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TEMPERATURE DEPENDENCE OF THE HYPERFINE FIELD AT IRON ATOMS NEAR 3d - IMPURITIES

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ABSTRACT

The temperature dependence of the hyperfine field at Fe atoms was determined by Mössbauer and continuous wave NMR methods for Fe-based alloys containing Ti, V, Cr, Mn, Co and Ni impurities. A marked anomaly was found in the case of Mn, and a smaller one for Ni. The temperature anomaly of the hyperfine field at iron atoms in the neighbourhood of these impurities was attributed to anomalous behaviour of the impurity moment reflected in the conduction electron polarization contribution of the hyperfine field.

РЕЗЮМЕ

С помощью эффекта Мессбауэра и постоянно возбужденного ЯМР исследовалась температурная зависимость сверхтонкого поля на ядрах железа в разбавленных сплавах железа с примесными атомами Ti, V, Cr, Mn, Co и Ni. В случае Mn найдено заметное аномальное поведение, а в случае Ni аномалия проявляется в меньшей степени. Аномальная температурная зависимость сверхтонкого поля на месте ядер железа вблизи атомов Mn и Ni объясняется аномальным поведением локальных магнитных моментов примесных атомов, влияние которых проявляется в изменении вклада поляризации электронов проводимости в сверхтонкое поле.

KIVONAT

Ti, V, Cr, Mn, Co és Ni szennyezéseket tartalmazó vas alapu ötvözetekben vizsgáltuk a vasatomok hiperfinom terének hőmérsékletfüggését Mössbauer és folytonos gerjesztésü NMR módszerekkel. Jellegzetes anomáliát találtunk a Mn, egy kisebbet pedig a Ni esetében. Az ezen szennyezések szomszédságában levő vasatomok hiperfinom terének hőmérsékleti anomáliáját a szennyezés-momentum anomális viselkedésének tulajdonitottuk, ami a hiperfinom tér vezetési elektron polarizációs járulékán keresztül tükröződik.

The temperature dependence of the moment of a magnetic impurity in a metallic ferromagnet may be different from that of the matrix. The first observation of such behaviour was of the anomalous temperature dependence of the Mn hyperfine field in iron [1]. According to Jaccarino et al. [2] the explanation of this fact given by the molecular field approximation of the Heisenberg model is that the impurity-host exchange is smaller than the host-host exchange interaction, so that the impurity moment decreases more rapidly with temperature than that of the matrix.

On the other hand, according to the Heisenberg model itself the magnetization of iron atoms around an impurity is different from that of the matrix because of the different exchange field acting on them. This leads to an anomalous behaviour of the hyperfine fields at iron atoms near the impurity through the H_{CP} core polarization contribution of the hyperfine field. Cranshaw et al. [3] interpreted the temperature dependences they found at the first neighbours of Mn impurities in a Fe-7,5 at%. Mn alloy between $80^{o}K$ and $500^{o}K$ in this way, but found no good agreement between the theory and experiment.

The aim of this paper is to show from measurements of the temperature dependence of the hyperfine field distribution around impurities that

i/ among the 3d - transition metal impurities only the Mn and Ni moments show anomalous temperature dependence and

ii/ the hyperfine field anomaly of the iron neighbours of the impurity is caused by an anomalous temperature dependence of the impurity moment due to the H_{CEP} conduction electron polarization contribution of the hyperfine field.

The Mössbauer effect measurements were performed on iron alloys with the following impurities: Ti /3.0 at%/, V /2.0 and 5.0 at%/, Cr /2.2 at%/, Mn /2.5 and 3.4 at%/, Co /3.0 at%/, and Ni /3.0 and 5.0 at%/, and the cwNMR experiments on alloys with V /0.5 at%/, Cr /2.2 at%/, Mn /1.0 at%/. For the ME and continuous wave nuclear magnetic resonance /cwNMR/ experiments conventional equipments [4, 5] were used, between $77^{o}K$ and the Curie point T_C and between $77^{o}K$ and room temperature, respectively.

The hyperfine field shifts at the first and second neighbours of the impurities were determined by decomposition of the Mössbauer spectra. The room temperature data are the following:

Ti : $\Delta H_1 = \Delta H_2 = -19.1 \pm 0.3$ kG,
V : $\Delta H_1 = \Delta H_2 = -24.4 \pm 0.4$ kG,
Cr : $\Delta H_1 = \Delta H_2 = -26.9 \pm 0.2$ kG.

