Quadrupole Coupling Constants for ^{100}Rh in Transition Metals from Perturbed Angular Correlation Spectroscopy

William J. Kemp[a], Adurafimihan A. Abiona[a,*], Patrick Kessler[b], Reiner Vianden[b] and Heiko Timmers[a,c]

[a] *School of Physical, Environmental and Mathematical Sciences, The University of New South Wales, Canberra Campus, ACT 2602, Canberra, Australia*
[b] *Helmholtz-Institut für Strahlen- und Kernphysik, Nußallee 14-16, 53115 Bonn, Germany*
[c] *Department of Nuclear Physics, Research School of Physics and Engineering, Australian National University, Canberra, ACT 200, Australia*

[*] *On leave from Centre for Energy Research and Development, Obafemi Awolowo University, Ile-Ife, Nigeria*

Time differential perturbed angular correlation spectroscopy of ^{100}Rh in zinc, rhodium, antimony, hafnium and rhenium has confirmed expectations for zinc and rhodium and provided the first measurements of quadrupole coupling constants for the three other transition metals with preliminary values of ν_Q = 4.3 MHz, 5.7 MHz, and 3.2 MHz, respectively. The three results appear to be consistent with published results for zirconium and ruthenium.

1. Introduction

The nuclear quadrupole moment Q has fundamental importance in nuclear structure physics and it is a crucial parameter for hyperfine interaction studies of condensed matter. Nuclear quadrupole moments may be calculated from measurements of the quadrupole coupling constant ν_Q in solids according to:

$$Q = \frac{h}{e}\frac{\nu_Q}{V_{zz}} \tag{1}$$

where h and e are Planck's constant and the positive elementary charge, respectively. This requires, however, that the principal component V_{zz} of the Electric Field Gradient (EFG) at the probe site is well known. Theoretical calculations of the EFG for solids have traditionally been difficult. Recent theoretical advances, such as the *WIEN2k* code [1], can now provide accurate predictions of electric field gradients in solids [2, 3]. In order to exploit such progress, a more complete compilation of quadrupole coupling constants than presented in Ref. [4] and improved experimental accuracy would be advantageous. The list of measurements of quadrupole coupling constants with time differential perturbed angular correlation spectroscopy (TDPAC) using the probe ^{100}Pd/^{100}Rh is particularly

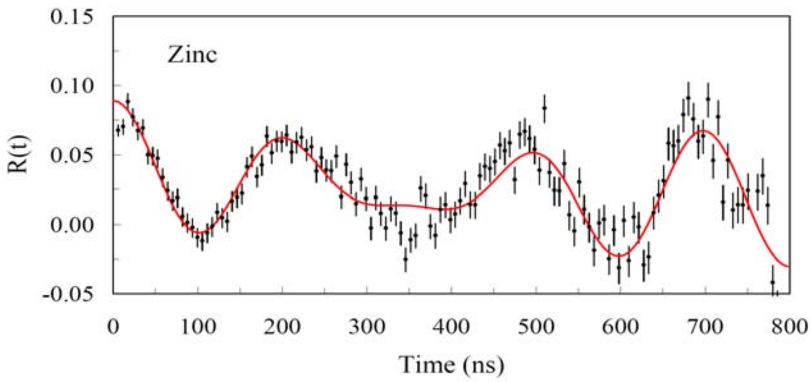

Fig. 1. Measured ratio function *R(t)* for ^{100}Rh in zinc. The fitted curve is shown in red.

sparse. The current accepted value of the nuclear quadrupole moment of the relevant 74 keV 2^+ state in ^{100}Rh ($t_{1/2}$ = 215 ns) is Q = 0.076(20) barn [5]. It may be noted that the relative uncertainty of this value is more than 25%. This project aims to provide several new TDPAC measurements of ν_Q for the ^{100}Pd/^{100}Rh probe while verifying existing results. Here preliminary results are presented for the transition metals zinc, rhodium, antimony, hafnium and rhenium.

2. Experimental Details

The 14 UD Pelletron accelerator at the Australian National University in Canberra was used to synthesize the ^{100}Pd/^{100}Rh probe nuclei via the fusion evaporation reaction ^{92}Zr(^{12}C, 4n)^{100}Pd. The 70 MeV ^{12}C beam was incident on the zirconium production target over 20 h at a beam current of 1 μA. Synthesized probe nuclei recoil-implanted at forward angles into polycrystalline samples of zinc, rhodium, antimony, hafnium and rhenium with recoil energies of several MeV [6].

