NUCLEAR MAGNETIC RESONANCE OF ^{8}Li IN $LiNbO_3$ AND THE QUADRUPOLE MOMENT OF ^{8}Li

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Nuclear magnetic resonance measurements were carried out on neutron activated ^{8}Li ($T_{1/2}$ = 0.84 s) nuclei in a single crystal of $LiNbO_3$. The quadrupolar splitted NMR spectrum, detected via the ^{8}Li β radiation, could be resolved. The quadrupole coupling constant was determined to $|e^2qQ/h| = 43 \pm 3$ kHz at room temperature. Comparison with the coupling constant of ^{7}Li in $LiNbO_3$ leads to the value of the quadrupole moment $|Q(^8\mathrm{Li})| = 32 \pm 6$ mb.

The nucleus ^{8}Li was the first to be investigated by an in-beam nuclear magnetic resonance method with nuclear radiation detection. In 1959 Connor [1] determined the magnetic moment of the β-emitter ^{8}Li after polarized neutron capture in cubic LiF. The present paper reports on the measurement of the quadrupole moment of ^{8}Li by extending the technique to a noncubic crystal, where the additional electric coupling produces a small quadrupolar splitting of the NMR line. We used the ferroelectric compound $LiNbO_3$. It is available as a single crystal and from several ^{7}Li NMR measurements [2,3, and refs. given there] the crystal electric field gradient at the Li site is known.

As ^{8}Li is a light nucleus – the lightest one whose quadrupole moment remained to be measured up to now – it exhibits only a weak electric interaction. In the present case of $LiNbO_3$ it was just possible to resolve the quadrupole pattern, whereas for ^{8}Li nuclei stopped in Be and Mg metal only a smeared resonance line was reported [4].

$LiNbO_3$ cristallizes in the trigonal space group R3c. The Li site possesses axial symmetry and the asymmetry parameter η vanishes. If further the quadrupolar interaction is small compared to the Zeeman energy first-order perturbation theory is sufficient. It yields for ^{8}Li with spin $I = 2$ [5] an NMR pattern consisting of four equally spaced $\Delta m_I = \pm 1$ curves with a frequency difference between neighbouring lines [6] of $\Delta\nu = (e^2qQ/8h)(3\cos^2\theta - 1)$, with quadrupole coupling constant e^2qQ, and angle θ between static field H_0 and crystallographic c-axis. For $\theta = 0°$ the line separation has its maximum $\Delta\nu(\theta{=}0) = e^2qQ/4h$ and for $\theta = 54.7°$ the lines collapse at the Larmor frequency $\gamma H_0/2\pi$.

The experimental technique was similar to that described in preceding papers [7,8]. A thermal neutron beam of the guide H 25 at the High Flux Reactor Grenoble was spin polarized by reflection from a magnetized $Co_{50}Fe_{50}$ mirror, yielding about 5×10^7 cm^{-2} s^{-1} polarized neutrons at the target. The $LiNbO_3$ target ($25 \times 25 \times 2.5$ mm^3, single domain crystal, c-axis perpendicular to the large surface with an accuracy better 0.5°) was mounted on a simple goniometer θ disk and was placed in an external magnetic field H_0. The rf coil consisted of 6.5 windings of aluminium wire (ϕ 0.4 mm) around the terget. The polarization of the ^{8}Li nuclei produced by neutron capture in the crystal was detected via the asymmetric β decay of ^{8}Li ($T_{1/2}$ = 0.84 s) to ^{8}Be. The β radiation was registered by two scintillator telescopes mounted on both sides of the target in the pole gap. The measurements were mainly performed at room temperature. The typical measuring time for one (single) resonance curve was about 24 h.

Fig. 1 shows the NMR spectrum for various angles θ. The single line observed at 54.7° broadens and finally splits into four components as θ decreases to 0°. The signal-to-noise ratio is rather poor for the splitted spectra and we did not evaluate e^2qQ from them. However, it demonstrates that the angular dependence of the frequency separation agrees with the expression

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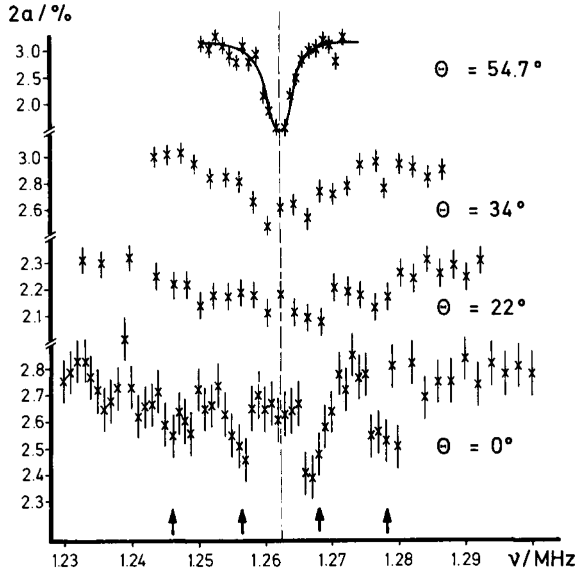