/In these cases the shifts at the first and second neighbours could not be resolved separately, because their magnitudes are nearly the same./

Mn : $\Delta H_1 = -23.0 \pm 0{,}1$ kG, $|\Delta H_2| < 3$ kG,
Co : $\Delta H_1 = 13.3 \pm 0.5$ kG, $\Delta H_2 = 6.0 \pm 1.0$ kG,
Ni : $\Delta H_1 = 9.4 \pm 0.3$ kG, $\Delta H_2 = 7.0 \pm 1.0$ kG.

All the above data are in good agreement with previous results of spin echo [6], cwNMR [7] and Mössbauer [8] measurements.

Fig. 1 shows the temperature dependence of the difference of the relative hyperfine field of Fe atoms without and with nearest-neighbour impurities, normalized to the value taken at 80^{o}K. There is a large anomaly in the case of Mn and a smaller one in the case of Ni impurities, while for other impurities no deviation was found within the experimental error. The temperature dependence of the hyperfine field at iron atoms without first-neighbour impurities is the same as that of the pure iron.

The anomaly found in the case of Ni is in agreement with that observed between 77^{o}K and 350^{o}K at the third - neighbour iron sites [9]. We could not follow the temperature dependences of the second - neighbour shifts in the case of the Mn, Ni and Co impurities by ME because of their small value.

The hyperfine field shifts at the more distant neighbours were detected by cwNMR method. The room-temperature spectra were similar to those measured by Mendis and Anderson [7]. Fig. 2 shows the temperature dependence of the central resonances and satellites in cases of Mn and Co impurities. For both impurities the temperature dependence is the same as the central resonance within experimental error /0.5 %o/.

At first sight it might seem possible to describe the anomalies found in the case of Mn and Ni impurities in terms of the Heisenberg model. However, according to this model a similar anomaly is expected with all the impurities, because the exchange between the impurity and the matrix is different from the exchange between the matrix atoms. Thus, the absence of the anomaly with Ti, V, Cr and Co and nonmagnetic impurities like Al, Ga and Sn |4| indicates that the anomalous temperature dependence of the hyperfine field found at the first neighbours of the Mn and Ni impurities has some other origin.

We suggest that the anomalous first-neighbour hyperfine field behaviour is the consequence of anomalous behaviour of the impurity moment. The change of the first-neighbour iron hyperfine field due to the impurity $/\Delta H_1/$ comes from two sources: the change of the core polarization ΔH_1^{CP} and the change of the conduction electron polarization component ΔH_1^{CEP}. ΔH_1^{CP} is proportional to the moment perturbation caused by the screening of the impurity in the d-band. Its temperature dependence is probably the same as that of the matrix, as is indicated by the absence of the anomaly with Ga and Sn impurities [4].

ΔH_1^{CEP} is connected with the perturbation caused by the impurity in the s-band and consists of two further components: one of these components is proportional to $/\mu_{Fe}-\mu_i/$ and reflects the spin perturbation around the impurity excess moment, the other comes from the charge perturbation and is proportional to the 4s-band polarization that is to μ_{Fe}. Thus, the temperature dependence of ΔH_1 has two components: one is proportional to μ_{Fe} and the other to $/\mu_{Fe}-\mu_i/$. If the impurity displays an anomaly, the temperature dependence of the latter is different from that of the matrix. As the temperature dependence of μ_i has not been measured by diffuse neutron scattering, we have only indirect information on $\mu_i(T)$. The dotted lines on Fig. 3 show the temperature dependence of the contribution proportional to $/\mu_{Fe}-\mu_i/$ given by making two different assumptions about the H_{CEP} contribution to the Mn hyperfine field. In calculation of curve 1 it was supposed that this contribution is equal to the H_{CEP} contribution of the iron, and thus $/H_{Fe}-H_{Mn}/ \sim /\mu_{Fe}-\mu_{Mn}/$, while for curve 2 the value $H_{CEP}^{Mn} = 160$ kG[10], the Mn moment at 80^oK $\mu_{Mn} \approx 1.1\mu_B$[11], and the core polarization coupling constant 60 kG/μ_B[10] are used. Different parameters alter only the steepness of the $/\mu_{Fe}-\mu_{Mn}/$ curve; the characteristic peak at $T/T_C = 0.6$ remains unchanged. The points show the contribution proportional to the matrix moment. The linear combination of the two curves describes the temperature dependence of ΔH_1 rather well /full line/. Of course, this description is not unambiguous, as equally good agreement can be obtained with other parameters as well. However, the curvature of the measured ΔH_1, and especially the strong peak around $T/T_C = 0.6$, supports the idea that the anomaly is caused by a conduction electron polarization proportional to $/\mu_{Fe}-\mu_{Mn}/$.

