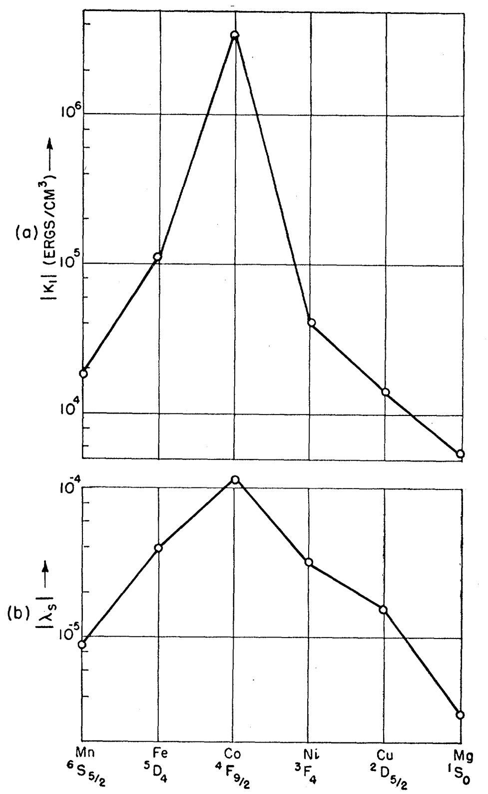

FIG. 1(a). Calculated anisotropy constant, K_1, (b) observed average magnetostriction constant, λ_s, plotted against M, for the ferromagnetic spinels, $M\mathrm{Fe_2O_4}$. Below each M is the ground-state term of M^{++}.

cooled slowly and are presumably nearly strain-free, with the exception of $\mathrm{CuFe_2O_4}$ which had to be quenched. Values of M_s at room temperature were obtained in these laboratories and from other appropriate sources.[9]

The calculated values of $|K_1|$ for $M\mathrm{Fe_2O_4}$ are plotted in Fig. 1(a) *versus* the ground-state term of M^{++}. One will note there the direct correspondence between K_1 and J, the inner quantum number of M^{++}. Such a relationship is expected in view of the dependence of magnetic anisotropy on spin-orbit coupling. Van Vleck[10] has discussed a similar behavior in the paramagnetic bivalent salts of the iron series.

We find by our calculations, $K_1 = -4.0\times10^4$ ergs/cm^3 for $\mathrm{NiFe_2O_4}$ and $K_1 = -3.4\times10^6$ for $\mathrm{CoFe_2O_4}$. Experimental values are, respectively,[11,1] -5.1×10^4 and -1.7×10^6. Since these experimental values were obtained on crystals containing some magnetite in solid-solution,[1] it seems reasonable that K_1 for $\mathrm{NiFe_2O_4}$ is higher and K_1 for $\mathrm{CoFe_2O_4}$, lower, respectively than what we calculated for pure materials.

Figure 1(b) is a plot of $|\lambda_s|$, the average value of the saturation magnetostriction for sintered, polycrystalline ferromagnetic spinels. (We have ignored the fact that λ_s is positive for $\mathrm{Fe_3O_4}$ and negative for the others). The values for λ_s were obtained here (with the exception of $\mathrm{CoFe_2O_4}$)[12] and are believed to be accurate to ±25 percent. One will note again the same type of dependence on J.

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Infrared Spectrum of Barium Titanate*

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THE infrared absorption of barium titanate ($\mathrm{BaTiO_3}$) has been studied between 2μ and 33μ. The spectrum obtained (Fig. 1) consists of two broad bands, one centered near 550 cm^{-1}, the other starting near 450 cm^{-1} and reaching a maximum beyond 300 cm^{-1}. The low transmission in the high-frequency end of the spectrum is due to scattering since the barium titanate was examined as a fine powder deposited on a KBr (or NaCl) plate from a suspension in isopropyl alcohol.

Several specimens of barium titanate were examined. The majority showed additional bands at 6.95, 9.45, and 11.65μ, which were proved to be due to carbonate ion impurities. Other impurity bands were noted at 7.1, 10.3, 11.05, 11.4, 11.85, and 12.85μ, but the impurities were not identified. The spectrum of a very

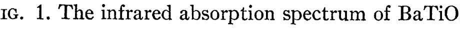

FIG. 1. The infrared absorption spectrum of $\mathrm{BaTiO_3}$.

