Quadrupole Moments of the ^{40}Ca Core Plus One Nucleon Nuclei ^{41}Sc and ^{41}Ca

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The electric-field-gradient (EFG) and anisotropic chemical shift of ^{45}Sc(I^π = 7/2$^-$, stable) in TiO_2 crystal were determined by detecting the FT-NMR of ^{45}Sc(0.5 atm% of Ti in TiO_2) doped in TiO_2 crystal at a high field of 7.0 T and 9.4 T. Using the EFG, an old β-NQR spectrum of ^{41}Sc was reanalyzed to obtain $eqQ(^{41}\text{Sc})/h$ which was combined with the renewed $Q(^{45}\text{Sc})$ = –(23.6 ± 0.2) fm^2 to obtain $|Q(^{41}\text{Sc}; I^\pi = 7/2^-, T_{1/2} = 0.596\text{ s})| = (15.6 \pm 0.3)$ fm^2. Also the atomic EFG in Ca was recalculated, using a finite-element multi configuration Hartree-Fock method to renew $Q(^{43}\text{Ca})$. Finally using the known hyperfine constants of ^{41}Ca, the $Q(^{41}\text{Ca})$ value has been renewed.

Key words: Quadrupole Moments of Sc and Ca Isotopes; Electric Field Gradients; Ca and Sc Atoms; TiO_2.

1. Introduction

Nuclear quadrupole moments have been an indispensable clue for the investigation of nuclear shell structure and nucleon interactions [1, 2] in the nucleus. Of particular interest is ^{41}Sc(I^π = 7/2$^-$, $T_{1/2}$ = 0.596 s) and ^{41}Ca(I^π = 7/2$^-$, $T_{1/2}$ = 10^5 y) because of their simple nuclear structure, i. e., each state is composed of a doubly closed-shell core, ^{40}Ca, and one extra nucleon attached to it. One of the problems in this system is that the doubly closed core of ^{40}Ca might be deformed. In spite of a theoretical prediction, this is still an open question [3]. This core deformation, if it exists, can be detected in the quadrupole moments of the ^{40}Ca + one nucleon nuclei. For this study the moment must be determined precisely, i. e., better than to a few% in the relative error $\delta Q/Q$. Then, applying the charge symmetry principle to the nuclear structure of the mirror pair, we may clearly discover the particular deformation effect in the quadrupole moments of ^{41}Sc and ^{41}Ca. Although their quadrupole moments have already been studied experimentally and theoretically [4 - 7], the precision of the found quadrupole moment of ^{41}Sc [4] was not sufficient due to the limit in the accuracy of the electric field gradient (EFG) at the Sc isotopes in TiO_2 crystal in which the short lived ^{41}Sc was implanted following the nuclear reaction. Also, the precision of the theoretical EFG in ^{41}Ca must be improved, using a more realistic atomic configuration.

2. EFG and FT-NMR of ^{45}Sc in TiO_2

The EFG tensor at ^{45}Sc located in the substitutional site of Ti in TiO_2 (tetragonal) crystal was studied by detecting FT-NMR [8] of ^{45}Sc at a high external magnetic field. Two fields H = 7.0 T and 9.4 T were employed to isolate the quadrupole effect from the anisotropic chemical shift. The sample was prepared by mixing proper amount of $^{45}Sc_2O_3$ powder and