In the case of Ni impurities, the detailed temperature dependence of the Ni hyperfine field is not known, so it is not possible to make such a detailed comparison as in the case of Mn. However, the anomaly seems to be well describable in the same way as in the Mn case if it is assumed that μ_{Ni} decreases a little more rapidly than μ_{Fe} and hence causes a rise in the absolute value of the negative contribution proportional to $/\mu_{Fe}-\mu_{Ni}/$.

Preliminary measurements show an anomalous temperature dependence of the first-neighbour iron hyperfine field similar to that of Mn in the case of Ru and Os, and a dependence similar to that of Ni in the case of Pd and Pt.

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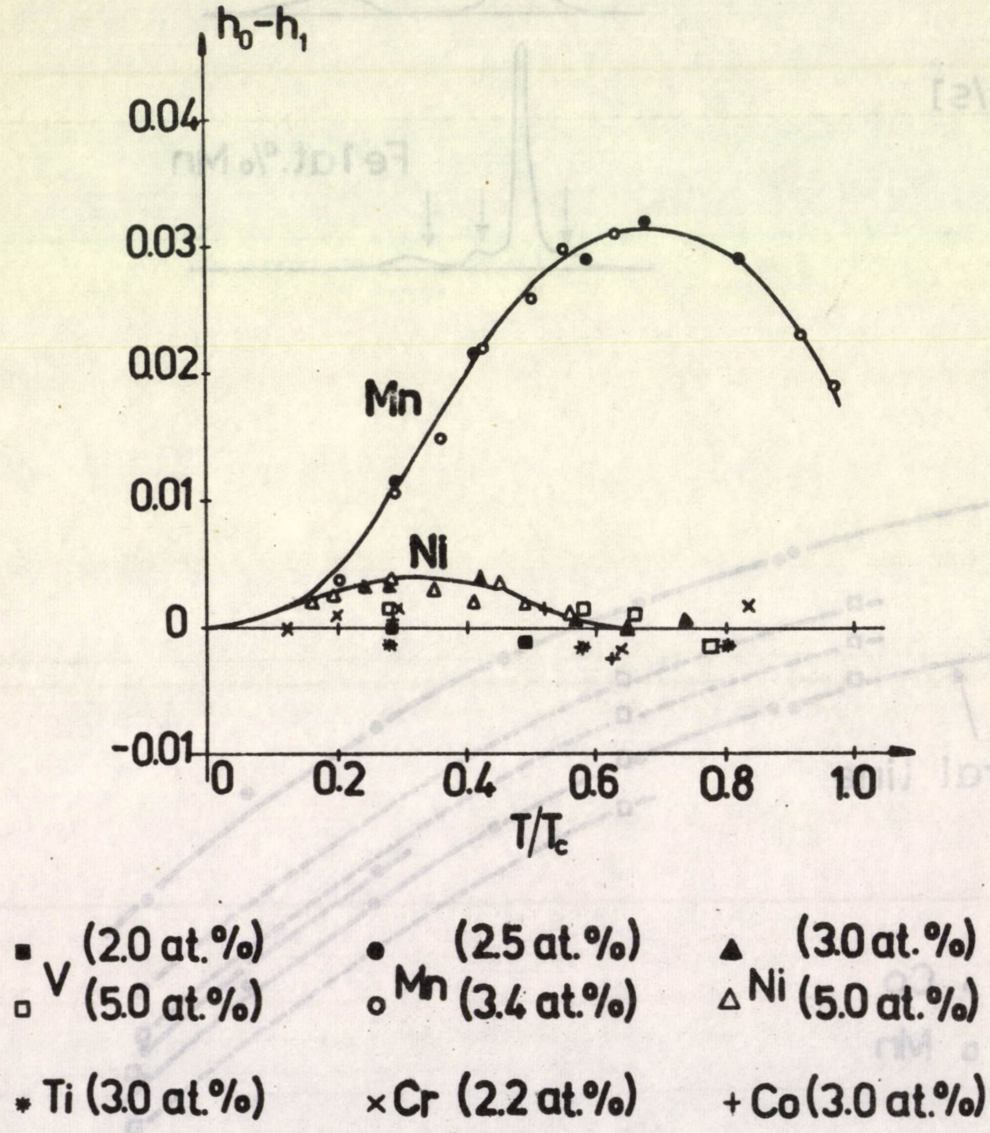


Fig. 1

The difference of the relative hyperfine field at iron atoms without $/h_0/$ and with $/h_1/$ impurity nearest neighbours.

