Magnetic moment of iron in Laves phases

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The nuclear magnetic resonance (NMR) method has been used to measure the shifts of the resonant frequencies of iron and yttrium nuclei in YFe_2 compounds at a pressure of 10 kbar. The magnetic moment of iron is divided into local and collectivized parts.

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Measurements of the hyperfine fields in Fe^{57} nuclei in RFe_2 intermetallic compounds, where R are rare earths ranging from Pr to Lu, show[1] that the iron atoms in these alloys retain a constant magnetic moment in first approximation. This result is considered as a confirmation of the almost complete localization of the atomic magnetic moment of iron. On the other hand, measurements of the magnetization of alloys of various stoichiometries (from RFe_2 to R_2Fe_{17}) indicate that the Curie tem-

TABLE I.

Nucleus	NMR frequency at $P=0$ [MHz]	NMR frequency at 10 kbar [MHz]
Y^{89}	45,90	46,37
Fe^{57}	28,80	28,54

perature decreases as the molar content of iron increases; this has occasionally been related to a decrease in the delocalized part of the magnetic moment of a 3*d* metal.[2,3] However, practical attempts to estimate the degree of this delocalization have not been undertaken until now, primarily because of a lack of experimental data that would make it possible to separate the "local" part from the collectivized part of the magnetic moment μ_{Fe}.

We made the first attempt to achieve such separation on the basis of a study of the influence of a high hydrostatic pressure on the nuclear magnetic resonance (NMR) frequency of the intermetallic compound YFe_2, in which the magnetic ordering is determined by one kind of atoms. The NMR spectra of Y^{89} and Fe^{57} nuclei were traced on a spin-echo spectrometer at 4.2 K. The hydrostatic pressure up to 10 kbar was produced in a beryllium-bronze chamber. The errors in the measurement of pressure did not exceed 5%, and the errors in the measurement of frequency did not exceed 0.1%. The frequency stability of the master oscillator and of the reference heterodyne was at least 10^{-5} during the measurements. The measurement results are given in Table I.

We can see in Table I that the applied pressure shifts the resonance frequencies of Y^{89} and Fe^{57} in opposite directions: the NMR frequency of Y^{89} increases with increasing pressure, and the NMR frequency of Fe^{57} decreases.

This is due to the fact that the hyperfine field H_{hf}^{Fe} in the iron atoms is directly proportional to the magnetic moment μ_{Fe} of the atoms, while the fields H_{hf}^{Y} in the nuclei of nonmagnetic yttrium ions are attributable to the influence of collectivized electrons.[4,5]

Thus, we can write

$$H_{hf}^{Fe} = A_{hf}^{Fe}\,\mu_{Fe}, \tag{1}$$

$$H_{hf}^{Y} = A_{hf}^{Y}\,\mu_{col}. \tag{2}$$

Here μ_{col} is the magnetic moment of collectivized electrons. It is clear that $\mu_{Fe} = \mu_{loc} \pm \mu_{col}$, where μ_{loc} is the localized part of the magnetic moment of the atoms. To explain the opposite tendencies in the variation of the hyperfine fields in the yttrium and iron nuclei, we must assume that $\mu_{Fe} = \mu_{loc} - \mu_{col}$. Thus, the increase of H_{hf}^{Y} with pressure is due to the increase of the quantity μ_{col}. This increase of μ_{col} leads to a decrease in the magnetic moment of iron and, in turn, to a decrease of the hyperfine field in the iron nuclei.

The total hyperfine field at a high pressure can be represented in the form

$$[H_{hf}^{Fe}]_p = [A_{hf}^{Fe}]_p(\mu_{loc} - \mu_{col} - \Delta\mu_{col}), \quad (3)$$

$$[H_{hf}^{Y}]_p = [A_{hf}^{Y}]_p(\mu_{col} + \Delta\mu_{col}), \quad (4)$$

where $[A_{hf}^{Fe}]_p$ and $[A_{hf}^{Y}]_p$ are the values of the hyperfine constants at a pressure of 10 kbar, and $\Delta\mu_{col}$ is the change in μ_{col} with pressure.