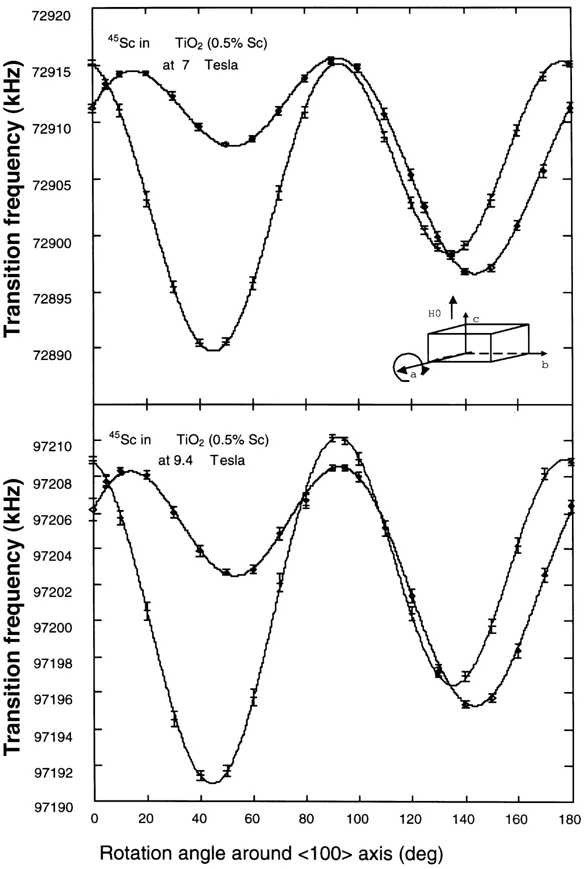

Fig. 1. FT-NMR of ^{45}Sc at H = 7.0 T and 9.4 T. Resonance frequencies of ^{45}Sc as a function of crystal orientation. The crystal was rotated around the axis placed almost parallel to <100> which was perpendicular to H_0. The $m = \pm 1/2 \leftrightarrow \mp 1/2$ transition frequencies were observed under the external fields of 7.0 T and 9.4 T.

TiO_2 before a TiO_2 (^{45}Sc) crystal was synthesized [9]. The concentration of the ^{45}Sc was 0.5 atom% of the Ti atoms in the crystal. The measurements of the transition between $m = \pm 1/2 \leftrightarrow \mp 1/2$ as a function of crystal orientation (the rotation axis was almost parallel to <100> placed vertical to H, the precise orientation of which was known also from the data fitting) were done at room temperature. The best fit of the theoretical curve to the data shown in Fig. 1 gave the coupling constant $|eqQ(^{45}\text{Sc}; 7/2^-)/h|$ = (11.02 ± 0.01) MHz with the V_{zz} direction being parallel to <110>, the asymmetry parameter η = (0.983 ± 0.003) and the second component V_{yy} being parallel to crystal c-axis [10]. As seen in the slight difference of the rotation pattern of the NMR the anisotropic chemical shift

Table 1. The experimental EFG and anisotropic chemical shift at the ^{45}Sc(0.5 atom% of Ti) site in TiO_2 (rutile).

$\lvert eqQ(^{45}\text{Sc})/h\rvert$ (MHz)	11.02 ± 0.01
$\eta\ (V_{ZZ} \parallel <110>)$	0.983 ± 0.003
V_{YY}	parallel to c-axis
$\lvert q\rvert$ (10^{15}V/cm^2)	193 ± 2
Anisotropic chemical shift (ppm)	
σ_{XX}	61.6 ± 0.6
σ_{YY}	3.6 ± 0.4
σ_{ZZ}	–65.2 ± 0.7

for the Sc isotope in the crystal was obtained simultaneously as given in Table 1. Also the EFG parameters are summarized in Table 1. Those parameters used in the old analyses [4] ($|eqQ(^{45}\text{Sc})/h|$, η) = (11.99 ± 0.12) MHz, (0.54 ± 0.02) have to be changed to the new set of {(11.02 ± 0.01) MHz, (0.983 ± 0.003)} to accordingly reanalyze the old data.

3. Reanalysis of the β-NQ(^{41}Sc)R Data

Using the present asymmetry parameter η of the EFG, the old β-NQR data [4] of ^{41}Sc implanted in a TiO_2 crystal placed in H_0 = 0.6 T were reanalyzed to renew the old ν_Q spectrum. First of all, the ν_Q frequency was recalculated using each RF set used for each data point as given in the figure and as a result a β-NQR spectrum is given in Figure 2. The solid curve is the best fit of the theoretical β-NQR curve for I = 7/2 to the data. The best fit gives $|eqQ(^{41}\text{Sc})/h|$ = (7.31 ± 0.07) MHz, $\Delta q/q$ = (8.7 ± 0.7)%. This

