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THE EFFECT OF PRESSURE ON THE POSITIVE MUON SPIN PRECESSION IN IRON AND NICKEL

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ABSTRACT

We have determined the pressure dependence of the local magnetic fields at μ^+ sites to be

$$\left(\frac{\partial \ln B}{\partial p}\right)_{298\text{ K}} = \begin{cases} -1.05(2) \times 10^{-3}/\text{kbar for Fe} \\ +0.43(6) \times 10^{-3}/\text{kbar for Ni}\ . \end{cases}$$

The dependence on temperature (also measured here) is discussed on the basis of these results.

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The hyperfine field B_{hf} at positive muon sites in iron and nickel exhibits marked deviations from the bulk magnetization M as a function of temperature [1-3]. Similar deviations have also been found for light interstitial impurities in Fe and Ni [4,5] as well as for heavier sp-impurities at substitutional sites in Fe, Co and Ni matrices [6,7]. Such deviations can partly be attributed to volume expansion effects, i.e. the change of the lattice parameter due to thermal expansion affects $B_{hf}(T)$ and M(T) in a different manner. The volume dependence of B_{hf} can be determined by pressure experiments. For Cd and Sn in nickel and Sn in iron the pressure dependence of B_{hf} does not follow that of the magnetization [8-10]. In connection with our efforts to understand the origin of $B_{hf}(\mu^+)$ in magnetic metals, we have now followed the local magnetic field at muon sites in high-purity polycrystalline Fe and Ni at 298 K and at hydrostatic pressures up to 7 kbars by the muon spin precession technique. We have also measured the temperature dependence of B_{hf} below 300 K with the same high-purity Fe and Ni to confirm earlier results [1-3].

The experiments were performed in a polarized muon beam from the 600 MeV Synchro-cyclotron (SC) at CERN. A pressure cell made of copper-beryllium, with two cavities (Ø 7 × 50 mm) and minimum 7 mm wall thickness, was used with an oil-kerosene mixture as the pressure-transmitting medium. The pressure was generated by a 7 kbar handpump (Nova Swiss) and measured with a Heise Bourdon tube gauge, claimed by the manufacturer to have an accuracy of ±0.01 kar. No polarizing magnetic field was used. The data were fitted to the expression

$$N(t) = N_0 \exp\left[-t/\tau_\mu\right]\left[1 + \sum_i a_i \exp(-\lambda_i t) \cos(2\pi\nu_i t + \phi_i)\right] . \qquad (1)$$

The low-temperature experiments were performed with a continuous-flow ^{4}He cryostat. The temperature was measured with calibrated platinum and carbon resistors. The zone-refined Fe and Ni samples are described elsewhere [11]. The muon precession frequency in nickel at 298 K and ambient pressure was found to be 18.416(3) MHz, corresponding to a field at the muon of 0.13587 T in good agreement with other experiments [3,12]. For iron under the same conditions, a precession frequency of 48.665(5) MHz was found, corresponding to 0.35905 T, also in good agreement with recent experiments [12,13]. The linewidths found at 298 K were $\lambda_{Fe} = 0.24(4)\ \mu s^{-1}$, $\lambda_{Ni} = 0.25(3)\ \mu s^{-1}$, verifying the high purity of the samples. The nickel linewidth remains constant at this low value down to 2 K.

The measured magnetic fields at 298 K and at different pressures were fitted to a straight line (fig. 1). The slopes yield

$$\frac{\partial \ln B_\mu}{\partial p} = \begin{cases} -1.05(2) \times 10^{-3}/\text{kbar for Fe} \\ +0.43(6) \times 10^{-3}/\text{kbar for Ni} . \end{cases}$$

