KFKI-73-31

K. Tompa

EFFECTIVE J VALUES IN DILUTE Cu-Mn AND Cu-Fe ALLOYS, AS DETERMINED IN TERMS OF NMR DATA

Hungarian Academy of Sciences

CENTRAL
RESEARCH
INSTITUTE FOR
PHYSICS

BUDAPEST

2017

KFKI-73-31

EFFECTIVE J VALUES IN DILUTE Cu-Mn AND Cu-Fe ALLOYS, AS DETERMINED IN TERMS OF NMR DATA

K. Tompa

Central Research Institute for Physics, Budapest, Hungary
Solid State Physics Depertment

Submitted to Journal of Phys. F

ABSTRACT

The values of the coupling constant $|J_{eff}| = 5\,|J_{sd}|$ have been calculated from susceptibility and NMR data by making use of the first order quadrupole wipe-out number in the case of Cu-Mn and Cu-Fe alloys. The thus obtained 2,1 and 3,8 eV /±10%/, respectively, are about 20% lower than the values determined from the broadening of the NMR spectrum. The systematic error of the latter method is probably due to the neglect of the contribution from the quadrupole effect to the broadening.

РЕЗЮМЕ

На основе данных ЯМР и восприимчивости впервые применяемым методом определили значение коэффициента связи $|J_{eff}| = 5\,|J_{sd}|$ в сверхразбавленных сплавах Cu-Mn и Cu-Fe. Полученные значения 2,1 и 3,8 эв /±10%/ были меньше предварительно определенных значений, вычисленных из расширения ЯМР-спектра, примерно на 20%. Предполагается, что причиной систематической ошибки определения вышеуказанных значений является пренебрежение квадрупольным эффектом.

ÖSSZEFOGLALÓ

NMR és szuszceptibilitás adatokból egy először most alkalmazott módszerrel meghatároztuk a $|J_{eff}| = 5\,|J_{sd}|$ csatolási állandó értékét Cu-Mn és Cu-Fe hig ötvözetekben. A kapott értékek 2,1 illetve 3,8 eV /±10%/, közelitőleg 20%-kal kisebbek a NMR spektrum kiszélesedéséből meghatározott értékeknél. Ez utóbbi értékek meghatározásának szisztematikus hibája feltehetően a kvadrupol effektus elhanyagolásából ered.

The energy of the interaction between two impurity atoms, and the energy difference between parallel and antiparallel alignments of two identical impurity spins in disordered dilute alloys can be expressed using the Caroli formula for double resonance scattering [1]. If one compares the latter expression with that formulated in terms of the s-d exchange interaction, the effective exchange constant can be defined as [2], [3]

$$5J_{sd} = J_{eff} = \frac{10E_F}{3\pi S} \sin\left(\eta_2^{\uparrow} - \eta_2^{\downarrow}\right) \qquad /1/$$

where J_{sd} is the sd coupling constant, E_F the Fermi energy, S the localized impurity spin and η_2^{σ} is the phase shift of the scattered electrons with spin σ.

On introducing the notation used by Souletie [4],

$$\eta_2^{\uparrow} = (1 + \xi)\eta_2,$$

$$\eta_2^{\downarrow} = (1 - \xi)\eta_2$$

equation /1/ can be simplified. In the case of polarized virtual state /$T=\infty$, $\xi = 1$/, we have $\eta_2^{\uparrow} = 2\eta_2$ and $\eta_2^{\downarrow} = 0$.

Then we find

$$J_{eff} = \frac{10E_F}{3\pi S} \sin 2\eta_2$$

The value of S is known from susceptibility measurements, and we intend to evaluate $\sin 2\eta_2$ from NMR data.

The density oscillation of conduction electrons with spin σ around the localized moment was expressed by Blandin [2] as

$$\Delta\rho^{\sigma}(r) = -\frac{5}{4\pi^2} \sin\eta_2^{\sigma}\, r^{-3} \cos\left(2k_F r + \eta_2^{\sigma}\right)$$

where r is the position vector and k_F is the Fermi wave number.

By making use of this expression, the total electron density oscillation is given as

$$\Delta n(r) = \Delta\rho^{\uparrow}(r) + \Delta\rho^{\downarrow}(r)$$

and the spin density oscillation as

$$\Delta s(r) = \Delta\rho^{\uparrow}(r) - \Delta\rho^{\downarrow}(r)$$

In the case of magnetic limit the charge density oscillation becomes equal to the spin density oscillation, i.e.

$$\Delta n(r) = \Delta s(r) = -\frac{5}{4\pi^2}\sin 2\eta_2\, r^{-3}\cos\left(2k_F r + 2\eta_2\right)$$

since the charge density oscillation is brought about by the electrons polarized in spin.

Thus in the case of magnetic limit the measurement of spin density is equivalent to that of charge density. It has been shown in our earlier NMR measurements [5] that the amplitude of the charge density oscillation can be evaluated from the wipe-out number of the first order quadrupole effect if the phase φ of the term $\cos/2k_F r+\varphi/$ is chosen to be zero. It follows that in the above specified case the amplitude of the spin density oscillation and thus J_{eff} can be evaluated from the measured wipe-out number of the first order quadrupole effect.

Out of the dilute Cu-3d transition metal alloys the wipe-out number of the first order quadrupole effect was measured on the Cu-Mn [6] and the Cu-Fe [7] alloys. At such a high temperature at which the wipe-out number becomes independent of the temperature we measured $n_1 = 1500 \pm 5\%$ and $n_1 = 2100 \pm 5\%$ on Cu-Mn and Cu-Fe, respectively. These values are taken to be characteristic of the magnetic limit case.