Fig. 1. ^{8}Li NMR signals in a $LiNbO_3$ crystal detected by the β decay asymmetry 2a for different angles θ. The solid curve for $\theta = 54.7°$ is a fitted Lorentzian with 1.2623(2) MHz center frequency, indicated by the dotted line. The arrows represent the positions of the four curves of fig. 2. Further data: H_0 = 2000 Oe; rf field strength $2H_1$ = 80 mOe, unmodulated; target at room temperature.

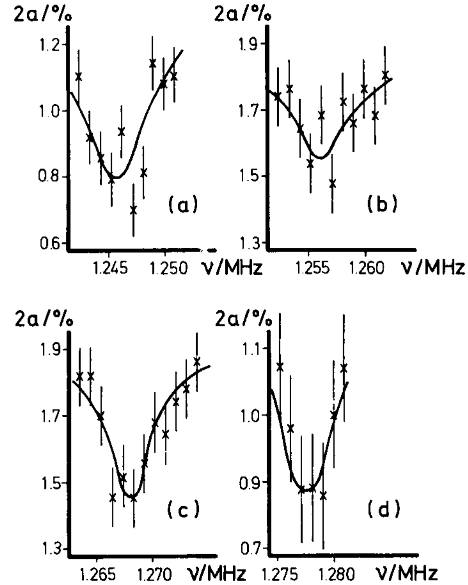

Fig. 2. The four single $\Delta m_I = \pm 1$ transitions of ^{8}Li in $LiNbO_3$. The β-decay asymmetry 2a is shown as a function of the unmodulated rf field. Its field strength was $2H_1$ = 0.28 Oe in diagram (a), and 80 mOe in diagrams (b) – (d). The field strength of the modulated rf field was $2H_1$ = 0.8 Oe. The solid curves are fitted Lorentzians. Further data: H_0 = 2000 Oe, target at room temperature.

given above. This fact, together with the small linewidth of the $\theta = 54.7°$ curve, is considered as a proof that those ^{8}Li nuclei which are observed in the NMR signal occupy normal, and practically undisturbed lattice sites. As the ^{8}Li nuclei are produced by the (n,γ) reaction they suffer a recoil by the γ-radiation with a maximum energy of 275 eV. It was therefore not self-evident whether the activated ^{8}Li atoms come to rest on normal Li lattice sites in an undisturbed environment†.

Fig. 2 shows the four single lines $\Delta m = \pm 1$ at $\theta = 0°$. In order to enhance the signal amplitude a technique developed in ref. [7] was applied: two different rf fields are applied simultaneously. One field is swept in steps over the transition to be measured. The other rf field is frequency modulated. Its constant center frequency and depth of modulation are chosen in a way that the adjacent two or three transitions on one side of the measured line become saturated.

The four transition frequencies were determined at H_0 = 2000 Oe and at room temperature‡ to 1278.2 ± 0.6, 1268.0 ± 0.6, 1256.5 ± 0.8 and 1246.1 ± 0.6 kHz, which results in the quadrupole coupling constant $e^2qQ/h = \pm 43 \pm 3$ kHz. The error cited is somewhat greater than the experimental error. This considers the fact that the modulated rf field may produce small shifts. Using the averaged value 54.5 ± 0.5 kHz for the coupling constant of ^{7}Li in $LiNbO_3$ from refs. [2,3], one obtains the ratio for the quadrupole moments $|Q(^8\mathrm{Li})/Q(^7\mathrm{Li})| = 0.79 \pm 0.06$. Inserting the value for $Q(^7\mathrm{Li}) = -41 \pm 6$ mb [9] one gets finally $|Q(^8\mathrm{Li})| = 32 \pm 6$ mb.

† In a previous NMR study on ^{20}F in tetragonal MgF_2 [7] we observed at room temperature undisturbed quadrupolar spectra. But no reliable conclusions can be drawn from the observation for $LiNbO_3$ with its more complicated structure.

‡ The NMR spectrum has also been recorded at 200°C, yielding a slightly larger quadrupole splitting, as was to be expected from ref. [3]. We cannot report a quantitative value for this shift, because our oven disturbed the field homogeneity.

The longitudinal spin-lattice relaxation time was determined at 27° and 200°C for H_0 = 2000 Oe with the results T_1 = 4.3 ± 1.2 s and 0.54 ± 0.04 s, respectively. A systematic investigation of the relaxation processes is presently under way.

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