Comments and Addenda

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Hyperfine Fields in Ni-Fe Alloys

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Recent measurements on the Ni hyperfine fields in Ni-Fe alloys are analyzed in terms of nearest-neighbor (nn) and next-nearest-neighbor (nnn) contributions. It is found that the nn contributions are dominant and that the nnn contributions play only a minor role.

RECENTLY, measurements on the Ni hyperfine (hf) fields in Ni-Fe alloys have become available.[1,2] The most striking result of these investigations is the difference in hf fields in the ordered Ni_3Fe alloy (-167 kOe)[2] as compared with the disordered Ni_3Fe alloy (-147 kOe).[1] In this paper, an attempt is made to explain this difference on the basis of nearest-neighbor (nn) and next-nearest-neighbor (nnn) interactions.

In the perfectly ordered Ni_3Fe structure, every Ni atom has four Fe nn, eight Ni nn, and six Ni nnn; in the disordered structure a Ni atom has three Fe nn, nine Ni nn, 1.5 Fe nnn, and 4.5 Ni nnn.

The hf fields in Ni metal (-80 kOe) and in ordered and disordered Ni_3Fe were analyzed under the following assumption. For low Fe concentrations the hf fields in the NiFe alloys at the Ni site can be described by[3]

$$H_{\mathrm{hf}}=-20\mu_{\mathrm{Ni}}-120\bar{\mu}\,, \tag{1a}$$

$$H_{\mathrm{hf}}=-20\mu_{\mathrm{Ni}}-pa-qa/x-rb-sb/x\,, \tag{1b}$$

where μ_{Ni} and $\bar{\mu}$ are the Ni moment and the average moment of the alloy, respectively. Here a is the contribution of a nn Ni atom to the hf field of a Ni atom, and b is the same contribution produced by a nn Fe atom. In addition, x is the fraction of the nn contribution to the hf field, which is produced by the nnn atoms, and $p(r)$ are the number of Ni (Fe) nn and $q(s)$ the number of Ni (Fe) nnn of a particular Ni atom. To determine the parameters a, b, and x, the following equations can be set up (in kOe):

$$\text{Ni} \qquad -80=-12-12a-6a/x\,, \tag{2a}$$

$$\text{Ni}_3\text{Fe ordered} \qquad -167=-12-8a-6a/x-4b\,, \tag{2b}$$

$$\text{Ni}_3\text{Fe disordered} \qquad -147=-12-9a-4.5a/x-3b-1.5b/x\,, \tag{2c}$$

where the 12 kOe are always the contribution of the own electrons of the Ni atom to the hf field calculated from Eq. (1a) with $\mu_{\mathrm{Ni}}=0.6\mu_B$. Equation (2c) refers to the most-probable-neighbor configuration of a Ni atom in the disordered Ni_3Fe alloy. This is the configuration corresponding to the observed hf field of -147 kOe. There are, of course, in the disordered alloy many other possible configurations, yielding other hf fields. But since none of these possible configurations could be detected with certainty either in the NMR spectra or in the Mössbauer spectra, no equations similar to Eq. (2c) were set up.

By solving Eq. (2a)–(2c) we find

$$a=5.5\text{ kOe},$$
$$b=27\text{ kOe},$$
$$x=16.$$

This shows the predominant contribution of the nn as compared with the nnn. This situation seems to hold for all Ni alloys, which lie on the Slater-Pauling curve. Collins and Low[4] find from their neutron-scattering experiments that, by adding Fe to Ni, the moment disturbance is confined to the solute atom in agreement with the above result. Cable *et al.*[5] find from neutron-scattering experiments in NiCu alloys that the moment disturbance at the Ni site is produced by nn Cu atoms only, again in agreement with the present results. It is

[1] U. Erich, E. Kankeleit, H. Prange, and S. Hüfner, J. Appl. Phys. **40**, 1491 (1969).
[2] T. J. Burch, J. I. Budnick, and S. Skalski, Phys. Rev. Letters **22**, 846 (1969).
[3] In Ref. 1, the following equation is given: $H_{\mathrm{hf}}=-20\,\mu_{\mathrm{Ni}}-100\,\mu$; a more careful analysis of the data yields Eq. (1a) [U. Erich, Z. Physik **227**, 25 (1969)].
[4] M. F. Collins and G. G. Low, Proc. Phys. Soc. (London) **86**, 535 (1965).
[5] J. W. Cable, E. O. Wollan, and H. R. Child, Phys. Rev. Letters **22**, 1256 (1969).

perhaps interesting to note that the H_{hf} contribution of a Fe nn equals roughly that determined in pure iron by adding small nonmagnetic impurities (e.g., 27 kOe for Al impurities).[6]

