilon_\infty = \frac{2}{\pi} \int_0^\infty \frac{\epsilon''(\omega',T)d\omega'}{\omega'}. \tag{1}$$

Here $\epsilon'(\omega,T)$ and $\epsilon''(\omega,T)$ are the real and imaginary parts of the dielectric constant and ϵ_∞ is the limiting dielectric constant for frequencies well above those where ferroelectric effects cease to be important. The value of ϵ'' in the integral is understood to include only contributions from modes in the frequency region of interest. For SrTiO₃ at room temperature the left side of (1) is about 300 and follows a Curie law behavior [ϵ_∞ can be neglected compared with $\epsilon'(0,T)$]. For the alkali halides or quartz the value of $\epsilon'(0,T) - \epsilon_\infty$ is 3 or 4 and is temperature insensitive. The point of interest is that previous spectroscopy of SrTiO₃ and related ferroelectrics has yielded an ϵ'' very little different from that of the alkali halides or quartz in terms of its contribution to $\epsilon'(0,T)$ via (1). Recently

Cochran[1] has proposed a theory of ferroelectricity which associates the ferroelectric transition in certain crystals with one of the optic modes of the lattice lowering its frequency and becoming unstable as the temperature is lowered toward T_c. Others, particularly P. W. Anderson, had discussed similar ideas previously in unpublished work. This paper reports a Cochran-type mode in SrTiO₃ whose contribution to ϵ'' satisfies (1) and which provides a resonant dispersion of ϵ'.

II. EXPERIMENTAL WORK

The reflectivity of strontium titanate has been measured over the range 2.5 to 250 cm⁻¹ at 93°K and from 2.5 to 3000 cm⁻¹ at 300°K. Figure 1 shows the
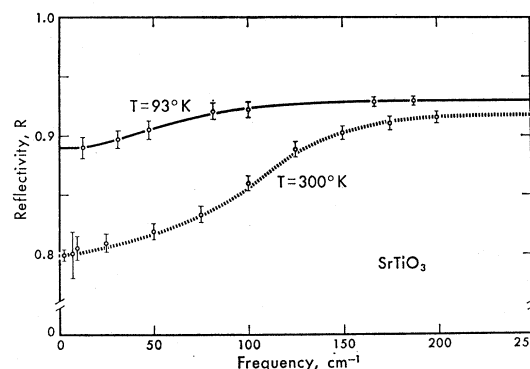

FIG. 1. Reflectivity of SrTiO₃ in the far infrared. The smooth curves are used in the dispersion analysis.

[1] W. Cochran, *Advances in Physics*, edited by N. F. Mott (Taylor and Francis, Ltd., London, 1960), Vol. 9, p. 387.
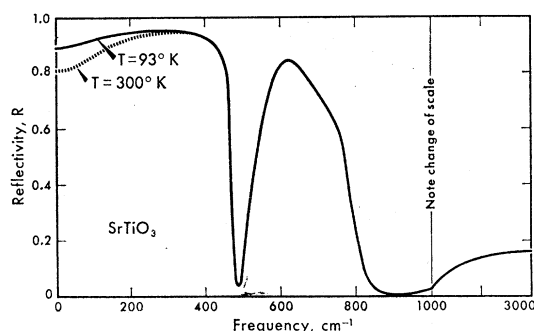
FIG. 2. Reflectivity of SrTiO$_3$ over the entire frequency range used in the dispersion analysis.

results in the region of most interest where measurements have not previously been made. The experimental methods are indicated in the following paragraphs.

A single-crystal boule of strontium titanate was cut to expose a face 12×16 mm and then polished on an optical lap by usual techniques. The polished surface was used as the diagonal reflector at a 90° bend in our standard light-pipe optics.[2] Provision was made in both the room-temperature and low-temperature experiment to replace the sample with a front-silvered mirror for normalization. Points were taken at 2.5 and 7.5 cm^{-1} using an 8-mm klystron and harmonic generator. An interference modulator[3] and helium-cooled carbon bolometer were used to separate and detect these harmonics. The same modulator was used for various points between 10 and 70 cm^{-1} using a high-pressure mercury arc source, while a vacuum grating monochromator and Perkin-Elmer prism monochromator were used over the higher frequency range.

Transmission measurements were attempted in the region 2.5 to 550 cm^{-1} with a sample 125 μ thick, at room temperature. Except for a point at 2.5 cm^{-1} however, the transmission was undetectable with our sensitivity (i.e., less than 0.1%). Room temperature and nitrogen temperature transmission measurements were made on powders of strontium titanate in wax. The results of all transmission measurements were consistent with the behavior of the optical absorption coefficient obtained from dispersion analysis except near 400 cm^{-1}. This discrepancy will be discussed below.