The total local field B_μ at the muon is given by

$$B_\mu = B_{hf} + B_L + B_{dip} , \qquad (2)$$

where B_L is the Lorentz field (298 K, Fe: 0.715 T and Ni: 0.203 T) and B_{dip} denotes the dipolar field; B_{dip} is zero for Ni because the μ^+ interstitial site has cubic symmetry. For Fe at room temperature, B_{dip} is considered to be averaged to zero owing to the rapid muon diffusion [14]. In order to obtain the relative change of B_{hf} with volume, the variation of $B_L = (4\pi/3)M$ with volume is required, i.e. the pressure-dependence of the host magnetization M_0 at $T = 0$ as well as a change in the Curie temperature T_C must be considered. The change in T_C for Ni is: $dT_C/dp = +0.32$ K/kbar, and for Fe ~ 0 [15]. Different values on the pressure dependence of M_0 at $T = 0$ have been reported for Ni [16-18]. We use the value $\partial \ln M_0/\partial p = -0.28 \times 10^{-3}$/kbar, and with knowledge of the slope of M(T) at 298 K and the change in T_C we derive the total pressure dependence of the magnetization in Ni at 298 K to be $\partial \ln M/\partial p = -0.20 \times 10^{-3}$/kbar. This is also in agreement with the value at 293 K quoted by Bloch and Pauthenet [19]. For Fe we use the value $\partial \ln M/\partial p = -0.28 \times 10^{-3}$/kbar [16]. With the compressibilities of Fe, $\partial \ln V/\partial p = -0.59 \times 10^{-3}$/kbar, and of Ni, $\partial \ln V/\partial p = -0.54 \times 10^{-3}$/kbar [20], we deduce:

$$\frac{\partial \ln B_{hf}}{\partial \ln V} = \begin{cases} -0.92(1) \text{ for Fe} \\ +4.0\ (2) \text{ for Ni} . \end{cases} \qquad (3)$$

The uncertainties of $\partial \ln M/\partial p$ and $\partial \ln V/\partial p$ have not been included in the errors given, but we estimate that they increase them by a factor of 2 or 3.

Conventionally one writes [21]

$$B_{hf} = -\frac{8\pi}{3}\mu_B\, \eta(0)(n_0^\uparrow - n_0^\downarrow) , \qquad (4)$$

where $(n_0^\uparrow - n_0^\downarrow)$ denotes the spin density at the muon site of the unperturbed system and $\eta(0)$ is the spin-density enhancement factor (SDEF) which accounts for the perturbation of the conduction electron polarization by presence of the muon. If we assume that $(n_0^\uparrow - n_0^\downarrow)$ is proportional to the bulk magnetization, we obtain a contribution of 0.47 (Fe) and 0.37 (Ni) to $\partial \ln B_{hf}/\partial \ln V$, to which about 0.3 should be added due to the volume dependence of $\eta(0)$ (estimated from fig. 3, ref. 21). This adds up to $\partial \ln B_{hf}/\partial \ln V \approx +0.8$ for Fe $\approx +0.7$ for Ni. While the Fe value agrees satisfactorily with the experimental value of +0.92, the Ni value of +4.0 cannot be explained within this approach. This discrepancy becomes even worse if it is assumed, as in Jena's theory [21], that the s-band has a very small polarization (which makes its spin density enhancement unimportant) and that most of the spin density arises from the d-band polarization (with a small SDEF [21,22]). In such a model, a strong radial dependence of the d-electron polarization would be required to explain our data. Furthermore, this model [21] cannot predict the absolute values for B_{hf} in Ni.

In Fig. 2 we present the temperature dependence, at ambient pressure, of the muon spin precession frequency, normalized to lowest temperature [Fe: 52.13(6) MHz, Ni: 20.253(3) MHz]. Using eq. (2) and assuming that $B_{hf}(T)$ can be expressed as $B_{hf}(T) = B_{hf}(0)\ A(T)\ M(T)/M_0$, we calculate the deviation from the bulk magnetization M(T) [23]. The result is shown in Fig. 3. It should be pointed out that for Ni about half of the slope of 300 K can be explained by the volume dependence of B_{hf} and thermal expansion. This clearly shows the importance of information on the volume dependence of B_{hf} for interpreting the temperature dependence. Moreover, it brings the theoretical predictions by Katayama et al. [24] (shown by the solid line in Fig. 3) much closer to the experimental results. The calculations of Katayama et al. are of an *ab initio* type, using "muffin-tin" potentials. The local spin density follows from the hybridization of 1s electrons on the μ^+ sites (assumed to be octahedral) and d-electron states from nickel.

However, for Fe the volume dependence of B_{hf} is too small -- and, above all, of opposite sign -- to bridge the gap between $B_{hf}(T)$ and M(T). So far no calculations of the type reported in ref. [24] exist for muons in this metal.

