

Mössbauer Effect at High Pressure for Fe<sup>57</sup> in Titanium, Vanadium, and Copper\*

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We have measured the effect of pressure to 250 kbar on the isomer shift of Fe<sup>57</sup> in dilute solution in titanium, vanadium, and copper. These results and previously published data on Fe<sup>57</sup> in iron indicate that for the bcc metals of the first transition-metal series, the 4s-electron density scales approximately with bulk density. For more closely packed phases the s-electron density changes less rapidly than the bulk density.

## I. INTRODUCTION

RECENTLY, Mössbauer experiments with Fe<sup>57</sup> in iron at high pressure have been done by Pound and Nicol and Jura,<sup>2</sup> and by Pipkorn *et al.*<sup>3</sup> The isomer-shift data obtained by these authors for the face-centered-cubic (fcc) phase of iron indicate that a change in lattice parameter up to 2% the only effect of the applied pressure is to scale the Fe<sup>57</sup> 4s-electron density proportional to the bulk density without affecting the 3d electrons. The experiments reported here show that the same behavior is found for a solid solution of Fe<sup>57</sup> in bcc vanadium, whereas the solid solutions of Fe<sup>57</sup> in titanium and in copper show a more complicated behavior.

The isomer shift  $\epsilon$  is defined as the difference in energy between the centers of gravity of the emission and of absorption lines.<sup>4</sup> It is here expressed in terms of the Doppler velocity at resonance measured with a stainless steel absorber. As pointed out by Pound *et al.*<sup>1</sup> The pressure coefficient of the isomer shift consists of a small contribution arising from the change in vibrational energy, which will be neglected, and of a term arising from the change in electron density at the Fe<sup>57</sup> nucleus,

$$\left(\frac{\partial \epsilon}{\partial p}\right)_T = \text{const} \left(\frac{\partial \psi(0)^2}{\partial(V/V_0)}\right)_T \left(\frac{\partial(V/V_0)}{\partial p}\right)_T. \quad (1)$$

Walker, Wertheim, and Jaccarino<sup>4</sup> have given a relationship between isomer shift and electron density. With their sign convention an increase in s-electron density corresponds to a decrease in isomer shift. If the electron density scales with volume  $V$ , the isomer shift due to the 4s electrons only will vary as<sup>3</sup>

$$\frac{\partial \epsilon}{\partial(V/V_0)} = 0.14 \text{ cm/sec}. \quad (2)$$

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<sup>1</sup> V. Pound, G. B. Benedek, and R. Drever, *Phys. Rev.* **123**, 7405 (1961).

<sup>2</sup> M. Nicol and G. Jura, *Science* **141**, 1035 (1963).

<sup>3</sup> N. Pipkorn, C. K. Edge, P. Debrunner, G. De Pasquali, H. G. Drickamer, and H. Frauenfelder, *Phys. Rev.* **135**, A1604 (1964).

<sup>4</sup> R. Walker, G. K. Wertheim, and V. Jaccarino, *Phys. Rev.* **123**, 698 (1961).

## II. EXPERIMENT

The method of source preparation was essentially identical with that described by Pipkorn *et al.*<sup>3</sup> Radioactive Co<sup>57</sup> was introduced into small foils of the sample metal by plating and diffusion. In all cases the concentration of Co<sup>57</sup> plus carrier was less than 1%. The absorber used was the same stainless steel foil enriched in Fe<sup>57</sup> used in the work on iron. The high-pressure cell and Mössbauer spectrometer are also described in detail by Pipkorn *et al.*<sup>3</sup> The isomer shifts were obtained by computer from a least-squares analysis of the experimental Mössbauer spectra.

## III. RESULTS

The isomer shifts at zero pressure for Fe<sup>57</sup> in the three host metals used in this study are listed in Table I.<sup>5</sup>

TABLE I. Atmospheric-pressure isomer shift for Fe<sup>57</sup> in various transition metals—relative to stainless steel absorber.

Metal	$\epsilon_0$ (cm/sec)
Ti	-0.0110 ± 0.0004
V	-0.0155 ± 0.0003
Fe	+0.0086 ± 0.0005
Cu	+0.029 ± <0.001

For comparison we also give the isomer shift at zero pressure relative to the same absorber for Fe<sup>57</sup> in iron.<sup>3</sup> Figure 1 shows the isomer shift versus pressure for Fe<sup>57</sup> in copper, titanium, and vanadium. Copper crystallizes in the face centered cubic (fcc) structure. Titanium is hexagonal close packed (hcp) at low pressure, but near 80-85 kbars it transforms (quite sluggishly) to a distorted cubic structure.<sup>6</sup> Vanadium crystallizes in the bcc structure as does iron below 130 kbar. At higher pressures iron assumes the hcp structure.

Figures 2 and 3 show the isomer shifts versus fractional volume change for the three host lattices plus that for pure iron. For iron the density data of Clendenen

<sup>5</sup> Here we use the sign convention that the velocity is positive when the absorber is moving away from the source. Thus as in conventional experiments with Fe<sup>57</sup> in which one varies the isomer shift of the absorber, a negative change in the isomer shift indicates increasing s-electron density at the nucleus.

<sup>6</sup> J. C. Jamieson, *Science* **140**, 72 (1963).