

Effect of uniaxial tensile stress on the isomer shift of ⁵⁷Fe in fcc stainless steels

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The electron wave-function response to uniaxial tensile stress in fcc steels (SS310 and SS316) was investigated through the isomer shift of the Mössbauer effect. Stresses up to 12 kbar (the ultimate tensile stress is approximately 14 kbar) were applied at room temperature. The isomer shift changes linearly in these circumstances. It is concluded that, as in the case of hydrostatic pressure, the paramount factor here is the volume strain of the wave functions of 4*S* electrons.

I. INTRODUCTION

The effect of hydrostatic pressure on the isomer shift (IS) has been the subject of extensive research.¹ Because of the extremely low sensitivity involved, and of inadequate accuracy in the spectra analysis, long counting time and high-pressure levels (over 15 kbar in α -Fe) were needed to produce measurable¹ IS values [over 0.01 mm/sec in α -Fe (see Table I)].

The changes of IS in Mössbauer-effect measurements are proportional to those in *S*-electron density $\rho(0)$ (also called contact electron density) at the

nuclei in an absorber or a source. Variation of $\rho(0)$ in compressed metals, alloys, and compounds is seen to involve several mechanisms, whose relative weight dictates the corresponding volume dependence. The main factors affecting the density of the 4*S* electrons are: (i) reduction of the crystal-lattice parameters² (volume scaling model) which is the paramount effect in a wide variety of transition²⁻¹⁰ and noble⁹ metals, (ii) screening of the 3*S* by the 3*d* electrons^{3,5,9} (a few percent at most), and possibly (iii) transitions from *s* to *d* states in the conduction band.^{3,5,9}

In contrast to the extensive work done on the

TABLE I. Shows the results of this and other investigations concerning the effect of stresses on the isomer shift.

Matrix	SS310	SS316	Stainless steel 1K \bar{h} 18N 9T	α -Fe
σ_t (unitest) ^a	σ_t	σ_t	σ_h	σ_h
σ_h (hydrostatic stress) (pressure)				
Crystal structure	fcc	fcc	fcc	bcc
β (compressibility) (10 ⁻⁴ kbar ⁻¹)	6.1±0.07	6.4±0.07	6.1±0.1	5.95
$\frac{\partial \Delta_{IS}}{\partial \sigma}$ (10 ⁻⁴ mm/sec kbar ⁻¹)	3.4	3.4	-10.1	-(7.5-9.1)
$\frac{\partial \Delta_{IS}}{\partial \ln V}$ mm/sec	experimental	1.66±0.1	1.59±0.1	1.6±0.1
	theoretical	1.50±0.1	1.49±0.1	1.54
$\partial \Delta_{IS}$ (mm/sec, relative to α -Fe) $\sigma=0, T_{room}$	-0.1	-0.09		0
<i>X</i> (number of 4 <i>S</i> electrons)	1.071	1.064	1.1	1
References	This work and 17	This work and 17	10	2-6

^aUniaxial tensile stress.

hydrostatic case, IS behavior under nonhydrostatic conditions was studied and analyzed on a more limited scale. The unitest (uniaxial tensile stress) case, which is confined to the 5–15-kbar range for various steels, was considered in several works^{11–13} but no theoretical analysis was attempted. Such an analysis would permit comparison with hydrostatic results, clear up the question as to the mechanism of $\rho(0)$ change under unitest conditions, and make it possible to evaluate the role of nonhydrostatic stress components, accompanying high-pressure hydrostatic experiments.

The present work, undertaken with the above ideas in mind, is concerned with applicability of the volume scaling model under unitest conditions. Results are discussed on the basis of the theory of elasticity and of the compressibility of the wave function of the 4*S* electrons. The amount of the latter was obtained from the IS calibration curve¹⁴ for the electronic configuration $3d^7 4s^x$. Mössbauer spectra were analyzed by means of a new quantitative analysis of difference spectrum (QADS) method, developed by the authors¹⁵ and already used for residual stress measurements in an overstrained cylinder.¹⁶ The method yields high accuracy of $\pm(0.1-0.2)$ kbar in a relatively short counting time.