We hope that our results will stimulate further theoretical efforts on the calculation of muon hyperfine fields, especially using cluster methods [25], which seem to be successful in explaining B_{hf} in transition metals.

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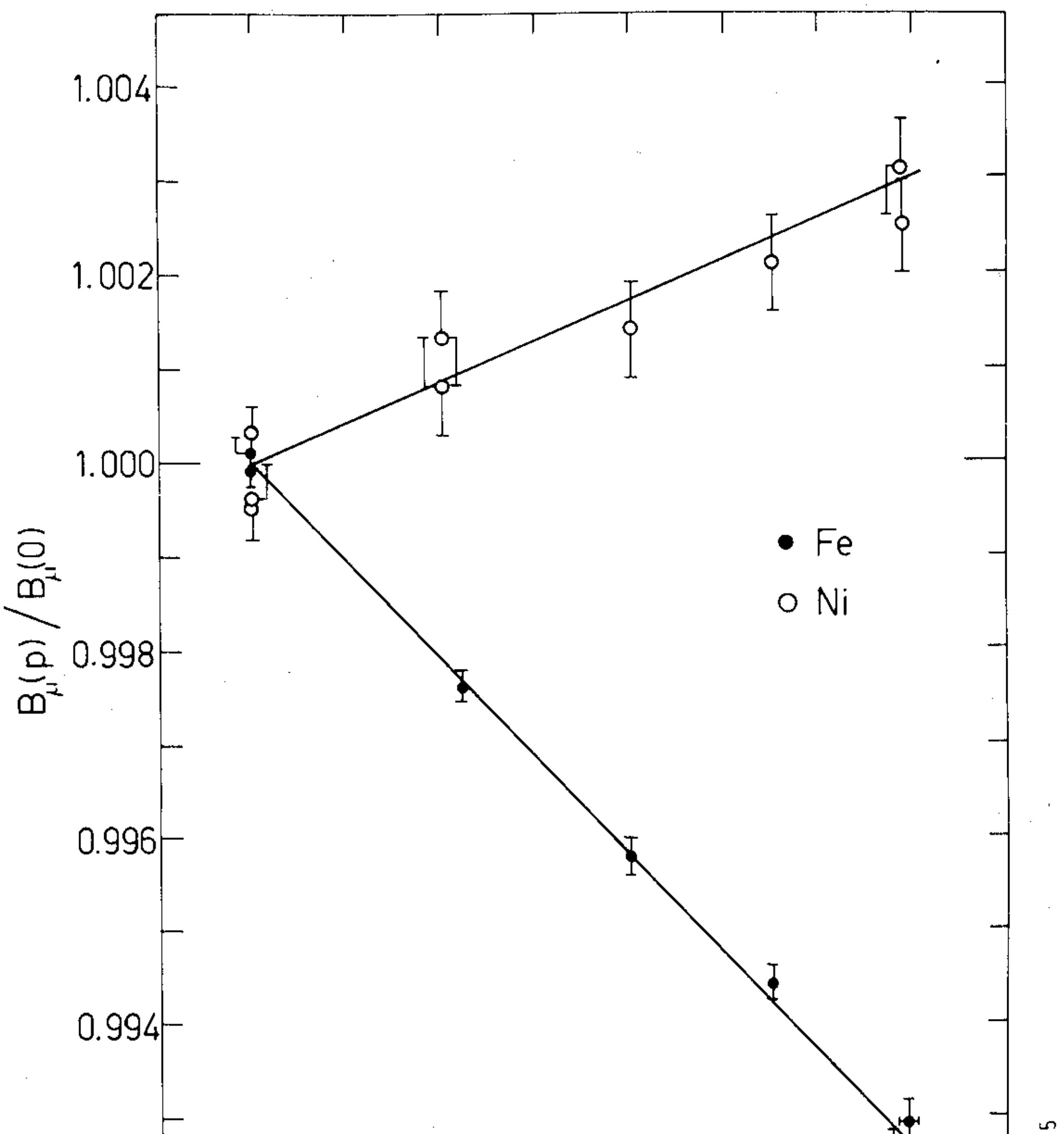
Figure captions

Fig. 1 : Normalized local field values at different pressures P. The solid lines are results from straight line fits.