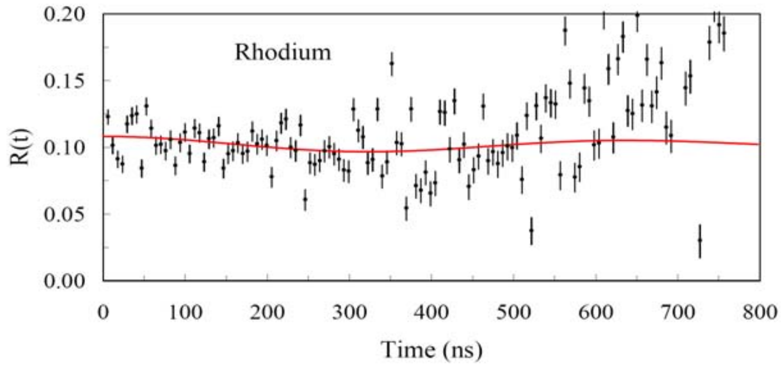

Fig. 2. Measured ratio function *R(t)* and fit for ^{100}Rh in rhodium.

As-implanted samples were studied with TDPAC spectroscopy [7] using a conventional set-up of four conical BaF_2 scintillation detectors forming a planar array with start/stop detector combinations at angles of 90° and 180°. For each detector combination the coincidence time distribution of the two gamma-rays in the 84 keV – 74 keV γ – γ cascade, populating and depopulating the intermediate 2^+ excited state in ^{100}Rh, were recorded using NIM-standard electronics. All time distributions obtained were corrected for statistical background events. The distributions for the 90° detector combinations and those for the 180° detector combinations were averaged, thus compensating for slight differences in detection solid angle and detector efficiency. Finally, using the conventional prescription, the ratio function $R(t) = A_{22}G(t)$ was extracted from the data [8]. The ratio function reflects the gamma-gamma anisotropy A_{22} of the probe and its time-dependent modulation $G(t)$ due to hyperfine interactions. The ratio functions were fitted using the code *Nightmare* which is based on the routine *NNFit* [9]. All fits assumed EFGs with no deviation from axial symmetry employing an axial asymmetry parameter η = 0. The non-physical rise of some measured ratio functions for large times is probably due to a saturation effect in the time-to-analogue converter (TAC). It is most pronounced for rhenium and antimony and is being investigated further.

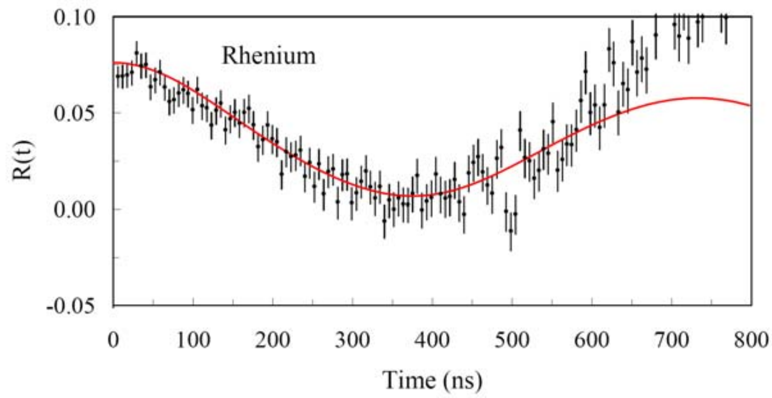

Fig. 3. Measured ratio function *R(t)* and fit for ^{100}Rh in rhenium.

3. Results

Figure 1 shows the measured ratio function $R(t)$ for ^{100}Rh in zinc. Zinc has a hexagonal lattice. It is apparent that

$R(t)$ is modulated as would be expected for a unique EFG with negligible damping. The fit reproduces the observed modulation pattern well with a quadrupole coupling constant of ν_Q = 11.4 MHz. This result agrees with the accepted value [4].

Rhodium has a cubic lattice. As there is no EFG for substitutional probe integration in cubic lattices, the ratio function should show no modulation, but the constant value of the experimental anisotropy. Figure 2 confirms that this is the case.

