PROC. JSSF-2, KYOTO, 1980
J. PHYS. SOC. JPN. **49** (1980) SUPPL. B, p. 98.

Structural Phase Transition in $Sr_2Nb_2O_7$

Kikuo OHI, Yukikuni AKISHIGE and Masaki HOTTA

Department of Physics, School of Science and Engineering, Waseda University, Okubo, Shinjuku-ku, Tokyo 160

Strontium niobate ($Sr_2Nb_2O_7$) is ferroelectric below the Curie temperature at 1342°C and has an incommensurate structure below 220°C.[1] In this report, we present the elastic and dielectric properties of $Sr_2Nb_2O_7$ and ESR study of the Fe doped crystal around the normal-incommensurate phase transition temperature.

The elastic compliance coefficients s_{11}^E and s_{22}^E have step like anomalies,[2] which are explained by the coupling between the incommensurate order parameter Q and the strain component x_i in the form QQ^*x_i. The dielectric constant ε_{33} has a small peak at the transition temperature.

Figure 1 shows angular dependence of ESR line in $Sr_2Nb_2O_7$:Fe at 230°C obtained by an x-band spectrometer. It seems that the lines correspond to the transition $M_s = 1/2 \leftarrow -1/2$ of Fe^{3+} ion in the strong orthorhombic field. The rotation spectrum can be analyzed in terms of the following spin Hamiltonian,

$$H_s = \beta H g S + D\left(S_z^2 - \frac{1}{3}\cdot S\cdot(S+1)\right) + E(S_x^2 - S_y^2).$$

The g tensor is assumed to be isotropic. The best fit parameters are as follows, $|2D| = 0.63 \pm 0.02\ \mathrm{cm}^{-1}$, $|E| = (2.54 \pm 0.02) \times 10^{-2}\ \mathrm{cm}^{-1}$, $\phi = 54.0 \pm 0.5$ deg., where ϕ is the angle between the principal axis z and the c-axis in the (100) plane. The principal axis x is parallel to the a-axis.[3] The calculated lines are shown in Fig. 1 by solid lines. The signs of D and E are not clear but they have opposite signs. The D value is several times as large as that of $BaTiO_3$ in the tetragonal and the orthorhombic phase,[4] but it is one fourth as large as that of Fe^{3+}–V_0 in $SrTiO_3$.[5] This result indicates that Fe^{3+} ion is sitting off the center of distorted octahedron of oxygen ions. The principal axis z coincides with the direction of Nb(2)–O(2)[3] within the experimental error. Therefore, it is assigned that Fe^{3+} ion substitutes on Nb (2) site.

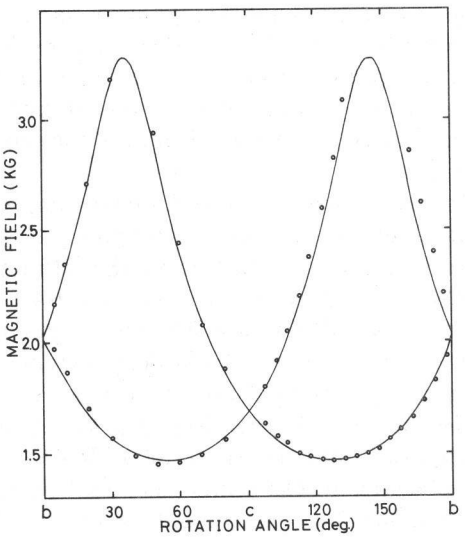

Fig. 1. Angular dependence of ESR lines of $Sr_2Nb_2O_7$: Fe at 230°C. Solid lines represent the values calculated by using the parameters described in the text.

Below 220°C the ESR line splits into two lines, which correspond to two different Nb (2) sites in the incommensurate phase.

The ESR linewidth of 55 gauss at 280°C increases with decreasing temperature and it reaches 95 gauss at the transition point.

References

1) N. Yamamoto, K. Yagi, G. Honjo, M. Kimura and T. Kawamura: J. Phys. Soc. Jpn. **48** (1980) 185.
2) K. Ohi, M. Kimura, H. Ishida and H. Kakinuma: J. Phys. Soc. Jpn. **46** (1979) 1387.
3) N. Ishizawa, F. Marumo, T. Kawamura and M. Kimura: Acta Cryst. **B31** (1975) 1932.
4) T. Sakudo: J. Phys: Soc. Jpn. **18** (1963) 1626.
5) Th. von Waldkirch, K. A. Müller and W. Berlinger: Phys. Rev. **B5** (1972) 4324.