Comments on Fe and Ni Hyperfine Fields in Ni_3Fe

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(Received 9 June 1969)

A model is presented to explain the observed hyperfine fields in Ni_3Fe.

RECENTLY, Burch *et al.*[1] reported on the Fe and Ni hyperfine fields in nearly ordered Ni_3Fe measured by nuclear magnetic resonance (NMR). They identified the most intense NMR line (at 63.5 MHz) as due to Ni in the ordered nearest-neighbor (nn) environment (i.e., Ni having eight Ni and four Fe first nn). We wish to point out that this identification can be rationalized by (i) noting that the Ni NMR as a dilute impurity in Fe occurs[2] at about 89 MHz, and (ii) assuming that in the pure ferromagnetic metals (Fe, Co, Ni) the hyperfine field arises approximately one-half from the atom itself and one-half from its nn, and (iii) assuming in an alloy that the hyperfine field due to the atom itself is the same as in the pure metal.

To apply this model, we note that the NMR frequency of Ni in pure Ni occurs at about 28.5 MHz. According to (ii) above, we attribute approximately 14.25 MHz of this to the Ni atom itself and about 1.19 MHz to each of the 12 nn atoms. The frequency for Ni in Fe [(i) above] is about 89 MHz. Of this amount, according to (iii), 14.25 MHz is due to the Ni atom itself; the remainder (74.75 MHz) due to the eight Fe nn atoms, i.e., 9.34 MHz per Fe nn atom. Thus the frequency of the Ni NMR in ordered Ni_3Fe is 14.25 MHz from the Ni atom itself; 8×1.19 MHz from the eight Ni nn atoms, and 4×9.34 MHz from the four Fe nn atoms. These contributions total 61.1 MHz, not far from the 63.5 MHz observed. The values in Table I are obtained on this model for the Fe NMR in ordered and disordered Ni_3Fe and for the Ni NMR in locally disordered nn environments.

TABLE I. Values for the Fe NMR in ordered and disordered Ni_3Fe and for the Ni NMR in locally disordered nn environments.

Site	No. of Fe nn's	Predicted NMR frequency (MHz)	Observed NMR frequency (MHz)
Fe	0	38.4	39.8
Fe	3[a]	43.2	43
Ni	1	36.7	
Ni	2	44.8	
Ni	3	53.0	55.0
Ni	4	61.1	63.5
Ni	5	69.3	70.8
Ni	6	77.4	

[a] Number of Fe nearest neighbors for the most likely Fe site in disordered Ni_3Fe.

The results are in remarkable agreement, considering the simplicity of our model. The corresponding Ni peaks in disordered Fe_3Ni are in even closer agreement with our predictions. Better agreement could be obtained by using a slightly different breakdown than 50-50, but this refinement seems unwarranted at this point. The difference in frequency for the same nn environments in ordered and disordered Ni_3Fe could be explained by including second nn. To obtain agreement, negative contributions must be used.

One application of the above considerations is in identifying the intensity near 45 MHz in "ordered" Ni_3Fe as due to Ni having two Fe nn. This would favor the model[1] M_2 over M_1.

The model we have presented is not entirely without precedent.[3] Watson[4] has suggested theoretical grounds for the approximate magnitude of this effect, and Beck[5] has mentioned a similar partitioning of hyperfine fields for other cases. The partitioning in (ii) above appears to work better than the assumption[3] of proportionality (with common coefficients) to the self- and nn moments for Fe, Co, and Ni, in themselves. Extension to other atoms (e.g., Al) has not been attempted here. Note that for the pure metals, any partitioning can be rationalized—it is only in the application to alloys that the separate identification of inter- and intra-atomic contributions to the hyperfine field has a physically unique meaning.

[1] T. J. Burch, J. I. Budnick, and S. Skalski, Phys. Rev. Letters **22**, 846 (1969).
[2] R. L. Streever, L. H. Bennett, R. C. LaForce, and G. F. Day, J. Appl. Phys. **34**, 1050 (1963).
[3] See, e.g., A. J. Freeman and R. E. Watson, *Magnetism*, edited by G. T. Rado and H. Suhl (Academic Press Inc., New York, 1965), Vol. II A, Chap. 4; M. B. Stearns and S. S. Wilson, Phys. Rev. Letters **13**, 313 (1964); G. K. Wertheim, V. Jaccarino, J. H. Wernick, and D. N. E. Buchanon, *ibid.* **12**, 24 (1964); S. Kobayasi, K. Asayama, and J. Itoh, J. Phys. Soc. Japan **21**, 65 (1966).
[4] R. E. Watson (private communication); see also R. E. Watson and A. J. Freeman, Phys. Rev. Letters **14**, 695 (1965); in *Hyperfine Interactions*, edited by A. J. Freeman and R. B. Frankel (Academic Press Inc., New York, 1965).
[5] P. A. Beck (private communication).