

Hyperfine interaction study of electric field gradient in hafnium phosphide using ^{181}Ta probe

VIVEK MANDOT, S N A JAAFFREY*, S S SHARMA and J VARMA

Department of Physics, College of Science M L Sukhadia University, Udaipur 313 001, India

* Address for correspondence: 2A, Sector 14, Hiran Magari (Goverdhan Vilas), Udaipur 313 001, India

Email: phy@mlsu.ac.in

MS received 1 May 1997; revised 13 January 1998

Abstract. The hyperfine interaction of ^{181}Ta in HfP has been investigated by time differential perturbed angular correlation method which yielded interaction frequency $\nu_Q = 630.20(15)$ MHz. The observed electric field gradient is calculated to be $1.66(25) \times 10^{20}$ V/m².

Keywords. Electric field gradient; asymmetry parameter; hafnium; phosphorus; hyperfine interaction; interaction frequency; quadrupole interaction; TDPAC.

PACS No.

1. Introduction

In recent years there has been increased interest in the hyperfine interaction studies of electric field gradient in compound systems [1–3]. A number of studies have been made in phosphides to understand the environment of phosphorus in compound such as TiP, ZrP, TaP, NbP, etc. [4]. The environment of the phosphorus in these compounds is more likely the trigonal prism. The tendency of phosphorus towards self-linkage is found only in these phosphorus rich phases in which pairs of atoms or chains usually occur [5, 6]. Authoritative reviews of metal phosphides are available, which cover the studies of the phosphides of group fourth, fifth and sixth and deal with the binary phosphides of all transition metals [7–9].

Moreover titanium and zirconium phosphides, to which the sodium chloride structures are ascribed, are reported to be probably phosphorus deficient [10]. The occurrence of this structure in transition metal monophosphides and the existence of an essentially undistorted octahedral environment for phosphorus in TiP seems to provide a transition from the lanthanide phosphide (all of which have the NaCl type structure) to the transition metal phosphides. Further it suggests that at least some of the phosphorus in group four B compounds could be in the ionic $\text{P}^{(-3)}$ form. Since Hf belongs to group four B and is very similar to Zr and Ti, the hyperfine interaction study was planned to find EFG in HfP system and to investigate if such phosphorus deficient and undistorted octahedral environment for P in HfP exist.

In the present work the hyperfine interaction of the 133 KeV (5/2+) level of ^{181}Ta in hafnium phosphide was studied using time differential perturbed angular correlation (TDPAC) technique. After beta decay, ^{181}Hf transforms into the excited state of ^{181}Ta . Further this excited ^{181}Ta nucleus emits two gamma rays of energies 133 KeV and 482 KeV and comes to ground state. Half-life of the intermediate state of ^{181}Ta is found to be 10.8 ns.

2. Experimental

Hafnium monophosphide systems were prepared by heating together hafnium powder and red phosphorus in sealed quartz tube under vacuum at 900°C for 12 h and quenched in water at 20°C. The TDPAC spectra of the samples were acquired at room temperature using a four counter set up. All spectra turned out to be same in identical conditions. The usual asymmetry ratio of the coincidence spectra at the angles 90° and 180° has been formed in each case. The time resolution of system was found to be 2.3 ns (FWHM). After subtracting the chance coincidence, the ratio $A_{22}G_{22}(t)$ was calculated as defined below

$$A_{22}G_{22}(t) = \frac{2*[W(180, t) - W(90, t)]}{[W(180, t) + 2*W(90, t)]}$$

where $W(180, t)$ and $W(90, t)$ are coincidence counts at angles 180° and 90° respectively and t is the time delay between the two gamma photons. The data in figure 1 were