III. ANALYSIS

The measured reflectivity R was transformed using a digital computer to obtain the associated phase angle,

$$\theta(\omega) = \frac{2\omega}{\pi} \int_0^\infty \frac{\ln[r(\omega')]d\omega'}{\omega^2 - \omega'^2}, \qquad (2)$$

where we characterize the reflecting surface by an

[2] R. C. Ohlmann, P. L. Richards, and M. Tinkham, J. Opt. Soc. Am. **48**, 531 (1958).
[3] A. S. Barker, Jr. and M. Tinkham, Bull. Am. Phys. Soc. **6**, 112 (1961).

amplitude reflection coefficient $re^{-i\theta}$, with $r = R^{\frac{1}{2}}$. The measurements were made at an angle of incidence of 45° using an unpolarized beam. Because of the complexity of the Fresnel formulas for this case, the formula for normal incidence was used to calculate n and k in a first approximation:

$$(n - ik - 1)/(n - ik + 1) = re^{-i\theta},$$

$$n = \frac{1 - r^2}{1 + r^2 - 2r \cos\theta}, \qquad (3)$$

$$k = \frac{2r \sin\theta}{1 + r^2 - 2r \cos\theta}.$$

At each frequency where the inversion was performed, the n and k calculated could be put into the Fresnel formulas for 45°. The result of averaging over the parallel and perpendicular reflectivity was then compared with the original experimental reflectivity. Tests of this kind always gave agreement within the experimental uncertainty, so the use of Eqs. (3) based on normal incidence was regarded as satisfactory.

Figure 2 shows the data used in the dispersion analysis. The reflectivity is taken to be constant from 3000 cm^{-1} to ∞. Figures 3–5 give the results of the analysis in terms of the dielectric constant, which is of more interest here than the index of refraction.

IV. DISCUSSION

Figure 3 shows the dispersion of the dielectric constant of strontium titanate. Prior to this work there had been many speculations concerning the nature and the frequency of the dispersion. We note from Figs. 3 and 4 that the dispersion is via a resonant, though rather low-Q, mode whose frequency and linewidth are very temperature dependent. Recently Cochran[1] has suggested that ferroelectricity in the perovskite titanates is connected with the lattice dynamics. Of central importance in Cochran's theory
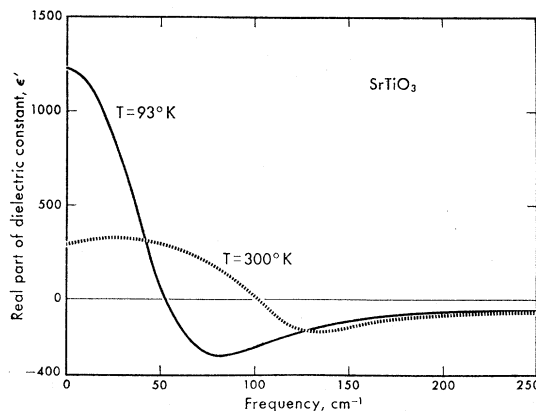

FIG. 3. Real part of the dielectric constant calculated from the reflectivity in Fig. 2.

is the Lyddane-Sachs-Teller[4] relation

$$\omega_L{}^2/\omega_T{}^2 = \epsilon(\omega=0)/\epsilon_\infty, \qquad (4)$$

written here for a diatomic lattice. ω_L and ω_T are the limiting frequencies of the long-wave longitudinal and transverse optic modes. Relation (4) has been extended to more general lattices by Cochran.[1] He associates the rapid rise of $\epsilon(\omega=0)$ with decreasing temperature (a hallmark of a ferroelectric) with the frequency of the transverse mode approaching zero. The reason for this decrease can be seen on examining the restoring force for ion motion for the two types of mode. In each case there is a nearest-neighbor contribution from overlap forces and a long-range part coming from the effective field at the ion due to all the other ions moving from their equilibrium positions. For the case of long-wave transverse ion displacements, this long-range restoring force is $Ze(-4\pi P/3)$, i.e., it is actually in the direction of the displacement and so lowers the frequency. (We have used the Lorentz from of the local field for illustration only.) For longitudinal displacements the force is $Ze(-4\pi P/3+4\pi P)$, i.e., the Lorentz force and the depolarization force. Thus the short-range and long-range forces could cancel in the transverse case. With near cancellation of the restoring force a small temperature dependence in the short-range force would cause ω_T to be very temperature dependent while ω_L would be insensitive to temperature. Equation (4) is a statement of this result in a form in which the short-range force does not appear explicitly. Figure 4 exhibits just this behavior. On going from 300 to 93°K the low-frequency dielectric constant has increased about 4 times and we note that the center frequency of the mode decreases about a factor of $\sqrt{4}$. Following Last[5] we might associate the low-frequency mode observed here with the $k=0$ Sr-TiO₃ transverse vibration.