Rhenium has a hexagonal lattice. Ignoring the spurious effect beyond 600 ns, the data can be well fitted. The fit shown in Figure 3 assumes a quadrupole coupling constant of ν_Q = 3.2 MHz. The rhenium sample was also measured following annealing in argon in a tube furnace at 800°C. After annealing the measured coupling constant was ν_Q = 3.7 MHz.

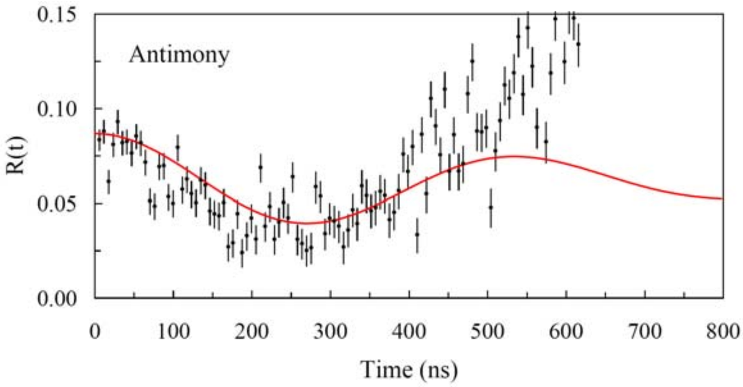

Fig. 4. The measured ratio function *R(t)* and a fit in red for ^{100}Rh in antimony.

Antimony has a rhombohedral lattice. Figure 4 shows that the data may be fitted below 400 ns, beyond which the non-physical rise of the data may be attributed to an artifice of the spectrometer. The fit assumes a quadrupole coupling constant of ν_Q = 4.3 MHz.

Hafnium has a hexagonal lattice. The measured ratio function in Figure 5 shows a slight modulation of the anisotropy. Some damping is apparent which is likely due to implantation induced lattice damage resulting in a non-unique EFG. The fit suggests ν_Q = 5.7 MHz.

4. Summary and Conclusions

The measured quadrupole coupling constants for the 2^+ state in ^{100}Rh have been compiled in Table 1 together with accepted values for zinc, zirconium and ruthenium. The measured value for zinc agrees with expectation. The new measurements for antimony, hafnium and rhenium are similar to accepted values for other transition metals such as zirconium and ruthenium. For example, the measured quadrupole coupling constant of ν_Q = 5.7 MHz is close to the value known for the isoelectronic metal zirconium of ν_Q = 8.1(4) MHz. Moreover, the elements ruthenium and rhenium which are in neighbouring groups in the periodic table both have relatively small quadrupole coupling constants.

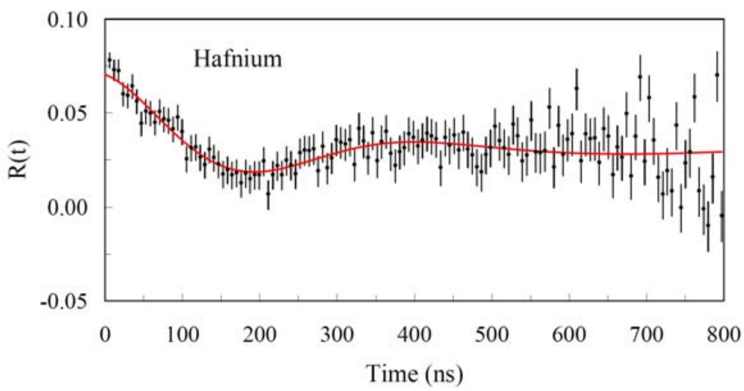

Fig. 5. The measured ratio function *R(t)* for ^{100}Rh in hafnium. The fit with the code *Nightmare* is shown in red.

Table 1. The quadrupole coupling constants measured in this work in comparison with literature values.

transition metal	atomic number Z	axial ratio *c*/*a*	measured ν_Q	accepted ν_Q (from Ref. [4])
Zinc	30	1.856	11.4	*11.4 (2)*
zirconium	*40*	*1.593*	-	*8.1 (4)*
ruthenium	*44*	*1.584*	-	*1.0 (3)*
antimony	51	(rhombohedral)	4.3	-
hafnium	72	1.582	5.7	-
rhenium	75	1.615	3.2	-

Besides confirming the new measurements, without the spurious effect in the ratio function for large times, future work, including measurements following annealing, will aim at establishing uncertainties for the measured quadrupole coupling constants. Measurements of ν_Q for additional transition metals may allow trends to be observed, which would test theory.

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