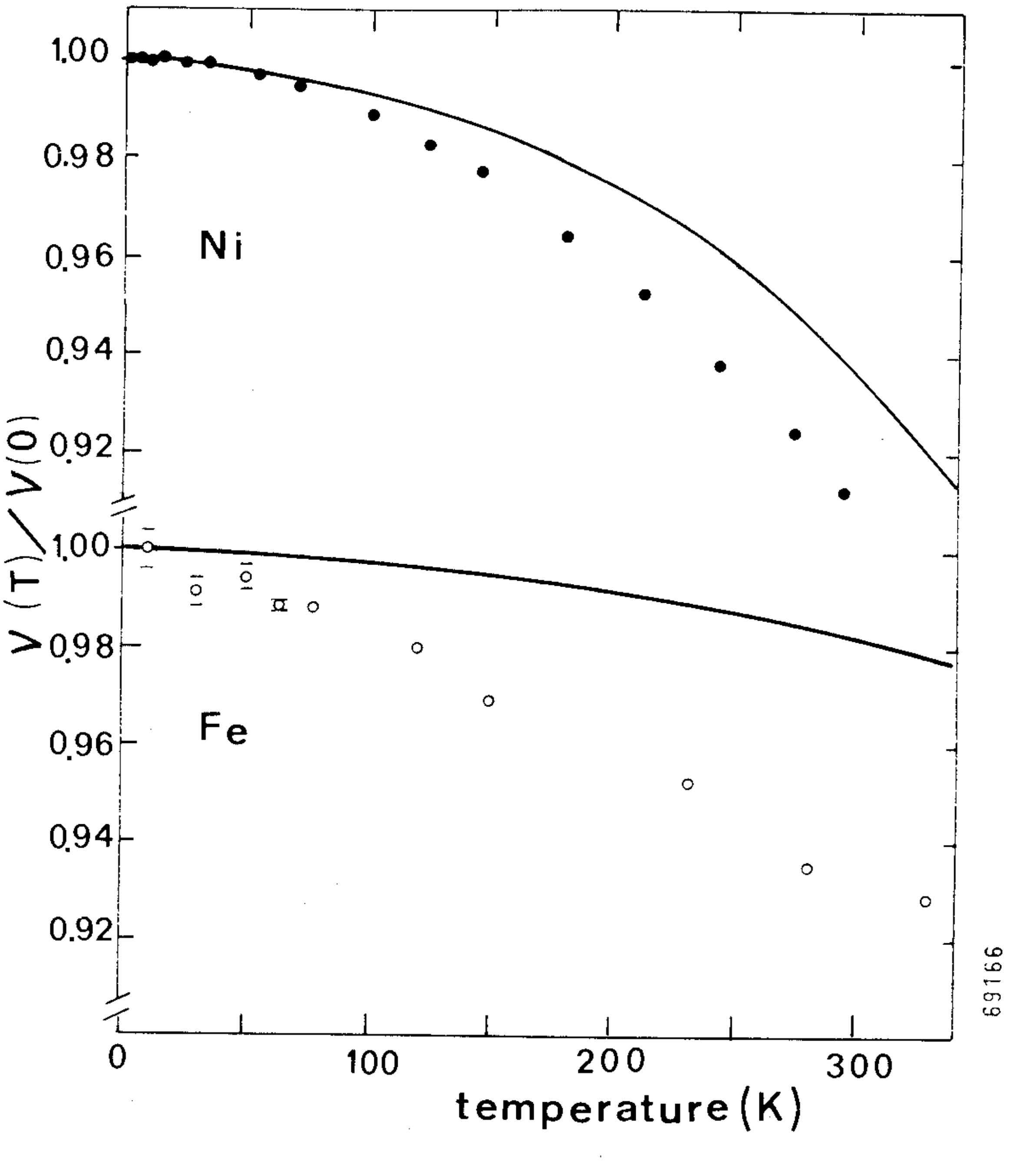
Fig. 2 : The temperature dependence of the spin precession frequencies in Fe and Ni, normalized to lowest temperature. The solid lines represent M(T).

Fig. 3 : The temperature dependence of A(T) defined by $B_{hf}(T) = B(0)\ A(T)\ M(T)/M_0$. The theoretical prediction (solid line) is taken from ref. 24.