[*Note added in proof*. We have been informed by W. G. Spitzer and R. C. Miller of the Bell Telephone Laboratories that they have found a dip in reflection associated with an optical mode near 175 cm⁻¹ in addi-
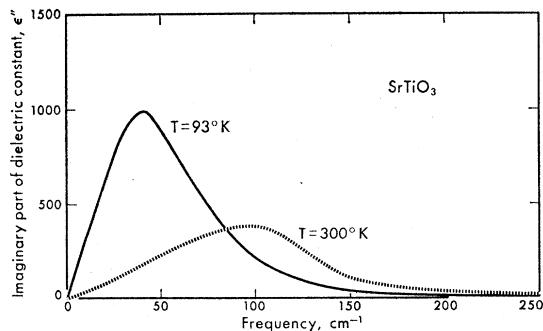

FIG. 4. Imaginary part of the dielectric constant calculated from the reflectivity in Fig. 2.

[4] R. H. Lyddane, R. G. Sachs, and E. Teller, Phys. Rev. **59**, 673 (1941).
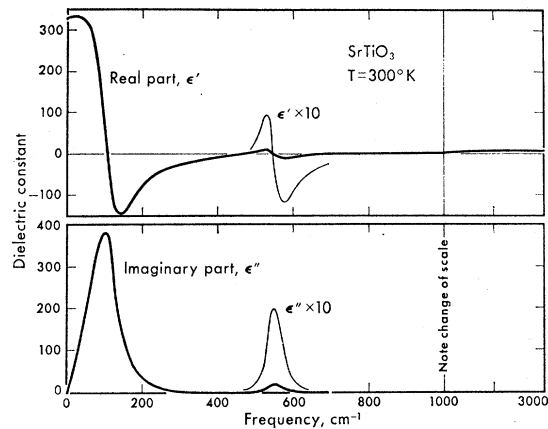[5] J. T. Last, Phys. Rev. **105**, 1740 (1957).

FIG. 5. Real and imaginary parts of the dielectric constant at room temperature over the entire frequency range investigated.

tion to the two modes reported in this paper. Subsequently, we have observed this mode in a higher resolution study of this region of the spectrum. Although not contributing significantly to the ferroelectricity, this additional mode does provide the third active mode expected on the basis of the symmetry of the unit cell, and it suggests a re-examination of the mode assignments.]

In Fig. 5 the dielectric constants are shown for the entire range of investigation at room temperature. Last[5] has reported modes at 395 and 610 cm⁻¹ for SrTiO₃ powder. Rupprecht[6] has measured single-crystal transmission over the range 500 to 4000 cm⁻¹ and finds that the vibration reported by Last at 610 cm⁻¹ is actually at 550 cm⁻¹, in good agreement with our result. We have seen the mode at 550 cm⁻¹ and a broad transmission minimum near 400 cm⁻¹ using 350-mesh powdered SrTiO₃ in wax. Unlike the 550-cm⁻¹ mode, however, the 400-cm⁻¹ transmission minimum depends critically on the powder density and might be a scattering effect. In an effort to find a mode near 400 cm⁻¹ we remeasured the reflectivity in this region looking for a small dip, only to obtain excellent agreement with Last's reflectivity which on inversion gives no mode at 400 cm⁻¹. Using another approach, a classical oscillator with center frequency 400 cm⁻¹, linewidth 100 cm⁻¹, and adjustable strength can be added to the dielectric constant shown in Fig. 5. R can then be calculated and compared with the measured R. A mode of even one-tenth the strength of the 550-cm⁻¹ mode causes a dip in R near 400 cm⁻¹ that would have been detectable. However, the explanation given above of the transmission dip seen by Last in terms of scattering is not entirely convincing, and a discrepancy may remain.

