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OSCILLATION OF CONDUCTION ELECTRON DENSITY NEAR THE SOLUTE ATOMS IN DILUTE Cu-Mn ALLOY*

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The "wipe-out" number characterizing the first order quadrupole effect of the ^{63}Cu NMR spectrum in dilute Cu-Mn alloys is 1500 ± 75. This value agrees quite well with the one calculated in terms of the Blandin-Caroli resonance scattering theory.

The properties of transition element impurities in nonmagnetic hosts have been the subject of numerous investigations [1], although the level of understanding is still unsatisfactory. This paper seeks to demonstrate that the measurement of the asymptotic excess conduction electron density /Friedel oscillation/ contributes to the solution of the problem of the "magnetic" impurity in a nonmagnetic host. The aim has been to observe Friedel oscillation around "magnetic" solute Mn atoms in copper-based alloys by measuring the first order quadrupole effect appearing in the ^{63}Cu NMR spectrum [2], and preliminary results for this Cu-Mn system are presented here. In this case the effect of Friedel oscillation is easily separated from that of the spin density oscillation. The theoretical prediction [3] that the Friedel oscillation is nonzero has been experimentally confirmed by the second order quadrupole measurements of Lumpkin [4].

The master alloy was prepared from 99,999 atomic % copper and 99,9 atomic % manganese by vacuum smelting. The measurements were performed on ∿15μ-thick foils produced by cold rolling. To remove dislocation effects the specimens were annealed for 1 hour at 400°C. The short duration and the relatively low temperature of the annealing were chosen to avoid the internal oxidation observed by Howling [5]. The Mn concentrations of the specimens prepared from the master alloy, as determined by spectro-

* The paper will appear in Low Temperature Physics, LT-12, Kyoto 1970.

photometric analysis, were found to be 52, 142, 270, 460, and 1040 atomic ppm / ± 5 % /. The wide line NMR spectrometer described in [6] was used.

The wipe-out number was determined from the NMR amplitude /D/-impurity concentration /c/ curve /Fig. 1/. The experimental points are averages taken over about 50 spectra. Simultaneously measured ^{27}Al NMR signals from Al foils were used as reference. The measured D amplitudes have been normalized to that of pure copper / D_o /, and the satellite contribution to the peak - to - peak amplitude of the derivative signal is given. The results measured at T = 150°C are shown. Below this temperature the log $\left(\frac{D}{D_o} - 0{,}4\right)/0{,}6$ - c curve deviates from the straight line characteristic of the first order quadrupole effect [7] owing to the spin density oscillation.

At 150°C our experiments gave the wipe-out number $n_1 = 1500 \pm 75$*.

Assuming the scattering to be predominantly d-resonance scattering, the excess density of the conduction electrons with spin near the impurity is given by [3] as

$$\Delta\rho^{\sigma}(r) = -\frac{5}{4\pi^2}\sin\delta_2^{\sigma}\, r^{-3}\cos\left(2k_F r + \delta_2^{\sigma}\right) ,$$

where r is the separation of matrix nucleus from impurity, k_F the Fermi wave number. The phase shifts δ_2^{σ} of the scattered partial waves $\ell = 2$, taken at the Fermi energy, are related to the number of localized 3d-electrons by the expression $N = \frac{5}{\pi}\left(\delta_2^{\uparrow} + \delta_2^{\downarrow}\right)$, and to the z component of the magnetic moment localized on the impurity atoms by the formula $M_z = \frac{5\mu_B}{\pi}\left(\delta_2^{\uparrow} - \delta_2^{\downarrow}\right)$, /$\mu_B$ is the Bohr magneton./

The difference in the number of spin-up and spin-down electrons gives the spin density, while their sum gives the charge density oscillation. Thus, the component z of the electric field gradient can be expressed as

$$q = \frac{8\pi}{3}\alpha\left[\Delta\rho^{\uparrow}(r) + \Delta\rho^{\downarrow}(r)\right]$$

where $\alpha = 25$ is the enhancement factor [8, 9].

$$\delta_2^{\uparrow} = \pi ; \quad \delta_2^{\downarrow} = \frac{\pi}{5} \cdot 0{,}7 = 0{,}44$$

Using the phase shifts given by Daniel [10] in his calculation of the residual resistivity in Cu-3d alloys, and the computer-calculated result [7] which relates the Friedel oscillation directly to the wipe-out number, we obtain the theoretical value $n_{1\ theor} = 1420$. This is in good agreement with the experimental value. /In terms of the "all -or- nothing" language the $q_{krit} = 1{,}8 \times 10^{21}$ cm^{-3} is the same as for Cu-Zn [7]./

The electronic structure proposed by Hurd [11] gives $n_{1\ theor} = 1840$

* The extrapolation method and the wipe out number published in the KFKI preprint 9/1969 are incorrect.

in satisfactory agreement with the experimental value.

