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HIGH-RESOLUTION TDPAC MEASUREMENT IN K_2ZrF_6

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A time resolution of $2\tau = 0.75$ ns, achieved with a conventional TDPAC setup with FCs detectors, allowed a determination of the very high electric field gradient at Hf impurity sites in K_2ZrF_6.

Simple theoretical calculations seem to indicate that nearest neighbours are responsible for the interaction observed.

1. Introduction

The 482 keV, $\frac{5}{2}^+$ state obtained in the decay of ^{181}Hf to ^{181}Ta constitutes one of the best probes for a TDPAC experiment, on account of its large quadrupole moment ($Q = 2.53$ b). Nevertheless, in the presence of intense *EFG*'s this advantage cannot be fully profitted by due to the finite time resolution of the NaI(Tl) detectors commonly used in the experimental setup.

In a previous e^--γ TDPAC experiment performed in order to measure the high magnetic hyperfine fields at Ta sites in Co and Fe hosts, the replacement of the NaI(Tl) detector by a plastic one was attempted [1]. The result was a satisfactory improvement in the resolution time, 0.8 ns, but a very poor overall efficiency.

Recently, Kočki et al. [2] using one plastic and one NaI(Tl) detector for the γ-γ cascade which yielded the same time resolution, have determined a large quadrupole interaction in $(SO_4)_2Hf$. In this case the plastic scintillator, an NE-140 one, was loaded with 5% Sn in order to enhance the photoelectric absorption of the 133 keV peak.

FCs detectors, which have just been commercially manufactured by Harshaw, exhibit, in addition to an excellent time resolution, an efficiency similar to that of

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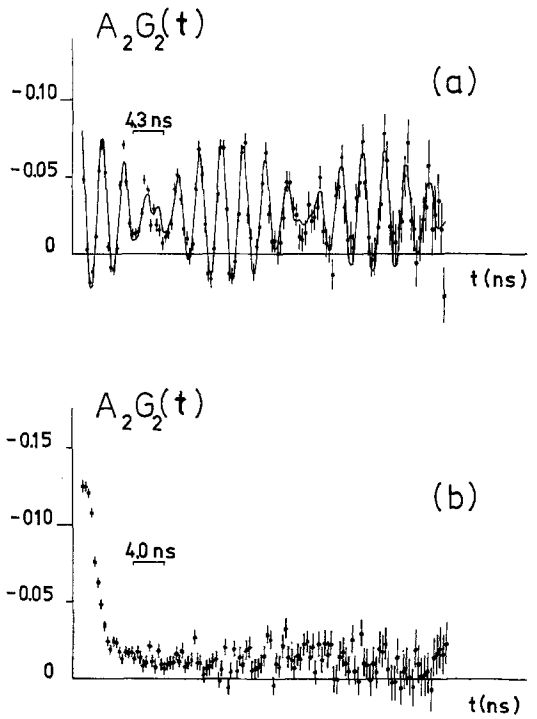

Fig. 1. (a) Spin rotation curve for ^{181}Ta in K_2ZrF_6 at room temperature obtained using FCs detectors. (b) Spin rotation curve for ^{181}Ta in K_2ZrF_6 at room temperature obtained using NaI(Tl) detectors.

the NaI(Tl) detectors and an energy resolution good enough to resolve the γ-ray energies of the more commonly used TDPAC probes.

In this work, using a conventional TDPAC setup with two FCs detectors and time resolution $2\tau = 0.75$ ns, we have determined the electric quadrupole interaction at the sites of Hf impurities in the K_2ZrF_6 compound at room temperature. This interaction could not be resolved at all in a previous experiment performed with NaI(Tl) crystals (see fig. 1b).

2. Experimental

A powder source of K_2ZrF_6 was irradiated with thermal neutrons ($\Phi \sim 10^{13}$ n/cm^2 · s) in the RA-3 reactor of the Comisión Nacional de Energía Atómica, Argentina. After irradiation, the source was melted and recrystallized.

Two integral lines assemblies with 3.75 cm × 3.75 cm FCs crystals coupled to RCA-8850 photomultipliers were used as γ-detectors. The resulting energy resolu-

tion, of about 22% for 662 keV, was sufficient to achieve a clean selection of the 133–482 keV γ-γ probe cascade. A typical fast-slow coincidence electronic array was used to determine the number of coincidences $C(\theta, t)$ involved in the cascade as a function of the angle θ subtended by the detectors and the delay time t between γ_2 and γ_1.

From the normalized and background-corrected measured coincidences $C_0(\theta, t)$ at $\theta = 90°$ and $\theta = 180°$ the function $A_2G_2(t)$ was obtained through the conventional ratio:

$$A_2G_2(t) = 2\,\frac{C_0(180, t) - C_0(90, t)}{C_0(180, t) + 2C_0(90, t)}\,. \tag{1}$$

Fig. 1a shows the corresponding spin rotation curve obtained with the setup described above. For comparison, fig. 1b exhibits the information obtained with a two NaI(Tl) detector array for the same sample at the same temperature.

The fitting procedure, which took into account the finite time resolution of the system, was performed using the fitting function:

$$A_2G_2(t) = A_2 \sum_{i=0}^{3} s_{2i}\, e^{-\delta\omega_i t} \cos(\omega_i t)\,, \tag{2}$$

and yielded the following values for the quadrupole parameters:

$$\omega_Q = 200 \pm 5 \text{ mrad/s}\,, \qquad (|V_{zz}| = (22.5 \pm 2.7) \times 10^{17}\ \text{V}\cdot\text{cm}^{-2})$$

$$\eta = 0.83 \pm 0.01\,.$$

The low fitted value of the distribution width around ω_Q ($\delta = 0.003 \pm 0.001$) indicated that the ^{181}Hf probes were located at very regular sites in the structure.

3. Discussion

According to the known crystalline data of the K_2ZrF_6 structure [3], two attempts at calculating the *EFG* at Hf sites were performed assuming a point-charge model. The first one, using the de Wette method [4], took into account the contribution of the whole lattice and the second was a simple electrostatic calculation over the nearest neighbours, e.g. the eight F^- ions of the pentagonal bipyramidal configuration surrounding the Hf probe. While the former yielded $V_{zz} = 19.43 \times 10^{17}\ \text{V}\cdot\text{cm}^{-2}$ and $\eta = 0.19$, the latter led to $V_{zz} = 8.33 \times 10^{17}\ \text{V}\cdot\text{cm}^{-2}$ and $\eta = 0.74$.

Since η, defined as the ratio $\eta = (V_{xx} - V_{yy})/V_{zz}$, is independent of any common multiplicative constant in the *EFG* components, the η values should be more heavily weighted than the V_{zz} ones, and the first simple model is to be eliminated. So, in the frame of this hypothesis, we think that the contribution of only the nearest neigh-

bours to the *EFG* is a better description of the actual situation. The corresponding V_{zz} values are smaller by a factor of about two than the experimental ones, which indicates that we have neglected an additional contribution to the *EFG* in this calculation.

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