This interpretation also explains the additional resonances found in the ordered Ni_3Fe at 145 and 186 kOe, and attributed by Burch *et al.*[2] to Ni with three and five Fe nn, respectively. The above figures show that replacement of one nn Ni by a nn Fe alters the field by 21.5 kOe, which then explains the additional resonances at 186 and 145 kOe with respect to the main resonance at 167 kOe. These results may also be used to interpret the somewhat complicated spectrum of the disordered sample of Ni_3Fe. The broad maximum at 55 MHz (which corresponds to 146 kOe) is certainly due to the resonance of Ni nuclei in a perfectly disordered environment; its field value of 146 kOe is in agreement with that obtained from the Mössbauer measurements (147 kOe). In the spectrum there are two additional sharp resonances, which can be attributed to Ni nuclei, namely at 155 and 177 kOe. We suggest that the 155-kOe resonance comes from Ni nuclei, which have three nn Fe, nine nn Ni, and six nnn Fe, and the 177-kOe resonance from Ni nuclei with four nn Fe, eight nn Ni, and six nnn Fe. We cannot as yet explain why these configurations are more stable than others.

[6] G. K. Wertheim, V. Jaccarino, J. H. Wernick, and D. N. E. Buchanan, Phys. Rev. Letters **12**, 24 (1964).

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Diamagnetic Susceptibility at the Transition to the Superconducting State*

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An expression of Schmid for the "extra" diamagnetic susceptibility is evaluated to facilitate comparison with the experiments of Gollub *et al.*

IN a paper of the same title, Schmid[1] has obtained an expression for the contribution to the diamagnetic susceptibility at zero field arising from fluctuations in the superconducting order parameter. The same result has been obtained by Schmidt.[2] We here generalize Schmid's result to the experimentally realized case of finite fields. Instead of the susceptibility, we calculate directly the magnetization, which is the measured quantity. The experiment has been carried out by Gollub *et al.*[3]

Our starting point is the expression for the free energy of Schmid:

$$\mathfrak{F}=-\frac{VkT}{4\pi}\tilde{B}\int\frac{dk}{2\pi}\sum_{n=0}^{\infty}\ln\frac{2m^*\pi kT/h^2}{k^2+\tilde{B}(n+\frac{1}{2})+\zeta^{-2}}, \quad (1)$$

where V is the volume of the system, m^* is the mass of the electron pair, ζ is the coherence length at zero field, and $\tilde{B}=4eB/hc$ is proportional to the magnetic field. The expression for $\mathfrak{F}$ is divergent, but the part of it which depends on field is not.

We now introduce the function $G(y)=[y]-y$, where $[y]$ is the integer part of y. Then we may write

$$\mathfrak{F}=-\frac{VkT}{4\pi}\int_0^{\infty}dx\int\frac{dk}{2\pi}\mathfrak{L}(k,x)\left[G'\left(\frac{x}{\tilde{B}}\right)+1\right]. \quad (2)$$

Here $\mathfrak{L}=\ln[2m^*\pi kTh^{-2}/(k^2+x+\zeta^{-2})]$ and G' is the derivative of G, which has δ-function contributions at $y=n+\frac{1}{2}$.

Thus we obtain

$$\mathfrak{M}=-\frac{\partial F}{\partial B}=-\frac{VkT}{4\pi}\frac{4e}{hc}\int_0^{\infty}dx\int\frac{dk}{2\pi}\frac{x}{\tilde{B}^2}\mathfrak{L}(k,x)G''\left(\frac{x}{\tilde{B}}\right)$$

$$=-\frac{VkT}{4\pi}\frac{4e}{hc}\int_0^{\infty}dx\int\frac{dk}{2\pi}G\left(\frac{x}{\tilde{B}}\right)\frac{d^2}{dx^2}x\mathfrak{L}(k,x). \quad (3)$$

Carrying out the differentiation, and the integral over k, replacing x by $y\tilde{B}$ and inserting the explicit expression for G, we obtain

$$-\frac{\mathfrak{M}}{\sqrt{B}}=\frac{VkT}{4\pi}\left(\frac{4e}{hc}\right)^{3/2}f(\gamma), \quad (4)$$

where

$$\gamma=(\tilde{B}\zeta^2)^{-1}=\frac{1}{2}\frac{T-T_{c0}}{B}\left|\frac{\partial H_{c2}}{\partial T}\right| \quad (5)$$

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[1] Albert Schmid, Phys. Rev. (to be published).
[2] H. Schmidt, Z. Physik **216**, 336 (1968). (There is a misprint of a factor of 4 in this result.)
[3] J. P. Gollub, M. R. Beasley, R. S. Newbower, and M. Tinkham, Phys. Rev. Letters **22**, 1288 (1969). We thank Professor Tinkham for communicating his results prior to publication.