1.004
1.002
1.000
0.998
0.996
0.994
0.992
$B_\mu(p)/B_\mu(0)$
0
1
2
3
4
5
6
7
p - kbar
● Fe
○ Ni
69165

Fig. 1



V(T)/V(0)
1.00
0.98
0.96
0.94
0.92
Ni
1.00
0.98
0.96
0.94
0.92
Fe
0
100
200
300
temperature (K)
69166

Fig. 2

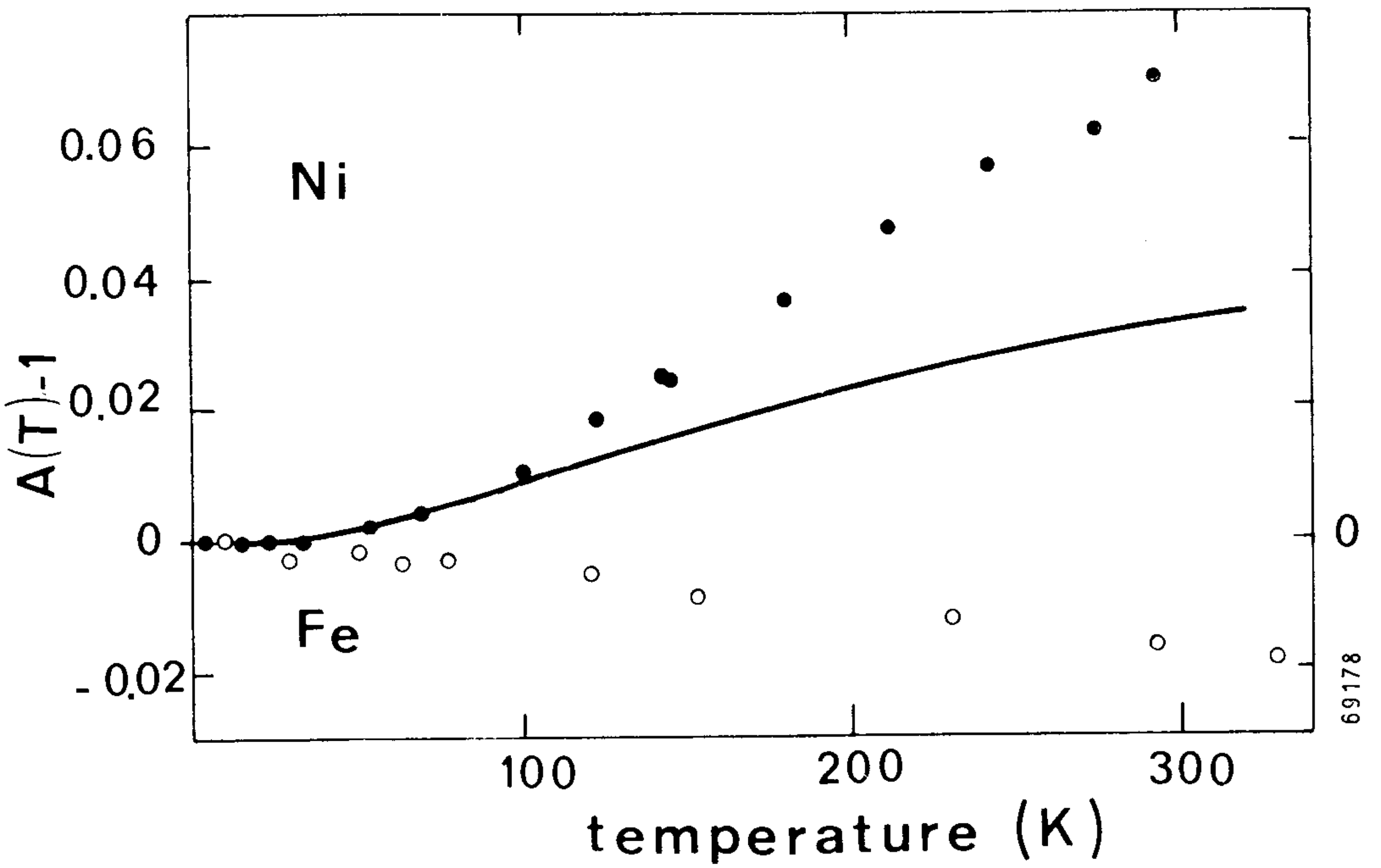


Fig. 3