The quadrupole effect of the NMR of the matrix nuclei in dilute alloys of copper with 3d - transition metals can be easily estimated from resonance scattering theory, e.g. by using the phase shifts given in [10] or by making use of assumption about the electronic structure of 3d - transition metals embedded in copper [1, 12].

Above the Kondo temperature the dependence of the excess charge density near the solute atoms on the atomic number of the latter yields a v-shaped curve with manganese at the minimum.

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REFERENCES

[1] Daybell, M.D., Steyert, W.A.: Rev.Mod.Phys., 40, 380 /1968/

[2] Cohen, M.H., Rief, F.: Solid State Physics, 5, p.321 /Academic Press, New York/

[3] Blandin, A.: J.Appl.Phys., 39, 1285 /1968/

[4] Lumpkin, O.J.: Phys.Rev., 164, 324 /1968/

[5] Howling, D.H.: Phys.Rev.Letters, 17, 253 /1966/

[6] Tompa, K., Tóth, F.: Magy.Fiz.Folyóirat, 11, 177 /1963/

[7] Tompa, K., Grüner, G., Jánossy, A., Tóth, F.: Solid State Communications 7, 697 /1969/

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

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

[10] Daniel, E.: J.Phys.Chem.Solids, 23, 975 /1962/

[11] Hurd, C.: J.Phys.Chem.Solids, 30, 539 /1968/

[12] Daybell, M.A., Steyert, W.A.: Sub-Kondo temperature properties, preprint.

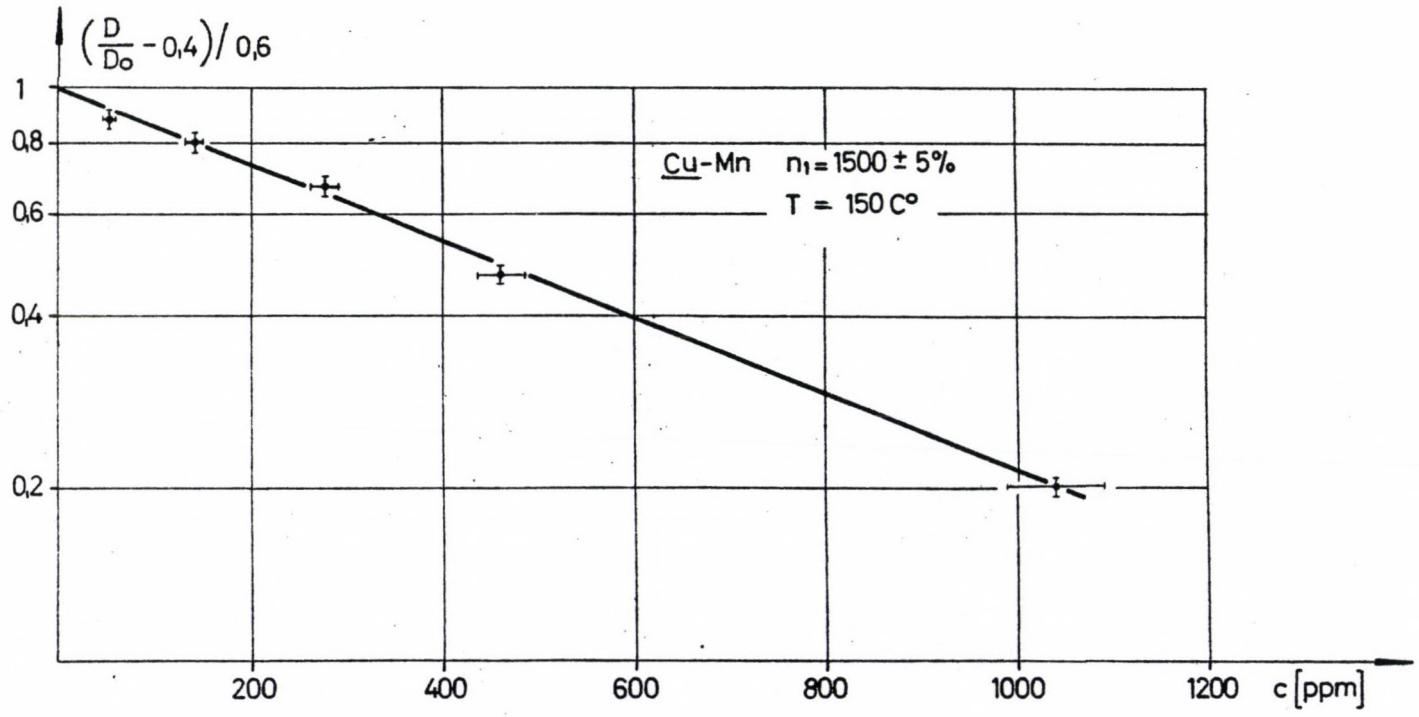

Figure 1.

First order quadrupole effect in copper based Cu-Mn dilute alloys, at T = 150 C°

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