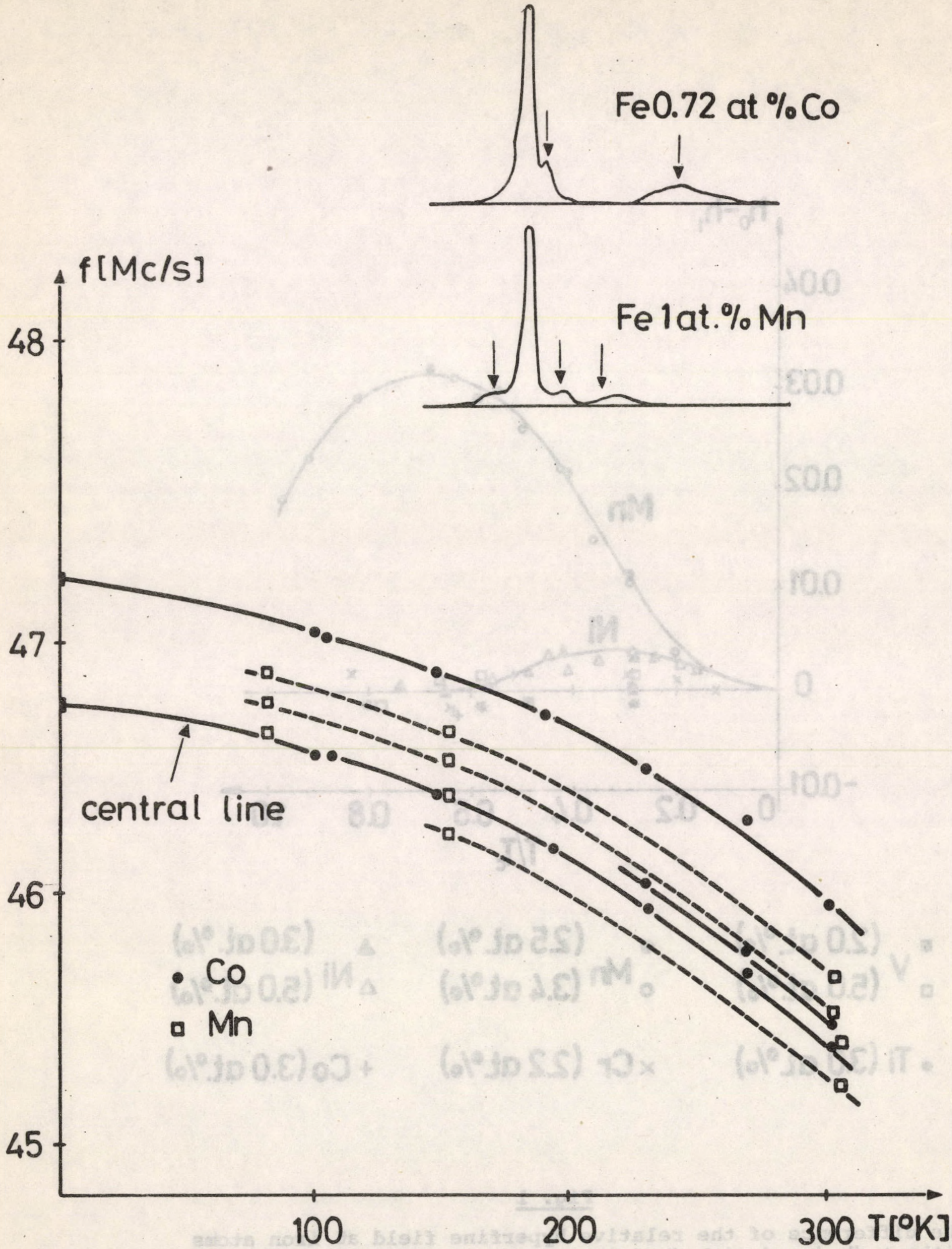
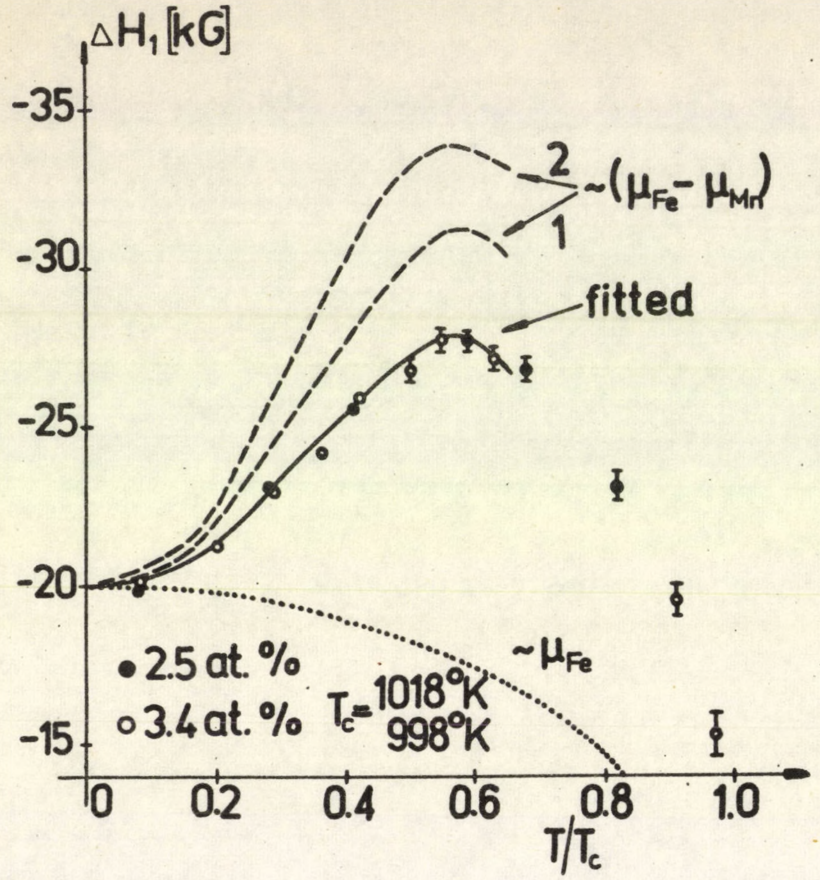
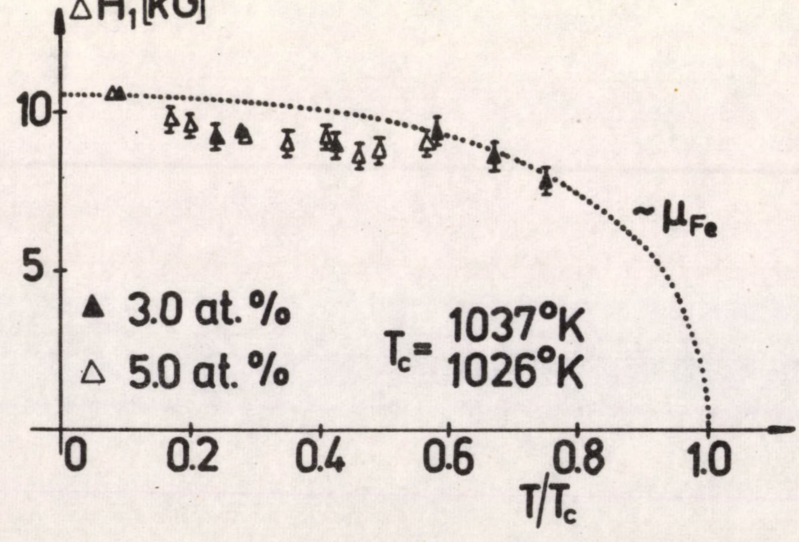


Fig. 2

Temperature dependence of the hyperfine field shifts in the case of Co and Mn impurities detected by cwNMR method. The SE data of FeCo alloys /Ref. 12/ taken at 1.3^{o}K are included in the figure too.



a. Mn



b. Ni

Fig. 3

The change of the hyperfine field due to the impurity at the first-neighbour iron atoms as a function of temperature. /The meaning of the curves is explained in the text./

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