II. EXPERIMENTAL

The Mössbauer effect was investigated at room temperature under unitest conditions in SS310 (Ref. 17) and SS316 (Ref. 17) [the lattice structure is fcc (γ -Fe), with a random distribution of Fe atoms] and stress levels up to 10 and 12.4 kbar, respectively. The source was 10 mCi ^{57}Co in a palladium matrix. The Mössbauer effect was approximately 30% in SS310 (foil thickness 28 μm) and 12.5% in SS316 (7.5 μm). The number N_∞ of "off-resonance" counts was approximately 2×10^5 and 4×10^5 , respectively.

III. RESULTS AND DISCUSSION

The Mössbauer spectra of both steels consist of a single broad line shifted under unitest conditions (positive shift values due to volume expansion). Figures 1 and 2 present the dependence of the IS on stress σ_t , which may be regarded as linear within the limits of experimental error. Our own results, and those of other investigations, are given in Table I. The slopes $\partial\Delta_{\text{IS}}/\partial\ln\sigma_t$, determined

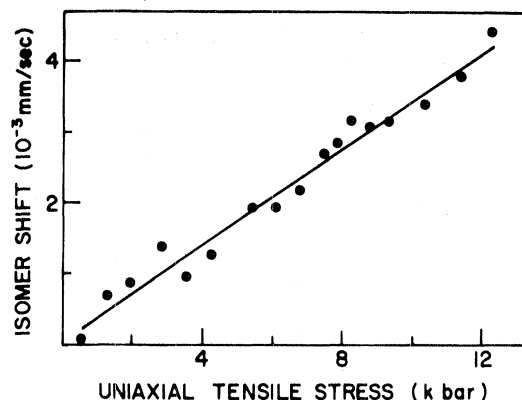


FIG. 1. Isomer shift of SS310 vs uniaxial tensile stress.

through a least-squares fit of the data yielded the volume dependence $\partial\Delta_{\text{IS}}/\partial\ln V_t$ required for the analysis which follows.

Letting σ_t lie along the x axis, we have according to the theory of elasticity:

$$\epsilon_x = \frac{1}{E}\sigma_t, \quad \epsilon_y = \epsilon_z = -\frac{\nu}{E}\sigma_t,$$

where E is Young's modulus, ν is Poisson's ratio, and $\epsilon_x, \epsilon_y, \epsilon_z$ are the principal strains (the others are zero). The relative volume is given by

$$\begin{aligned} \Delta\ln V_t &= \left[\frac{\Delta V}{V} \right]_t = \epsilon_x + \epsilon_y + \epsilon_z \\ &= \frac{1-2\nu}{E}\sigma_t = \frac{1}{3}\beta\sigma_t, \end{aligned} \quad (1)$$

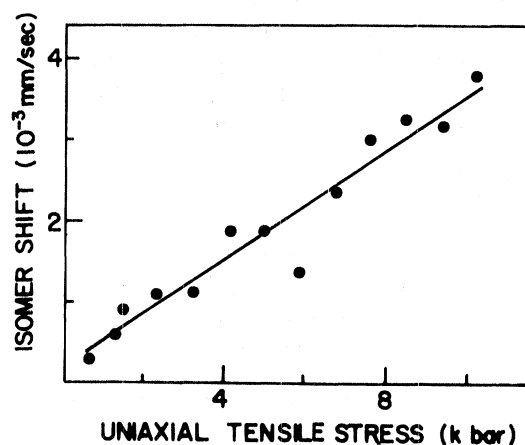


FIG. 2. Isomer shift of SS316 vs uniaxial tensile stress.

where β is the compressibility. With the aid of Eq. (1), we find the relation between $\partial\Delta_{IS}/\partial\sigma_t$ and $\partial\Delta_{IS}/\partial\ln V_t$,

$$\frac{\partial\Delta_{IS}}{\partial\sigma_t} = \frac{\partial\Delta_{IS}}{\partial\ln V_t} \frac{d\ln V_t}{d\sigma_t} = \frac{1}{3}\beta \frac{\partial\Delta_{IS}}{\partial\ln V_t}, \quad (2)$$

$$\frac{\partial\Delta_{IS}}{\partial\ln V_t} = \frac{3}{\beta} \frac{\partial\Delta_{IS}}{\partial\sigma_t}.$$

For a hydrostatic stress σ_h , we have

$$\frac{\partial\Delta_{IS}}{\partial\ln V_h} = \frac{1}{\beta} \frac{\partial\Delta_{IS}}{\partial\sigma_h}. \quad (3)$$

By Eqs. (2) and (3), the IS change expected in the unitest should be as small as one-third of its value for the corresponding hydrostatic pressure. Table I shows this to be the case for $\partial\Delta_{IS}/\partial\sigma_t$ and $\partial\Delta_{IS}/\partial\sigma_h$ for the three stainless steels despite the differences in their chemical composition.