It must be emphasized that the presence or absence or temperature dependence of modes at 400 cm⁻¹ has little effect on the inferred form of the low-frequency

[6] G. Rupprecht (private communication).

vibration. The dispersion relation (2) has a somewhat local character because of its frequency dependence. The effect of adding a classical mode at 400 cm^{-1} was carefully checked. Within experimental uncertainty, even a strong mode at 400 cm^{-1} does not affect the inversion of the over-all reflectivity (with the extra mode included) to obtain the dielectric constant in the region of the low-frequency mode.

Recently, some success has been achieved in explaining the linewidth of optical modes in alkali halides in terms of anharmonic damping.[7] This work suggests that the very broad line in SrTiO$_3$ may result partly from the form of the acoustic phonon dispersion curves. Anharmonic potential terms in the Hamiltonian allow the $k=0$ optic mode to dissipate energy to phonons of other wave vectors. The damping is particularly strong at frequencies $\omega_{1a}-\omega_{ta}$ and $\omega_{1a}+\omega_{ta}$, where ω_{1a} and ω_{ta} are the frequencies of the longitudinal and transverse acoustic phonon branches at the zone boundary.[7,8] For the alkali halides the natural frequency of the optic mode falls in a region of low damping about midway between the above regions of high damping. In SrTiO$_3$, however, a rough calculation using the elastic constants indicates the optic mode frequency to be within 30% of $\omega_{1a}-\omega_{ta}$ which is right in the region of large damping.[7,8]

The behavior of $\tan\delta=\epsilon''/\epsilon'$ is of considerable practical interest at frequencies below the dispersion. Here SrTiO$_3$ exhibits nonlinear effects and may be used for harmonic generation, modulation, parametric amplification, etc., with an efficiency usually governed by $\tan\delta$. Rupprecht et al.[9] have measured $\tan\delta$ over a wide range of microwave frequencies. Fitting a classical dispersion form to the low-frequency mode observed here gives the frequency and temperature dependence of $\tan\delta$ in the microwave region below 150°K seen by them, namely $\tan\delta\sim\omega/(T-T_c)$. At frequencies so far from the infrared resonance, however, the anharmonic damping factor has decreased considerably,[7] and other damping mechanisms[9] may be important.

[7] H. Bilz, L. Genzel, and H. Happ, Z. Physik **160**, 535 (1960).
[8] M. Blackman, Z. Physik **86**, 421 (1933).

[9] G. Rupprecht, R. O. Bell, and B. D. Silverman, Phys. Rev. **123**, 97 (1961).

Moving Edge Dislocations in Cubic and Hexagonal Materials*

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Numerical values of the threshold and limiting velocities of edge dislocations in various cubic and hexagonal materials are presented; a number of orientations and directions of motion of the edge dislocation are considered. At the limiting velocity C_∞, the energy of the dislocation becomes infinite; in many instances it is found that the limiting velocity is less than the corresponding velocity of shear sound. At the threshold (Rayleigh) velocity C_R, the shear stress of the moving edge dislocation vanishes on the slip plane. Edge dislocations of like sign moving at velocities between C_R and C_∞ attract rather than repel one another. The lower the value of the ratio C_R/C_∞, the easier it should be to bring edge dislocations into the anomalous velocity range. Theoretically this ratio has zero as a lower limit; however, no value of C_R/C_∞ less than 0.85 was found for those materials and orientations considered.

I. INTRODUCTION

IN a previous paper[1] the dynamical behavior of uniformly moving dislocations in anisotropic media was discussed for those crystal systems for which the edge and screw components can be considered separately. It was found that a screw dislocation behaves normally at all velocities up to its limiting velocity. An edge dislocation, however, displays an anomalous behavior; in general there is a range of velocities for which the shear stress on the slip plane of the moving edge dislocation is negative and edge dislocations of like sign attract rather than repel one another. The existence of this anomalous velocity range in isotropic materials was first pointed out by Weertman.[2] In an isotropic material, the upper limit of this velocity range is the velocity of shear sound, which is also the limiting velocity of the edge dislocation; the lower limit is the Rayleigh wave velocity which can never be less than 0.69 the velocity of shear sound. In the anisotropic case it is possible for both the upper limit (C_∞, the limiting velocity) and the lower limit (C_R, the threshold velocity) to be any velocity from zero up to the shear wave velocity, depending on the elastic constants of the material and the orientation considered.

[1] L. J. Teutonico, Phys. Rev. **124**, 1039 (1961).

[2] J. Weertman, *Response of Metals to High Velocity Deformation*, edited by P. G. Shewmon and V. F. Zackay (Interscience Publishers, Inc., New York, 1961).