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Publication Date
1972-03-01

Submitted to Physics Letters A

LBL-641
Preprint

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March 1972

AEC Contract No. W-7405-eng-48

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ELECTRIC QUADRUPOLE INTERACTION OF Ta-181 IN HEXAGONAL TRANSITION METALS[†]

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March 1972

The electric quadrupole interaction of ^{181}Ta impurity atoms in the hexagonal transition metals Re, Os, Hf, and Ru has been studied at room temperature. From the resolved Mössbauer absorption spectra values for the electric field gradients at the ^{181}Ta nucleus and for the isomer shifts of the 6.2 keV gamma rays were obtained.

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Recently, the electric quadrupole hyperfine splitting of the 6.2 keV gamma rays of ^{181}Ta has been observed for the first time, using a source of ^{181}W diffused into single-crystal Re metal [1]. From the completely resolved Mössbauer spectra the ratio of the electric quadrupole moments, the electric quadrupole interaction (EQI) of ^{181}Ta in Re metal, and the isomer shift (IS) of the 6.2 keV gamma rays of ^{181}Ta(Re) relative to Ta metal were derived. The high potential resolution inherent in the 6.2 keV gamma resonance, when applied to the study of EQI's, has thus clearly been demonstrated. It is a consequence of the small natural linewidth of the 6.2 keV gamma rays ($2\frac{\hbar}{\tau} = 0.0065$ mm/s) and the large electric quadrupole moments of the ^{181}Ta nucleus in both nuclear states [1].

[†]Work performed under the auspices of the U. S. Atomic Energy Commission.

In the present paper we report on measurements of the hyperfine spectra of the 6.2 keV gamma rays in sources of ^{181}W diffused into single crystal Hf metal, and polycrystalline Os and Ru metal. The Mössbauer experiments were performed at room temperature in the same way as described previously [1], and a Ta metal foil (4 mg/cm^2) was used as a single line absorber.

Some typical velocity spectra are presented in fig. 1: in (a) for a single-crystal ^{181}W(Re) source with direction of observation perpendicular to the [0001]-direction [1], in (b) for a polycrystalline ^{181}W(Os) source, and in (c) for a polycrystalline ^{181}W(Ru) source. For the assignment of individual transitions to the observed lines we refer to ref. 1. From least-squares fits of a superposition of dispersion-modified Lorentzian lines [2] to the data, values for the EQI of the ^{181}Ta ground-state, $e^2qQ(7/2)$, and for the IS of the 6.2 keV gamma rays were obtained. In all cases, the electric field gradients (EFG) were assumed to be axially symmetric. The amplitude of the dispersion term, $2\xi = 0.30\pm0.01$ [2], and - for the Os, Ru, and Hf spectra - the ratio of the electric quadrupole moments $Q(9/2)/Q(7/2) = 1.133\pm0.010$ [1], were kept constant during the fit procedure.

The experimental results, including those for Re metal (from ref. 1), are summarized in table 1. The observed ISs cover a range of 27 mm/s, and fit well in the systematics found for ^{181}Ta impurities in host metals of the d-transition elements [3]. Despite the fact that the total experimental linewidths are still from ~ 100 times (Re) to ~ 300 times (Os) wider than the natural linewidth, the obtained resolution is rather good. The values for the z-component eq of the axially symmetric EFG, given in column 3, were obtained with $Q(7/2) = +3.9\pm0.4$b [4] for the electric quadrupole moment of the

groundstate of ^{181}Ta, and the error bars of eq are mainly due to the 10% uncertainty in Q(7/2). For all the studied cases the sign of eq was also determined.

Presently, no satisfactory theory exists for EFG's in hexagonal transition metals. Our result shows that a simple "point-ion and uniform background model" [5] alone is not sufficient, since the EFGs calculated with its help are positive for all the studied metals, while the experimental values are negative for Re, Os, and Ru. Such a model considers only the lattice contribution q_{latt} to the EFG. Obviously, the local contributions, caused by a non-uniform arrangement of localized charge around the central atom, as well as by a non-uniform distribution of conduction electrons within the central cell, play an essential role. The latter effect has been discussed by Watson et al. [6], who predicted an "overshielding effect", caused by the conduction electrons, especially in cases with a high density of states at the Fermi energy. According to them this local conduction electron contribution should be linearly related to the lattic field gradient, $q_{loc} = r.q_{latt}$, so that we may write for the total EFG $q = q_{latt}[1 - \gamma_\infty) + r(1 - R_Q)]$, where γ_∞ and R_Q are the lattice and atomic Sternheimer factors, respectively. With $\gamma_\infty \sim -60$ [7] and $R_Q \sim -0.2$ [8] for Ta, and using q_{latt} values calculated with ref. 5, we may derive overshielding factors r of -160, -85, and -75 for Ta in Re, Os, and Ru, respectively. These values are not too different from those predicted for the pure metals, $r \sim -100$ for Re, and $r \sim -55$ for Os [6].

On the other hand, the EFG for ^{181}Ta(Re) is positive and even bigger than $q_{latt}(1 - \gamma_\infty)$, and its temperature dependence, measured by TDPAC of the $5/2^+$-state at 482 keV of ^{181}Ta [9], is well described by the anisotropic

variation of the lattice parameters with temperature. This means that in this case the lattice contribution may play an essential role. In order to clarify the situation further, a study of the temperature dependence of the EFG for these host metals is under way.