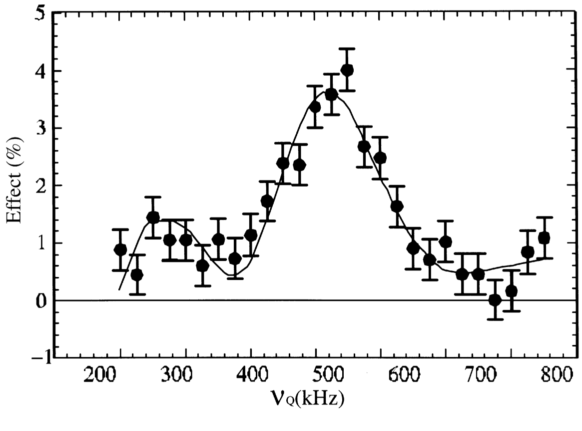

Fig. 2. Quadrupole spectrum of ^{41}Sc implanted in TiO_2 at high field. The asymmetry change was measured as a function of the quadrupole coupling frequency, $\nu_Q = 3eqQ/2I(2I-1)$. The solid curve is the best fit of the theoretical curve to the data.

rather wide spread of Δq can be understood by the evenly spreaded crystal defects and damages due to the implantation as discussed for the case of implantation of ^{12}N into an insulator BN(hexagonal) crystal [11]. For the present $\Delta q/q$ we add a systematic error of $\pm$60 kHz to the result. Finally we obtain $|eqQ(^{41}\text{Sc})/h|$ = (7.31 $\pm$ 0.07(stat) $\pm$ 0.06(syst)). As a result we have a ratio of the coupling constants for ^{41}Sc and ^{45}Sc to be $|eqQ(^{41}\text{Sc})/eqQ(^{45}\text{Sc})|_{\text{new}}$ = 0.66 $\pm$ 0.01.

4. Quadrupole Moment of ^{41}Sc

Before using $Q(^{45}\text{Sc})$ as a reference a newer atomic hyperfine constant for the ^{45}Sc atom was adopted: $B(^{2S+1}L_J) = b_{nl}(2J-1)/2(J+1) = eqQ(^{45}\text{Sc})$ [12, 13], where q is the valence only atomic field gradient at the nucleus with a newer Sternheimer polarization effect [14]. Here b_{nl} is the hyperfine constant defined by the above equation for a valence only configuration in the n-th shell with an orbital angular momentum l. Using the realistic configuration mixing and the off-diagonal hyperfine effect in b_{nl} given by Childs [13] and a valence only q by Fricke [12] we obtained $Q(^{45}\text{Sc}; 7/2^-)$ = –(21.41 $\pm$ 0.08) fm^2. We define this value further as $Q(^{45}\text{Sc}; 7/2^-) = Q_\text{u}$ where subscript u stands for a value uncorrected for the Sternheimer polarization. Here, since the Sternheimer correction for the ground state of ^{45}Sc was independently calculated by Sternheimer and Gupta [14], we adopted a correction factor $1/(1-R)$ = (1.102 $\pm$ 0.009). Then, $Q_{\text{cor}}(^{45}\text{Sc}; 7/2^-) = Q_\text{u}/(1-R)$ = –(23.6 $\pm$ 0.2) fm^2 is obtained, where the subscript cor stands for the value corrected for the Sternheimer polarization. Finally, using the present $Q_{\text{cor}}(^{45}\text{Sc}; 7/2^-)$ value, we determined a corrected value for ^{41}Sc as $|Q(^{41}\text{Sc}; 7/2^-)|$ = (15.6 $\pm$ 0.3) fm^2, which agrees with the old value (16.6 $\pm$ 0.8) fm^2 within the error, although the present value is by 6% smaller than the previously reported one.