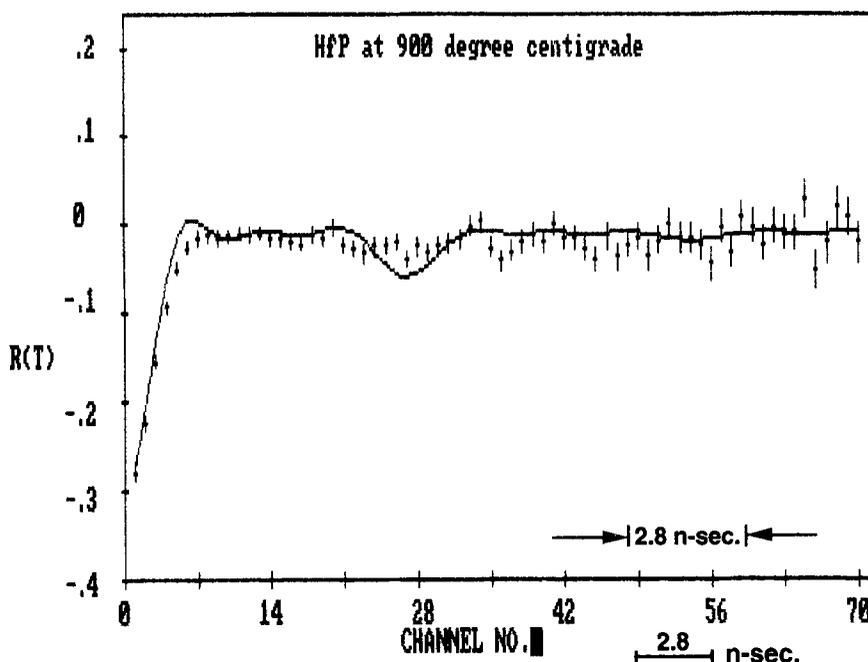


Figure 1. TDPAC spectrum of HfP at 900°C (calibration 0.4 n-sec per channel).

computer analysed using standard function of randomly oriented electric field gradient (EFG) for spin ($5/2+$) keeping the asymmetry parameter as floating [10].

3. Results and conclusion

The figure shows one of the spectra of the sample treated at temperature 900°C which developed into well-defined frequency. Computer analysis yielded frequency 630.20 (15) MHz and very small spread in interaction frequency of 1.5%, which clearly rules out the possibility of phosphorus deficient structure of HfP. From the interaction frequency, EFG in HfP is estimated using Sterheimer antishielding factor $(1 - \gamma_{\infty}) = 62$ [11, 12] and quadrupole moment 2.5 (0.15) barn [13] to be $1.66(0.25) \times 10^{20}$ volt/m². This EFG was compared with theoretically obtained EFG 1.72×10^{20} volt/m² for well known hexagonal closed pack HfP system using lattice parameters $a = 3.65 \text{ \AA}$, $c/a = 3.39 \text{ \AA}$ and phosphorus in $\text{P}^{(-5)}$ form [14–16]. The consistency between the observed and computed EFG's allowed us to draw conclusion about the phosphorus ionic form in HfP system to be more likely the $\text{P}^{(-5)}$ rather than the $\text{P}^{(-3)}$ form.

Moreover the high value of $A_{22}(t) = -0.25$ at $t = 0$ and asymmetry parameter $\eta = 0$ also support the strong quadrupole interaction of ^{181}Ta with EFG in HfP and non-existence of undistorted environment. The inherent value of $\lambda = -0.015$ could probably be attributed to the relaxation of charges in the system during beta decay of ^{181}Hf nuclei. It could be explained by the time dependent electric quadrupole interaction during charge neutralization process of ions ($\tau = 5 \times 10^{(-8)}$ s) [17].

Acknowledgement

The authors are thankful to Drs Gufran Beig and K Venugopalan for valuable discussion and computer analysis of data.

References

- [1] A Lerf and T Butz, *Hyperfine Interaction* **36**, 275 (1987)
- [2] J W Ball and M Kaplan, *J. Chem. Phys.* **69**, 117 (1978)
- [3] A Baudry, P Boyer and J P Boilot, *Solid State Commun.* **56**, 91 (1985)
- [4] *M T P International Review of Science (Inorganic Chemistry Series One) Transition Metals – Part 1* edited by W A Sharp (University Park Press, Baltimore, 1972) vol. 5, pp. 152–162
- [5] P O Snell, *Acta chem. Scand.* **21**, 1773 (1967)
- [6] N Schonberg, *Acta chem. Scand.* **8**, 226 (1954)
- [7] T Lundström, *Ark. Kemi.* **31**, 227 (1969)
- [8] S Rundquist, *Ark. Kemi.* **20**, 67 (1963)
- [9] I Engström, *Thesis* (University of Uppsala, 1970)
- [10] R Steffen and H Frauenfelder, *Alpha, beta and gamma ray spectroscopy* edited by Kai Siegbahn (North-Holland Publishing Company, Amsterdam, 1965), vol. 2, p. 997
- [11] K Sen and P T Narasimhan, *Phys. Rev.* **B15**, 96 (1977)
- [12] F D Feiock and W R Johnson, *Phys. Rev.* **187**, 39 (1969)
- [13] G Netz and E Bodenstedt, *Nucl. Phys.* **A208**, 503 (1973)
- [14] W B Pearson, *A hand book of lattice spacings and structures of metals and alloys* (Pergamon Press Ltd., 1967) vol. 2, p. 278

- [15] R P Sharma, M B Kurup and K G Prasad, *Hyperfine interactions* **4**, 622 (1978)
- [16] P Jena, S D Mahanti and T P Das, *Phys. Rev.* **137**, 973 (1973)
- [17] A Weiss, *Magnetic resonance and relaxation* edited by R Blinc (North Holland, Amsterdam, 1967) pp. 1076