Comparing Eqs. (1) and (3), as well as Eqs. (2) and (4), we obtain

$$\frac{[H_{hf}^{Fe}]_o}{[H_{hf}^{Fe}]_p} = \frac{[A_{hf}^{Fe}]_o(\mu_{loc} - \mu_{col})}{[A_{hf}^{Fe}]_p(\mu_{loc} - \mu_{col} - \Delta\mu_{col}}, \quad (5)$$

$$\frac{[H_{hf}^{Y}]_o}{[H_{hf}^{Y}]_p} = \frac{[A_{hf}^{Y}]_o\,\mu_{col}}{[A_{hf}^{Y}]_p(\mu_{col} + \Delta\mu_{col})}. \quad (6)$$

The value of μ_{col} can be easily determined from Eqs. (5) and (6)

$$\mu_{col} = \frac{[H_{hf}^{Y}]_o[A_{hf}^{Y}]_p\{[H_{hf}^{Fe}]_o[A_{hf}^{Fe}]_p - [H_{hf}^{Fe}]_p[A_{hf}^{Fe}]_o\}\mu_{Fe}}{[H_{hf}^{Fe}]_o[A_{hf}^{Fe}]_p\{[H_{hf}^{Y}]_p[A_{hf}^{Y}]_o - [H_{hf}^{Y}]_o[A_{hf}^{Y}]_p\}}. \quad (7a)$$

It is easy to evaluate this expression numerically in two limiting cases: when the change in the hyperfine field is caused entirely by the change in the hyperfine constant and, conversely, when these constants remain unchanged and the shift of the resonance frequencies due to pressure is attributed only to a change in the magnetic moment.

It seems that the representation (7a) has no meaning in the first case, since

$$\frac{[H_{hf}^{Fe}]_p}{[H_{hf}^{Fe}]_o} = \frac{[A_{hf}^{Fe}]_p}{[A_{hf}^{Fe}]_o}, \quad \frac{[H_{hf}^{Y}]_p}{[H_{hf}^{Y}]_o} = \frac{[A_{hf}^{Y}]_p}{[A_{hf}^{Y}]_o}$$

and the quantity μ_{col} is undefined.

In the second case $[A_{hf}^{Y}]_p = [A_{hf}^{Y}]_o$ and $[A_{hf}^{Fe}]_p = [A_{hf}^{Fe}]_o$ and Eq. (7a) has a simpler form

$$\mu_{col} = \frac{[H_{hf}^{Y}]_o\{[H_{hf}^{Fe}]_o - [H_{hf}^{Fe}]_p\}\mu_{Fe}}{[H_{hf}^{Fe}]_o\{[H_{hf}^{Y}]_p - [H_{hf}^{Y}]_o\}}. \quad (7b)$$

By substituting the experimental values of $[H_{hf}^{Fe}]_p$, $[H_{hf}^{Fe}]_o$, $[H_{hf}^{Y}]_p$, $[H_{hf}^{Y}]_o$, and[6] $\mu_{Fe} = 1.45\,\mu_B$ in this expression, we find that μ_{col} is equal to $1.25\,\mu_B$. It follows from measurements of the magnetization that $\mu_{loc} = \mu_{col} + \mu_{Fe} = 2.7 \pm 0.3\,\mu_B$. Generally, the hyperfine field changes because of the action of both factors, but at pres-

sures up to 10 kbar we can assume that a decrease in volume is due primarily to a change in the interatomic spacing, rather than due to a deformation of the electronic shells of the atoms. This is consistent with the data of our previous measurements,[7] which showed that a change in the hyperfine constants with pressure is at least an order of magnitude smaller than the change in the magnetic moment.

Thus, by using the NMR method under a pressure we have been able to separate the localized part from the collectivized part of the magnetic moment of iron. The obtained results open up new possibilities for studying the nature of the moment of 3*d* metals in intermetallic compounds.

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