TEMPERATURE DEPENDENCE OF ESR PARAMETERS OF IRON GROUP IMPURITIES IN LITHIUM NIOBATE CRYSTALS AND A MODEL OF DEFECTS♠

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INTRODUCTION

The electron spin resonance of paramagnetic impurities of Cr^{3+}, Mn^{2+}, and Fe^{3+} in $LiNbO_3$ single crystals grown by the Czochralski method, independently doped with 0.01, 0.05, 0.10, and 0.50 wt % of Cr, 0.01 wt % of Mn, and 0.01, 0.08, and 0.39 wt % of Fe, respectively, has been investigated by employing a Varian X-band ESR spectrometer. The rotation patterns of the resonance fields for these three impurities, respectively, were measured in the two mutually perpendicular principal planes and found to be axially symmetric about the c-axis for all these impurities.

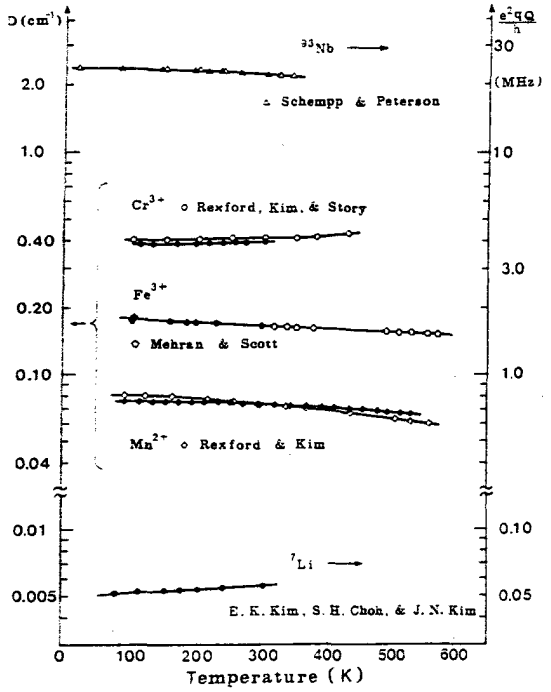
EXPERIMENTAL RESULTS AND ANALYSIS

Resonance data were analyzed in terms of the usual spin Hamiltonian :

$$\mathcal{H} = g\beta \mathbf{B}\cdot\mathbf{S} + B_2^0 O_2^0 + B_4^0 O_4^0 + B_4^3 O_4^3 + \mathbf{S}\cdot\overleftrightarrow{A}\cdot\mathbf{I},$$

and the parameters determined at room temperature are shown below. These parameters appear to be insensitive to the impurity concentration.

As the temperature is increased, the value of B_2^0 is found to be strongly temperature dependent as shown in the last column of the table. These dependences turn out to be closely related to the temperature dependence of the nuclear quadrupole coupling constant, e^2qQ/h, of ^7Li and ^{93}Nb in the pure $LiNbO_3$ crystal [1], where e^2qQ/h of ^7Li increases with increasing temperature whereas that of ^{93}Nb decreases and $\eta = 0$ for both at all



temperatures. By comparing similarities of B_2^0 and e^2qQ/h in mathematical formulae in ESR and NMR Hamiltonian, respectively, and from these temperature dependences as shown above, we propose that the Cr^{3+} ion substitutes for Li and the Mn^{2+} and Fe^{3+} impurities substitute for Nb. These conclusions are in partial agreement with a recent report [2].

REFERENCES

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impurity	S	g	B_2^0/h(GHz)	B_4^0/h(GHz)	B_4^3/h(GHz)	A/h(GHz)	as temp. incr.
Cr^{3+}	3/2	1.972	3.947				B_2^0 incr.
Mn^{2+}	5/2	2.006	0.730	-0.0001	0.047	0.230	B_2^0 decr.
Fe^{3+}	5/2	1.993	1.65	0.0084	0.068		B_2^0 decr.

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