As regards electron response, we assume that the unitest effect is due to strain of the 4S conduction electrons and there is no *s-d* transfer, and moreover that their density at the nucleus, $\rho_{4S}(0)$ scales inversely with volume²:

$$\frac{\partial\ln\rho_{4S}(0)}{\partial\ln V_t} = -1. \quad (4)$$

With the aid of Eq. (4) we get

$$\frac{\partial\Delta_{IS}}{\partial\ln V_t} = \frac{\partial\Delta_{IS}}{\partial\ln\rho_{4S}(0)} \frac{d\ln\rho_{4S}(0)}{d\ln V_t} = \frac{-\partial\Delta_{IS}}{\partial\ln\rho_{4S}(0)}. \quad (5)$$

Suppose that in our case an increase and/or decrease of $\rho_{4S}(0)$ is equivalent, in terms of its influence on the IS, to addition and/or subtraction of 4S electrons. That is, denoting by X the number of 4S electrons per atom, then $\rho_{4S}(0) = KX$ (where K is a proportionality factor) and

$$\frac{\partial\ln X}{\partial\ln\rho_{4S}(0)} = 1. \quad (6)$$

In the above, shielding and other effects are disregarded for simplicity, but Eq. (6) is justified so long as our model is in agreement with experimental results. In turn, it yields

$$\frac{\partial\Delta_{IS}}{\partial\ln\rho_{4S}(0)} = \frac{\partial\Delta_{IS}}{\partial\ln X} \frac{d\ln X}{d\ln\rho_{4S}(0)} = \frac{\partial\Delta_{IS}}{\partial\ln X}. \quad (7)$$

In iron alloys and compounds with electronic configuration $3d^7 4s^X$, a change ΔX induces a

change in the isomer shifts, $\partial\Delta_{IS}$, such that¹⁴

$$\partial\Delta_{IS} = -1.4\Delta X \quad (8)$$

in units of mm/sec. From (5), (7), and (8) we get

$$\frac{\partial\Delta_{IS}}{\partial\ln V_t} = 1.4X. \quad (9)$$

Using the known IS for unstrained stainless steels (the shift of the center of gravity of the Mössbauer line, Table I) relative to α -Fe, Eq. (8) yields the number X of 4S electrons:

$$\Delta X_{SS310} = \frac{-\partial\Delta_{IS}}{1.4} = \frac{0.1}{1.4} \approx 0.071,$$

whence

$$X_{SS310} = 1 + 0.071 = 1.071,$$

and similarly

$$X_{SS316} = 1.064,$$

it being assumed that α -Fe has a single 4S electron.^{3,14}

Table I shows that the values of $\partial\Delta_{IS}/\partial\ln V_t$ according to Eq. (9) agree with their measured counterparts [Eq. (2)] within the limits of uncertainty. The main uncertainty in Eq. (9) involves the accuracy of the measured¹⁴ number 1.4, which is $\partial\Delta_{IS}/\Delta X$ in Eq. (8). Setting this error at about 5–10% and recalling that $X \approx 1$, we have from Eq. (9), in mm/sec:

$$\left| \Delta \frac{\partial\Delta_{IS}}{\partial\ln V_t} \right| \approx X \left| \Delta \frac{\partial\Delta_{IS}}{\Delta X} \right| \sim 0.1.$$

Experimental uncertainties are given in accordance with their fit to the data of Fig. 1 and 2.

IV. CONCLUSION

It is apparent that within the studied unitest range, volume scaling of the 4S electrons is the paramount factor. Contributions to IS due to nonhydrostatic stress components in high-pressure experiments may also be evaluated by the volume-scaling model.

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