The authors would like to thank Prof. D. A. Shirley for his constant interest.

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Table 1. Summary of experimental results, obtained for the EQI of the ground-state of ^{181}Ta, $e^2qQ(7/2)$, the EFG eq at the Ta nucleus, the IS relative to Ta metal, and the total experimental linewidth W.

host	$e^2qQ(7/2)$ (10^{-6} eV)	eq (10^{17} V/cm^2)	IS (mm/s)	W (mm/s)
Re	-2.15±0.02	-5.5±0.5	-14.0±0.1	0.60±0.04
Os	-2.35±0.04	-6.0±0.7	-2.9±0.2	1.8 ±0.2
Hf	+1.83±0.10	+4.7±0.7	-0.6±0.3	1.6 ±0.4
Ru	-1.56±0.04	-4.0±0.5	-27.6±0.3	1.3 ±0.2

Figure Caption

Fig. 1. Mössbauer absorption spectra of the 6.2 keV gamma rays of ^{181}Ta for sources of ^{181}W(Re) (a), ^{181}W(Os) (b), and ^{181}W(Ru) (c), analyzed with a single-line absorber of Ta metal.

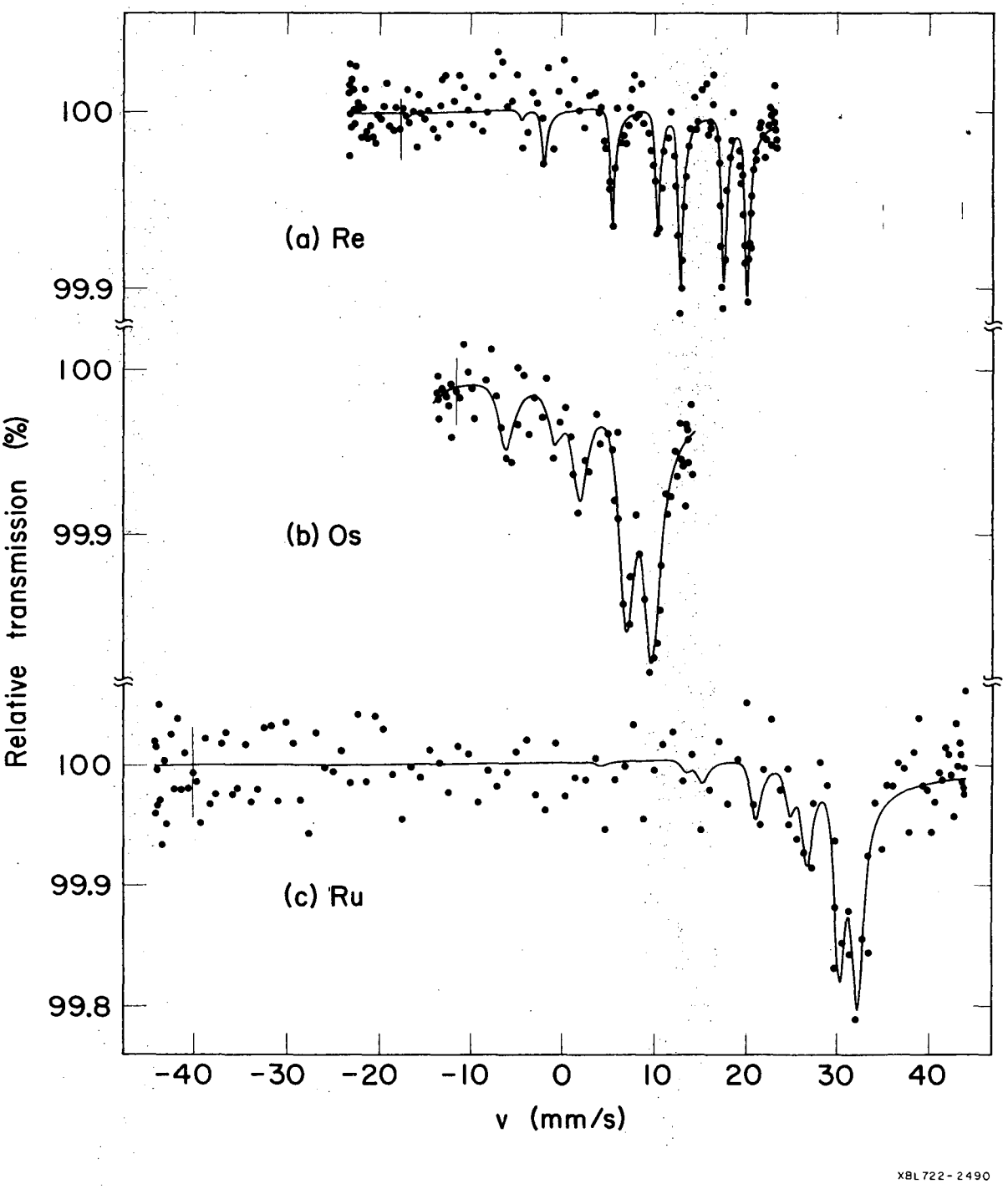
100
99.9
(a) Re
100
99.9
(b) Os
100
99.9
99.8
(c) Ru
Relative transmission (%)
-40
-30
-20
-10
0
10
20
30
40
v (mm/s)
XBL722-2490

Fig. 1

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