Before the numerical results, let us consider the errors involved in this calculation:

a/ an uncertainty of about 10% for neglecting the phase factor in the evaluation of the charge density oscillation amplitude from n_1 /first order quadrupole wipe-out number/;

b/ ± 5% accuracy of the wipe-out number measurement;

c/ an unknown correction arising from the formula relating the field gradient to the charge density oscillation /see e.g. [8]/ due to the uncertainty of the factor α used in this expression [9];

d/ a correction of about 20% if one uses for the nonresonant phase shifts, which have to be taken into account in the evaluation of the first order quadrupole effect, the values measured on Cu-Ni since no such measurements have been performed on Cu-Mn or Cu-Fe.

In spite of these corrections it turned out that the thus calculated values of $|J_{eff}|$ are in better agreement with those obtained by other physical methods than the results of NMR spectrum broadening.

Table 1. shows the values of the coupling constants as calculated for dilute Cu-Mn and Cu-Fe alloys by different methods.

Table 1.

$|J_{sd}|$ and $|J_{eff}|$ coupling constants /reported values/

Alloy	$|J_{sd}|$ [eV] from impurity resistivity and susceptibility data		$|J_{eff}| = 5\ |J_{sd}|$ [eV] from NMR spectrum broadening	
Cu-Mn	0,24 0,29	[10] [11] [12]	2,6 2,6	[13] [14] [15]
Cu-Fe	0,34 0,4 0,8	[12] [14] [16]	5	[14] [15]

Table 2. shows the numerical data used in the present calculation along with the thus obtained values of $|J_{eff}|$.

Table 2.

Coupling constants, as evaluated by the present method

Alloy	Effective Bohn magneton		S	sin $2\eta_2$	$|J_{eff}|$ |eV|
Cu-Mn	$4,93 \pm 0,2$	[12]	2	0,59	2,1
Cu-Fe	$3,68 \pm 0,2$	[17]	1,4	0,72	3,8

As to the values of sin $2\eta_2$ in column 4 of Table 2, it has to be noted that they have been calculated from the measured wipe-out numbers [6] [7] taking $\alpha = 25$ and using the phase shifts η_0 and η_1 measured for Cu-Ni in the evaluation of the non-resonant scattering contribution. A similar calculation gives $J_{eff} = 1,6$ eV for Cu-Mn and $J_{eff} = 3,2$ eV fpr Cu-Fe in the case of $\eta_0 = \eta_1 = 0$.

It can be seen that the values of $|J_{eff}|$ is in either case lower than that obtained in any reported calculation from the NMR spectrum broadening. This is probably due to the fact that in those cases the broadening of the spectrum was attributed exclusively to magnetic interactions without taking into account the contribution from the quadrupole effect. Our estimates are in a reasonable agreement with those obtained for 5 $|J_{sd}|$, than the earlier NMR results, but this agreement is not as good as that one for Ag-Mn /Mizuno, 1971/.

Acknowledgements

Thanks are due to Prof. L. Pál and to Dr. B. Vasvári for the support of this work and to colleague Dr. C. Hargitai for useful discussions.

References

[1] B. Caroli, J. Phys.Chem. Solids, 28, 1427 /1967/

[2] A. Blandin, J.Appl.Phys. 39, 1285 /1964/

[3] A. Narath, Preprint, submitted to CRC Critical Reviews in Solid State Sciences

A. Narath, A.C. Gossard, Phys.Rev. 183, 391 /1969/

[4] J. Souletie, J. of Low Temp.Phys. 7, 141 /1972/

[5] K. Tompa, J. Phys.Chem. Solids, 33, 163 /1972/

[6] K. Tompa, Proc. of the 12th International Conference on Low Temp. Physics, Kyoto, Japan, 1971. p: 783

[7] K. Tompa, A. Lovas, L.Zámbó, Phys. Status Solidi /b/ 54, K17 /1972/

[8] W. Kohn, S.H. Vosko, Phys.Rev. 119, 912 /1960/

[9] K. Tompa, F. Tóth, E. Nagy, Phys.Status Solidi 41, 413 /1970/

[10] J.A. Campbell, J.P. Compton, J.R. Williams, G.V.H. Wilson, Phys.Rev. Letters 19, 1319 /1967/

[11] W.P. Pratt, R.I. Schermer, W.A. Steyert, J.Low Temp. Phys. 1, 469 /1969/

[12] C.M. Hurd, J. Phys.Chem.Solids 30, 539 /1969/

[13] A.C. Chapman, E.F.W. Seymour, Proc.Phys.Soc. 72, 797 /1952/

[14] K. Mizuno, J. Phys.Soc. Japan 30, 742 /1971/

[15] T. Sugawara, J. Phys.Soc. Japan 14, 643 /1959/

[16] M.D. Dybell, W.A. Steyert, Phys.Rev. 167, 536 /1968/

[17] C.M. Hurd, J. Phys.Chem.Solids 28, 1345 /1967/

Kiadja a Központi Fizikai Kutató Intézet
Felelős kiadó: Vasvári Béla igazgató-helyettes
Szakmai lektor: Hargitai Csaba
Nyelvi lektor: Kovács Jenőné
Példányszám: 290 Törzsszám: 73-8619
Készült a KFKI sokszorosító üzemében
Budapest, 1973. junius hó