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HYPERFINE INTERACTIONS IN DyFe$_2$

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Intermetallic RM$_2$ compounds were investigated by many authors. The obtained results suggest, that in a particular series e.g. RFe$_2$, the magnetic properties depend weakly on the kind of R atom. A crystalline anisotropy of rare earth element is responsible however for the easy axis direction. In a case when the easy axis and a local direction of the EFG main axis do not coincide and at the same time quadrupole interaction is not much smaller than the magnetic one, any approximations used for the description of nuclear energy levels may be unsatisfactory. From our investigation arises, that DyFe$_2$ is an example of such a case.

In DyFe$_2$ structure / space group Fd$ar{3}$m/ all Fe atoms are crystallographically equivalent. If we assume that the EFG tensor for particular atom has the same type of symmetry as the point symmetry of the atom site then the EFG tensor in DyFe$_2$ should posses axial symmetry. Because the easy direction is [100], there is the same angle $\theta$ between the easy direction and the local EFG main axis for each Fe atom. One can expect an identical value of hyperfine interaction for all atoms and the Mössbauer spectrum should contain only one sextet.

The solution for energy eigenvalues in case of axially symmetric EFG tensor in the first approximation is given by the formula

$$\Delta E_m = -\frac{q}{n} m H_{\text{eff}} + (-1)^{m+q} \frac{e^2 q Q (3 \cos^2 \theta - 1)}{4} /1/$$

The expression $\frac{e^2 q Q (3 \cos^2 \theta - 1)}{2}$ will be referred to as $QS$ and spectrum fits according to formula /1/ we call "diagonal sextets". If $q = 0$ or $\cos \theta = 1/\sqrt{3}$, the spectrum should not exhibit any quadrupole splitting because $QS$ is equal to zero.

In DyFe$_2$ the angle $\theta$ fulfills the condition that $\cos \theta = 1/\sqrt{3}$. The numerical fits indicate however significant contribution of the quadrupole splitting to the measured spectra. The obtained $QS$ value does not depend on temperature and equals 0.03 mm/s. Moreover, all our spectra show 0.04 mm/s shift of the observed positions of 2 and 5 lines with respect to those expected from formula /1/. These results prove that expression /1/ is not sufficient for correct nuclear energy levels.
description of $^{57}\text{Fe}$ in DyFe$_2$ structure. According to [1] the full Hamiltonian of hyperfine interactions may be written in the form:

$$H = H_\text{w} + P_{20}O_{20} + \sum P_{2\alpha}O_{2\alpha}/2$$

where $P_{2\alpha}$ are real coefficients describing the EFG tensor. The third component of formula /2/ one can treat as diagonal Hamiltonian perturbation. In the DyFe$_2$ case it is convenient to chose the EFG tensor principal axes system because the only nonvanishing $e_{2\alpha}$ are here $P_{20}$ and $P_{22}$/diagonal element and asymmetry parameter/. After transformation to magnetic coordinates system the EFG tensor is defined by five new $P_{2\alpha}$ coefficients / or three, if the EFG tensor has the axial symmetry/. The $\mu$sbaure spectra were fitted according to the program, in which the energy eigenvalues were given by the solutions of Hamiltonian /2/. Our results are as follows:

/1/ the fits with $P_{22}=0$ /axial symmetry of $\omega$G tensor/ are not satisfactory, 
/2/ the fits with free $P_{22}$ parameter are far better as diagonal sextet fits. 
$\chi^2$ values are in this case same as for six independent lines fits.

The $P_{20}$ and $P_{22}$ do not depend on temperature /Fig.1/. $P_{20}$ parameter fulfils the relation

$$\omega_{\theta=0} = -3 P_{20}$$

For DyFe$_2$ we get then $\omega_{\theta=0} = -0.306$ mm/s. This value is close to $\omega_{\theta=0} = -0.38$ mm/s obtained by Gubbens et al.[2] for YFe$_2$, in accordance with the tendency that hyperfine interaction parameters depend only weakly on $\alpha$ atom.

![Fig.1. $P_{20}$ and $P_{22}$ coefficients vs. temperature /for DyFe$_2$/](image)

In conclusion, the application of aproximation /1/ in the case of DyFe$_2$ leads to the incorrect values of hyperfine interaction parameters. The correct values are obtained by taking into account off-diagonal elements of EFG tensor. The derived results indicate moreover that the $\omega$G tensor in DyFe$_2$ has not axial symmetry.

References: