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LETTER TO THE EDITOR

A ^{57}Fe high-pressure Mössbauer study of the ferromagnetic intermetallic compound $\text{Gd}_2\text{Fe}_{17}$

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Abstract. The effect of pressure up to 5.5 GPa on the magnetic behaviour of $\text{Gd}_2\text{Fe}_{17}$ has been investigated using the ^{57}Fe high-pressure Mössbauer effect technique. We show that the decrease of the average magnetic hyperfine field at 300 K can be well explained by the decrease of Curie temperature with pressure, while the Fe local magnetic moment remains almost stable in this pressure range. The decrease of the isomer shift with increasing pressure indicates a corresponding increase of the *s*-electron density at the ^{57}Fe nucleus, which is mainly caused by the volume compression of the 4*s* conduction electrons.

Recently, the interstitial rare-earth (R) iron compounds have attracted more interest because of their possible application as permanent magnet materials [1-6]. It has been shown that the magnetic properties of R_2Fe_{17} compounds can be greatly improved by interstitial atoms of carbon [1-3] and nitrogen [4-6]. The interstitial atoms cause an expansion of the unit-cell volume (e.g. about 6-7% for $\text{R}_2\text{Fe}_{17}\text{N}_{3-8}$) [6], and thereby give rise to large values of the magnetization, uniaxial anisotropy, Curie temperature (T_C) and coercivity. Therefore, the study of these compounds under high pressure—by which the volume of the unit cell can be reduced—is very helpful for obtaining a deeper understanding of the influence of the interstitial atoms on the magnetic properties.

In this work, we have used the ^{57}Fe high-pressure Mössbauer effect (ME) technique (up to 5.5 GPa and at 300 K) in order to investigate the effect of pressure on the magnetic and electronic properties of the $\text{Gd}_2\text{Fe}_{17}$ compound. The ^{57}Fe high-pressure ME spectroscopy offers us the possibility of investigating pressure-induced changes of the magnetic properties (via the effective magnetic hyperfine (HF) field at the ^{57}Fe nuclei, B_{eff}) and of the electronic properties (via the ME isomer shift, *S*).

The ingot of $\text{Gd}_2\text{Fe}_{17}$ was prepared by arc melting of iron (purity 99.99%) and gadolinium (purity 99.9%) in a pure argon atmosphere; followed by annealing at 980 °C in a vacuum of 10^{-5} Torr for about 14 h. The x-ray diffraction pattern obtained using $\text{Co K}\alpha$ radiation shows that $\text{Gd}_2\text{Fe}_{17}$ is single phase with the $\text{Th}_2\text{Zn}_{17}$ -type structure. The ^{57}Fe high-pressure ME experiments were performed in a Chester-Jones-type high-pressure setup with B_4C anvils. The sample in the high-pressure cell was mixed with epoxy and placed in a pyrophyllite ring supported from outside by a steel belt. This type of pressure cell allows quasi-hydrostatic pressures up to about 7.0 GPa to be attained. The pressure

calibration at room temperature was performed by measuring the Mössbauer isomer shift of a β -Sn foil, whose pressure dependence has been calibrated [7, 8]. The B_4C anvils contain ^{57}Fe impurities that cannot be removed without destroying the mechanical properties of this material. Because of the presence of these impurities, there is a complicated ME spectrum superimposed on the ME spectrum of the sample studied. For this reason, all the spectra were obtained by subtracting the spectrum of the anvils from those collected at each pressure point.

There are four non-equivalent sites of the iron atoms in the Th_2Zn_{17} structure, denoted by 6c, 9d, 18f and 18h. Because the magnetization of the Gd_2Fe_{17} compound lies in the basal plane, the Mössbauer subspectra for the 18f and 18h sites are split into two additional subspectra with an intensity ratio of 1:2 [9]. Therefore, six subspectra for 6c, 9d, 6f, 12f, 6h and 12h were used to fit the Mössbauer spectra of the compound. Some selected Mössbauer spectra at different pressure points are shown in figure 1. We have deduced the average values of B_{eff} , \bar{B}_{eff} , from the weighted average values of B_{eff} of each subspectrum. The same analysis has been used to calculate the average values of the isomer shift (\bar{S}).

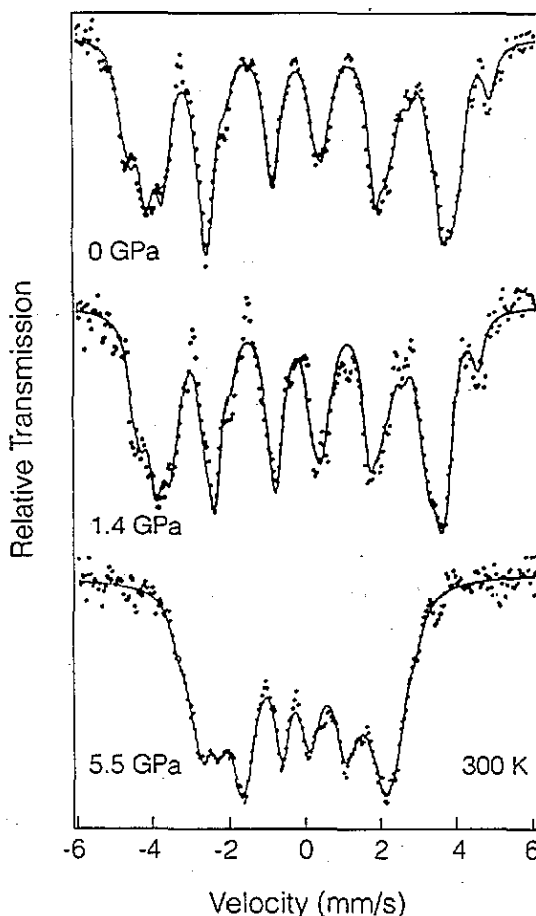


Figure 1. ^{57}Fe Mössbauer spectra of Gd_2Fe_{17} at 300 K and at pressures of 0, 1.4 and 5.5 GPa.

The average values of the isomer shift \bar{S} and the hyperfine field \bar{B}_{eff} at room temperature as a function of pressure are shown in figure 2 and figure 3, respectively. It can be seen

that both \bar{S} and \bar{B}_{eff} decrease with increasing pressure. The decrease of \bar{S} due to increasing pressure results from the increase of the s-electron density at the ^{57}Fe nucleus $\rho(0)$ [10]. The linear pressure-induced decrease of isomer shift can be fitted well by using the formula, $\bar{S}(p) = \bar{S}(0) - ap$, where a is the slope, $a = \partial\bar{S}/\partial p \simeq 1.4 \times 10^{-2} \text{ mm s}^{-1} \text{ GPa}^{-1}$ and $\bar{S}(0)$ at $p = 0 \text{ GPa}$, $\bar{S}(0) = -0.10(1) \text{ mm s}^{-1}$. Different mechanisms can contribute to an increase of $\rho(0)$ with increasing pressure. Using a value of the compressibility (κ) of about $8 \times 10^{-3} \text{ GPa}^{-1}$ for R_2Fe_{17} [11], one obtains $\partial\bar{S}/\partial \ln V \simeq 1.8 \text{ mm s}^{-1}$, where V is the volume. This value is comparable with that for $\alpha\text{-Fe}$ at 300 K ($\partial\bar{S}/\partial \ln V = 1.4 \text{ mm s}^{-1}$ [12]). We can therefore explain the pressure-induced increase of $\rho(0)$ in the same way as for $\alpha\text{-Fe}$: the main contribution to the increase of $\rho(0)$ is due to volume compression of the 4s conduction electrons. Other contributions, e.g. changes of the screening of the 3s electrons by the 3d electrons and changes of charge transfer (s \rightarrow d), are of less importance.

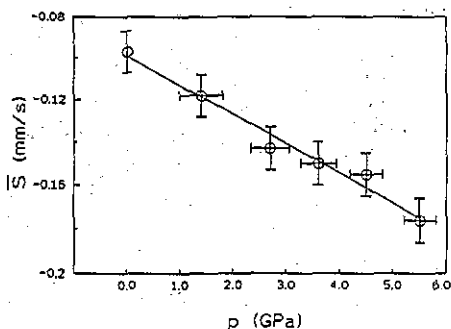


Figure 2. The pressure dependence of the average isomer shift \bar{S} in $\text{Gd}_2\text{Fe}_{17}$ at 300 K. The solid line through the data points is only a guide to the eye.

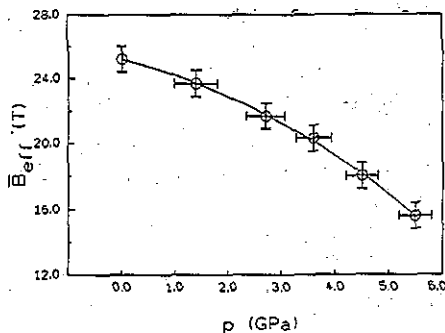


Figure 3. The pressure dependence of the average magnetic hyperfine field \bar{B}_{eff} in $\text{Gd}_2\text{Fe}_{17}$ at 300 K. The solid line through the data points is only a guide to the eye.

The decrease of \bar{B}_{eff} caused by decreasing the unit-cell volume of $\text{Gd}_2\text{Fe}_{17}$ under high pressure and at 300 K is evident from figure 3. On the other hand, all R_2Fe_{17} compounds are known to exhibit large magneto-volume effects [11, 13], e.g. a large decrease of their Curie temperature T_C with decreasing volume [13]. Therefore, the measured values of B_{eff} at room temperature and at different pressures will be affected by the decrease of T_C with pressure, since the value of T_C for $\text{Gd}_2\text{Fe}_{17}$ at ambient pressure ($T_C = 477 \text{ K}$) is close to 300 K. On the basis of this experimental fact, we have assumed that the reduction of B_{eff} with increasing pressure is mainly caused by the corresponding reduction of T_C , while the Fe local magnetic moment remains almost constant. In order to prove the validity of our assumption, we perform the following analysis: we estimate the required reduction of T_C at the maximum pressure (5.5 GPa) which gives the experimental value of \bar{B}_{eff} (at 5.5 GPa) at 300 K by using the known temperature dependence of the magnetization (Brillouin curve for $J = \frac{5}{2}$). We then obtain a value of $T_C = 342 \text{ K}$ at 5.5 GPa which leads to a value of $\partial T_C/\partial p = -25 \text{ K GPa}^{-1}$. This value of $\partial T_C/\partial p$ is very close to the experimentally measured values of $\partial T_C/\partial p$ in related R_2Fe_{17} compounds [13], e.g. $\partial T_C/\partial p = -26 \text{ K GPa}^{-1}$ for $\text{Pr}_2\text{Fe}_{17}$ and -30 K GPa^{-1} for $\text{Nd}_2\text{Fe}_{17}$. This strongly supports our assumption that the pressure-induced decrease of \bar{B}_{eff} at 300 K up to 5.5 GPa in $\text{Gd}_2\text{Fe}_{17}$ is mainly caused by the corresponding reduction of T_C with pressure, while the Fe local magnetic moment remains almost unchanged.

Finally, we want to refer to an interesting aspect regarding the difference between the effect of external pressure (our experiment) and that of 'lattice pressure' (expansion) due

to alloying with carbon on the Curie temperature in $\text{Gd}_2\text{Fe}_{17}$ [14]. For this purpose, we compare in the following the values of the volume-induced changes of T_C in $\text{Gd}_2\text{Fe}_{17}$ from our experimental results with those obtained from alloying with carbon, i.e. $\text{Gd}_2\text{Fe}_{17}\text{C}_x$, $0 \leq x \leq 1.5$ [14]. According to [14], alloying $\text{Gd}_2\text{Fe}_{17}$ with carbon (C) ($\text{Gd}_2\text{Fe}_{17}\text{C}_x$, $0 \leq x \leq 1.5$) results in an enhancement of T_C with increasing volume (C concentration) of $\partial \ln T_C / \partial \ln V = 8$ [14]. In order to compare the volume-induced changes of T_C , we have to convert our measured value of $\partial T_C / \partial p$ to $\partial \ln T_C / \partial \ln V$ using a value of the compressibility $\kappa = 8 \times 10^{-3} \text{ GPa}^{-1}$ [11]. This value of κ is commonly taken for R_2Fe_{17} [16] since the volume changes due to alloying with C or N have been found to be fairly constant within the R_2Fe_{17} series [16]. Using this value of κ , we obtain a value of $\partial \ln T_C / \partial \ln V = 7.7$, which is very close to the value obtained from alloying with carbon (see above). The near equality of these two values shows that the effect of interstitial atoms (C) in $\text{Gd}_2\text{Fe}_{17}\text{C}_x$ is nearly a pure volume expansion (i.e. without chemical or electronic disturbance). A detailed study of this last point will be published in a forthcoming paper [17].

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