5. Recalculation of the Atomic EFG in Ca and $Q(^{41}\text{Ca}; 7/2^-)$

An improvement in the calculation of the atomic q of ^{43}Ca used for the derivation of $Q(^{43}\text{Ca}; 7/2^-)$ was made here [15] since two q values with almost 15% difference have been reported in 1992 and 93 by Salomonsson and Sundholm et al., respectively [16]. Salomonsson used a many-body perturbation calculation on the atomic 4s3d and 4s4p configurations of Ca. On the other hand, Sundholm et al. performed a finite-element multi configuration Hartree-Fock calculation (MCHF) for the active space extended to a range which includes the 2p orbit. In this calculation they found the importance of the polarization effect of 2p to the atomic q value. To confirm this, we have recalculated q by use of the MCHF developed by Fisher [17] with a larger active space for Ca(3d4s, $^1D_2$), for which atomic hyperfine interactions were studied. In this framework, f- and g-shell contributions and relativistic effects, as well as the 2p configuration are included as for the Sundholm calculation. The calculated q value obtained as a function of the active space showed good agreements with the one given by Sundholm as q(spd limit) = –0.4090 a. u., q(f-shell) = –0.0142 a.u., and q(g-shell) = –0.0010 a.u., q(relativistic) = –0.0014 a. u. except for the present q(p-shell) = +0.0373 a. u., which showed a non negligible change from the pld value q(p-shell; Sundholm) = –0.08899 a. u. Here the field gradient q(a. u.) expressed by a. u. units is equivalent to q(MKS) = q (a. u.) $\cdot$ 9.717 $\cdot$ 10^{21} V/m^2. Thus we obtained q(Ca: 3d4s, $^1D_2$) = (0.3579 $\pm$ 0.0075) a. u. with theoretical uncertainty of 2.1%. As a result, $Q(^{43}\text{Ca}; 7/2^-)$ = –(5.52 $\pm$ 0.11) fm^2 is concluded. From the experimental ratio $Q(^{41}\text{Ca}; 7/2^-)/Q(^{43}\text{Ca}; 7/2^-)$ = (1.63 $\pm$ 0.01) [5], we obtain $|Q(^{41}\text{Ca}; 7/2^-)|$ = –(9.00 $\pm$ 0.18) fm^2.

6. Discussion on the Mirror Quadrupole Moments of ^{41}Sc and ^{41}Ca

With respect to the nuclear quadrupole moment, the value of a state in a nucleus is given [2] by the sum of quadrupole moments of the proton group and that of the neutron group in the nucleus as $Q(N_\text{p}, N_\text{n}) = e_\text{n}^{\text{eff}} \cdot Q(N_\text{n}) + e_\text{p}^{\text{eff}} \cdot Q(N_\text{p})$. The effective charges e_p^{eff} = +1.31 e and e_n^{eff} = +0.525 e for proton and neutron, respectively, in the 0f-1p shell have been given by Dahr and Bhatt [18] from their projected Hartree-Fock calculations which reproduce B(E2) data well.

A set of theoretical predictions on the mass $A = 41$ system has been made also by Sagawa and Kitagawa [20] by use of the Woods-Saxon potential for a valence nucleon besides the ^{40}Ca core which has been assumed to be spherical. In their calculation, the wave functions for the protons and neutrons in the ^{40}Ca core in ^{41}Sc and ^{41}Ca are obtained by use of a harmonic oscillator potential. Aside from the potential depth the parameters of the Woods-Saxon potential are taken from [20]. The depth is adjusted to reproduce the experimental separation energy of the single particle state in each shell model configuration [19]. They concluded that the loosely bound proton in ^{41}Sc with a small separation energy of 1.1 MeV is spatially extended to the out side of the ^{40}Ca core. The nuclear structure of ^{41}Sc is not identical with that of ^{41}Ca as to the meaning of its radial extensions, at least. Such distributions give for the deeply bound proton and neutron in ^{41}Ca with separation energies of 8.9 MeV and 8.4 MeV, respectively, $Q_{\text{th}}(21) = -10.75\ \text{fm}^2$ and $Q_{\text{th}}(20) = 0\ \text{fm}^2$, respectively. The theoretical $Q_{\text{th}}(^{41}\text{Ca}; 7/2^-) = -6.88\ \text{fm}^2$ differs by about 24% from the experimental one $Q_{\text{exp}}(^{41}\text{Ca}; 7/2^-) = -(9.0 \pm 0.2)\ \text{fm}^2$. On the other hand, for the deeply bound neutrons and loosely bound protons in ^{41}Sc they obtain theoretical values as $Q_{\text{th}}(20) = 0\ \text{fm}^2$ and $Q_{\text{th}}(21) = -11.5\ \text{fm}^2$, respectively. The values give $Q_{\text{th}}(^{41}\text{Sc}; 7/2^-) = -15.1\ \text{fm}^2$, which agrees well with the experimental value, i. e., only 0.5 fm^2, or 3%, smaller than the experimental value, 15.6 fm^2.

