Discontinuity of the hyperfine field at Co^{59} nuclei in intermetallic compounds with gadolinium

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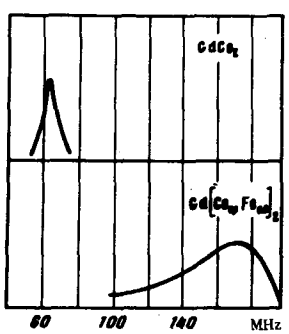
A discontinuity of the hyperfine field at Co^{59} nuclei in intermetallic $Gd(Co_xFe_{1-x})_2$ compounds was observed by the NMR method. This discontinuity is attributed to a change in the degree of delocalization of the 3*d* electrons.

We obtained nuclear magnetic resonance (NMR) spectra of certain samples of the system $Gd(Co_xFe_{1-x})_2$, which have a crystal lattice of the Laves cubic phase type.

The NMR lines of the $GdCo_2$ and $Gd(Co_{0.1}Fe_{0.9})_2$ samples were recorded with a spin-echo spectrometer at 4.2 °K. The duration of the first and second pulses was 10 μsec, the delay between them was 60 μsec, and the repetition frequency of the series was 1 Hz. The contours of the NMR signals of these samples are shown in the figure, and the values of the hyperfine fields are listed in the table, which gives also the results of the magnetic measurements. It is seen from the figure that the gravity centers of the NMR lines of Co^{59} in the $GdCo_2$ and $Gd(Co_{0.1}Fe_{0.9})_2$ samples lie close to 62 and 165 MHz, respectively, i. e., the average hyperfine field at the Co^{59} nuclei changes by a factor 2.7, which is much larger than the change observed in other iron-cobalt compounds.[1–4]



NMR line contours of $GdCo_2$ and $Gd(Co_{0.1}Fe_{0.9})_2$ samples.

At the same time, the average magnetic moment $\bar{\mu}_{3d}$, of the 3*d* sublattice, calculated by us from measurements of the magnetization show that the change of $\bar{\mu}_{3d}$ on going from $GdCo_2$ to $Gd(Co_{0.1}Fe_{0.9})_2$ does not exceed 80%. To compare the change of the hyperfine field with the change of the magnetic moment of the cobalt, we have separated μ_{Co} from the values of μ_{3d}, representing the latter in the form

$$\bar{\mu}_{3d} = x\mu_{Co} + (1-x)\mu_{Fe}. \qquad (1)$$

It must be recognized here that the electron structure of the Fe atoms in compounds of the RFe_2 type is

Magnetic characteristics of the alloys $GdCo_2$ and $Gd(Co_{0.1}Fe_{0.9})_2$

Composition	Hyperfine field, kOe	Saturation magnetization, G-cm³/g	Magnetic moment of 3*d* sublattice	Curie temperature, °K
$GdCo_2$	67.0	67.0	1.1	408
$Gd(Co_{0.1}Fe_{0.9})_2$	170	96.0	1.85	812

stable, as a result of which the ratio $H_{hf}^{Fe}/\mu_{Fe}=\text{const}$ remains in force for the considered class of compounds. Our measurements of the NMR of Fe^{57} show that the hyperfine fields at the iron change only by a factor 1.08 on going from $GdFe_2$ to $Gd(Co_{0.1}Fe_{0.9})_2$. Since $\mu_{Fe}=1.7\ \mu_B$ in the $GdFe_2$ compound,[2] we find on the basis of[1] the values $\mu_{Fe}=1.83\mu_B$ and $\mu_{Co}=1.8\mu_B$ for $Gd(Co_{0.1}Fe_{0.9})_2$.

Thus, the change of the hyperfine field at the Co^{59} nuclei in the investigated samples is not proportional to the change of the magnetic moment of the cobalt atoms. This anomalous behavior of the hyperfine field can be explained by recognizing that the field H_{hf} has several sources, namely

$$H_{hf}=H_{ep}+H_{orb}+H_{Co}^{4s}+H_{3d}^{neighb}+H_{4f}^{neighb}, \qquad (2)$$

where H_{ep} is the field resulting from the exchange polarization of the atomic core by the atom's own magnetic moment, H_{orb} and H_{Co}^{4s} are the contributions connected with the orbital momentum and the polarization of the 4*s* electrons by the self-moment of the Co atom, and H_{4f}^{neighb} and H_{3d}^{neighb} are the contributions of the neighboring atoms from the 4*f* and 3*d* sublattice, respectively.

The contributions H_{ep}, H_{orb}, and H_{Co}^{4s} are proportional, in one degree or another, to the magnetic moment of the atom, and for cobalt H_{ep} is close to the theoretical value 125 kOe/μ_B.[5] Using this circumstance, Christopher and Taylor[4] estimated the contribution of H_{4f}^{neighb} in the $GdCo_2$ compound and found it to be +80 kOe. As to the contribution H_{3d}^{neighb}, it is known[6] that the neighboring Fe atoms produce a negative hyperfine field, whereas for Co[7] the contributions from the environment are positive up to the fourth coordination sphere.

Thus, it can be concluded that the discontinuity of the hyperfine field at the Co^{59} nuclei is due to an abrupt change in the value of H_{3d}^{neighb}. A comparison of the Curie temperatures of the investigated samples show that on going from $Gd(Co_{0.1}Fe_{0.9})_2$ to $GdCo_2$ the exchange-interaction energy decreases. Within the framework of Friedel's theory[8] this means a change in the wavelength λ and in the amplitude of the oscillations of the spin density of the collectivized 3*d* electrons, and this should lead to a shift of the modes of these oscillations owing to the increase in the value of $\lambda/d\sim 1/k_f d$, where d is the lattice constant and k_f is the Fermi wave vector for the d band. It is this change of the spin density which leads to the strong change of the contribution of H_{3d}^{neighb} to the hyperfine field.

[1] A. Piercy and K. Taylor, J. Phys. 4C, 1112 (1968).
[2] K. N. R. Taylor, Adv. Phys. 87, 551 (1971).
[3] S. Kobayshi and K. Asayama, J. Phys. 21, 65 (1966).
[4] K. Taylor and J. Christopher, J. Phys. 2C, 2237 (1967).
[5] A. Freeman and R. Watson, Phys. Rev. 123, 2027 (1961).
[6] M. B. Stearns, Phys. Rev. 4B, 4081 (1961).
[7] G. Gruner and K. Tompa, J. Phys. 3F, 189 (1973).
[8] T. Friedel, G. Leman and S. Olszewski, J. Appl. Phys. 32, 325S (1961).