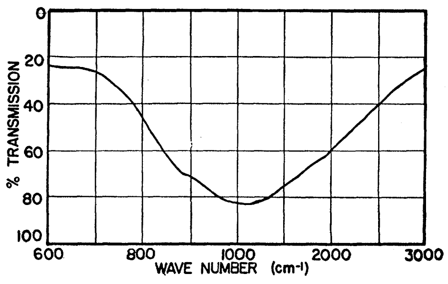

FIG. 2. The infrared absorption spectrum of $SrTiO_3$.

pure specimen of powdered strontium titanate ($SrTiO_3$) was observed between 2μ and 15μ (Fig. 2). It is identical with that of barium titanate obtained under similar conditions over that region of the spectrum. Noland[1] has recently reported the spectrum of a single crystal of strontium titanate between 1μ and 10.5μ, at which wavelength the extinction coefficient is greater than 100 cm^{-1} and is still increasing. He finds two weak bands near 5.5μ and 7.5μ. These could easily have been missed by us since our effective thickness was much less than the thickness he used. We might add that the spectrum of a single crystal of barium titanate just run in this laboratory by M. Haas shows a weak band at 8μ and a "cutoff" near 11.2μ. The spectrum of ilmenite ($FeTiO_3$) has been recorded by Hunt and others.[2] With the exception of a weak band at 1000 cm^{-1}, it is also very similar to that of barium titanate.

Apart from impurity bands, there appears to be no difference between the spectrum of barium titanate in the hexagonal and in the tetragonal form over the range 2μ to 15μ. No change was observed in the spectrum of barium titanate (ceramic) when heated to 150°C.

The foregoing observations may be considered in the light of recent theories about the ferroelectric character of barium titanate.

Jaynes[3] has predicted from an electronic theory that there should be an infrared absorption at 1000 cm^{-1}. There is definitely no *strong* absorption band in the neighborhood of 1000 cm^{-1}. Although a few specimens have shown a very weak absorption near 1000 cm^{-1}, this is most probably due to BaO impurity.

Megaw[4] has proposed that the change from the cubic form (above the Curie point of 120°C) to the tetragonal form corresponds to a change in the character of the bonds round the Ti and O atoms. If this were so, one might expect a change in the spectrum on heating to 150°C and also differences between the spectra of the tetragonal and hexagonal forms of $BaTiO_3$ since the latter is not ferroelectric. This change should be very marked in the strong band near 600 cm^{-1} since this band [which is common to all titanates and is found also in rutile (TiO_2)] is undoubtedly connected with a vibration of the TiO_4 tetrahedra. No such change was observed. It is possible, of course, that changes may have occurred at lower frequencies beyond our range of detection.

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Hyperfine Splitting of Donor States in Silicon

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ELECTRON spin resonances exhibiting hyperfine structure have recently been observed in *n*-type Si by Fletcher *et al.*[1] The number of hyperfine lines of these resonances corresponds exactly to the nuclear spin of the added Group V atoms, showing conclusively that the resonances are due to electrons localized near such atoms. It has therefore been assumed[1] that the resonances arise from the well-known donor states with ionization energies of about 0.04 to 0.05 ev. We have made a theoretical estimate of the hyperfine splitting of phosphorus donor states to be expected on this assumption and find agreement with experiment within a factor of ~2.5. (We estimate the uncertainty of our theoretical result as about a factor of 5.)

Following is a brief summary of our calculations; a detailed report will be published shortly. The conduction band of Si has 6 minima on the (1,0,0) and equivalent axes.[2] The effective masses at one of these minima are $0.19m$ (twice) and $0.99m$.[3] Let $\psi(\mathbf{k}^{(i)},\mathbf{r})$ be the Bloch function corresponding to the energy minimum at $\mathbf{k}^{(i)}$, so normalized that

$$\int_{\text{cell}} |\psi(\mathbf{k}^{(i)},\mathbf{r})|^2 d\tau = \text{volume of unit cell}, \qquad (1)$$

and phased so as to be real at $\mathbf{r}=0$. It may then be shown that in the so-called effective mass approximation, the normalized ground-state wave function of the donor electron has the following form:

$$\psi(\mathbf{r}) = \frac{1}{(6)^{\frac{1}{2}}} \sum_{i=1}^{6} F^{(i)}(\mathbf{r})\psi(\mathbf{k}^{(i)},\mathbf{r}). \qquad (2)$$

The $F^{(i)}(\mathbf{r})$ satisfy effective mass equations with the above masses and the potential $-e^2/\kappa r$ (κ = dielectric constant). They are taken as real and are normalized to unity over all space. The hyperfine splitting is then determined by the value of

$$|\psi(0)|^2 = 6|F^{(1)}(0)|^2|\psi(\mathbf{k}^{(1)},0)|^2. \qquad (3)$$