The theoretical value of ^{41}Ca does not reproduce the experimental one at all. If an irregular effective charge is assumed to account for this discrepancy, $e_{\text{n}}^{\text{eff}} = 0.85\ e$ is needed, which is almost 1.5 times the known value, which is quite abnormal. To account for the discrepancy we may suggest a core deformation in spite of the good agreement of theory and experiment for ^{41}Sc. Using the above theoretical $Q_{\text{th}}(21)$ for ^{41}Sc and ^{41}Ca given by Kitagawa et al. [19] and the effective charges given by Dahr et al. [18], we derive quadrupole moments Q_{def} due to the core deformation as

$$\begin{aligned} Q_{\text{exp}}(^{41}\text{Ca}; 7/2^-) &= -(9.0 \pm 0.2)\ \text{fm}^2 \\ &= Q_{\text{th}}(\text{neutron})e_{\text{n}}^{\text{eff}} + Q_{\text{def}} \text{ and} \\ Q_{\text{exp}}(^{41}\text{Sc}; 7/2^-) &= -(15.6 \pm 0.3)\ \text{fm}^2 \\ &= Q_{\text{th}}(\text{proton})e_{\text{p}}^{\text{eff}} + Q_{\text{def}}. \end{aligned}$$

We obtain Q_{def} (from ^{41}Ca) = $-(3.0 \pm 0.2)$ fm^2 and Q_{def} (from ^{41}Sc) = $-(0.5 \pm 0.4)$ fm^2. Thus, two different Q_{def} values may imply a finite iso vector component if the soft ^{40}Ca core exists.

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[1] H. Sagawa and B. A. Brown, Nucl. Phys. **A430**, 84 (1984).
[2] T. Minamisono, T. Ohtsubo, I. Minami, S. Fukuda, A. Kitagawa, M. Fukuda, K. Matsuta, Y. Nojiri, S. Takeda, H. Sagawa, and H. Kitagawa, Phys. Rev. Letters **69**, 2058 (1992).
[3] W. J. Grace and A. M. Green, Nucl. Phys. **A93**, 110 (1967).
[4] T. Minamisono, Y. Nojiri, K. Matsuta, K. Takeyama, A. Kitagawa, T. Ohtsubo, A. Ozawa, and M. Izumi, Nucl. Phys. **A516**, 365 (1990); Nucl. Phys. **A559**, 239 (1993).
[5] M. Arnold, K. Kowalsky, T. Stehlin, F. Traeger, and zu Putlitz, Z. Phys. A, Atoms and Nuclei **314**, 303 (1983).
[6] S. Ichii, W. Bentz, and A. Arima, Nucl. Phys. **A464**, 575 (1987).
[7] I. S. Towner and F. C. Khanna, Nucl. Phys. **A399**, 334 (1983); Phys. Reports **155**, 264 (1987).
[8] E. Fukuda and D. W. Roeder, Experimental Pulse NMR – A Nut and Bolt Approach, Addison-Wesley, Reading, MA 1981.
[9] Synthesized and offered by Earth Jewelry Co., Ikeda, Osaka, Japan.
[10] K. Sato, S. Takeda, S. Fukuda, T. Minamisono, M. Tanigaki, T. Miyake, Y. Maruyama, K. Matsuta, M. Fukuda, and Y. Nojiri, Z. Naturforsch. **53a**, 549 (1998).
[11] T. Minamisono, K. Sato, H. Akai, S. Takeda, Y. Maruyama, K. Matsuta, M. Fukuda, T. Miyake, A. Morishita, T. Izumikawa, and Y. Nojiri, Phys. Lett. **B 420**, 31 (1998).
[12] G. Fricke, H. Kopfermann, S. Penselin, and K. Schlupmann, Z. Phys. **156**, 416 (1959).
[13] W. J. Childs, Phys. Rev. **A4**, 1767 (1971).
[14] R. P. Gupta and S. K. Sen, Phys. Rev. **A7**, 850 (1973); R. M. Sternheimer, Phys. Rev. **A6**, 1702 (1972).
[15] S. Fukuda, Ph.D. Thesis, Graduate School of Science, Osaka University, Osaka 1995.
[16] S. Salomonsson, Z. Phys. **A316**, 135 (1994); D. Sundholm and J. Olsen, J. Chem. Phys. **38**, 1 (1993).
[17] C.F. Fisher, Comput. Phys. Commun. **64**, 431 (1991); P. Jonsson, Comput. Phys. Commun. **74**, 399 (1993).
[18] A. K. Dahr and K. H. Bhatt, Phys. Rev. **C16**, 792 (1977).
[19] H. Kitagawa and H. Sagawa, Nucl. Phys. **A551**, 16 (1993).
[20] A. Bohr and B.R. Mottelson, Nucl. Structure Vol. 1, Benjamin, New York 1969, p. 239.