Contents

1 Introduction

The ^{57}Co in α-iron is a source with considerable selfabsorption by the natural abundance of ^{57}Fe of 0.0214. A thickness of 1μ of iron foil gives an effective thickness of

1μ·7.8748g/cm^3 · σ_0·6.022 ·10^{23}/atomic_weight·abundance·f-factor= 0.465·f-factor. W. Sturhahn and A. Chumakov measured the f-factor of polycrystalline iron foils [1] in the temperature range of 4.2K up to 400K. The f-factor at RT is f=0.8 such that the effective thickness of 1μ iron becomes $t_{eff} = 0.372$ If the diffusion depth is large enough emission lines will be absorbed dependent on their polarization and intensity. The stronger and less polarized lines lose the most. In case of a magnetized iron foil parallel and the γ-direction orthonormal to the surface the emission lines 2,5 of the sextet are mainly concerned. Disregarding selfabsorption the surface of the source seems to be oriented at an angle less than $\theta = 90^o$ with respect to the γ-direction. Calculating the source function with an angle less than $\theta = 90^o$, the polarization of the emission lines is also changed, so that measurements with polarized absorbers cannot be accurately simulated.

2 Emission

The source spectrum is the sum of Lorentzians multiplied by the 2x2 density matrices r_i:

$$\rho_r(E) = \frac{2}{\Gamma\pi}\sum_i \frac{1}{2}r_i \cdot \frac{(\Gamma/2)^2}{(E-E_i)^2+(\Gamma/2)^2} \qquad (1)$$

$$1 = Tr\left(\sum_i \frac{1}{2}r_i\right)$$

$$\begin{pmatrix} 1/2 & 0 \\ 0 & 1/2 \end{pmatrix} = \int_{-\infty}^{\infty}\rho_r(E)dE$$

The total intensity, sum over all Lorentzians, is normalized to 1. Γ is the natural linewidth. Since the Lorentz function is real and the density matrix r_i of a transition is hermitian, the diagonal elements of $\rho_r(E)$ are real numbers.

The sum can be taken a double sum over inequivalent sites j with weights w_j and transitions E_i^j.

$$\rho_r(E) = \frac{2}{\Gamma\pi}\sum_j w_j \sum_i \frac{1}{2}r_i^j \cdot \frac{(\Gamma/2)^2}{(E-E_i^j)^2+(\Gamma/2)^2} \qquad (2)$$

$$\sum_j w_j = 1$$

The radiation travels through a material of refraction index $\mathbf{n}(E)$:

$$\mathbf{n} = \underline{1} - \frac{\sigma f(\mathbf{k})}{2k}\sum_j N_j \sum_i R_i^j \cdot \frac{\Gamma/2}{E-E_i^j - i\Gamma/2} \qquad (3)$$

with the unit 2x2 matrix $\underline{1}$, the cross section σ, the Lamb-Mossbauer factor f in direction $\mathbf{k}$, the density N_j of nuclei of type j. The density matrix at position z (travelling from 0 to z) is given by

$$\rho(E,z) = e^{i\mathbf{n}kz}\rho_r(E)e^{-i\mathbf{n}^\dagger kz} \qquad (4)$$

The electronic absorption $exp(-\mu_e z)$ shall be included later. In the following the double sum is is written aa a sum over i only for simplicity. Several simplifications for the selfabsorption of a ^{57}Co in α-iron are introduced. First of all the f-factor is taken to be isotropic. The profile of the distribution of the ^{57}Co diffused into the α-iron foil is simplified to a) an δ-function, b) uniform distribution, and a distribution given by some function C(z), i.e a diifusion profile (see section 4). The integrations will be approximated by summations over up to 128 integration points.

The case a) is already described by eq. 4 where z is the depth d. Inserting the refraction index of α-iron which is assumed to be homogeneously magnetized, such that the $R_i = r_i$ and the E_i are the same, eq.3 is rewritten as

$$\rho(E,z) = e^{-\frac{i}{2}tz(A(E)+h(E))}\rho_r(E)e^{\frac{i}{2}tz\left(A^\dagger(E)+h^\dagger(E)\right)} \tag{5}$$

$$A(E) = \sum_i \left(r_i - \frac{1}{2}Tr(r_i)\cdot\underline{1} \right)\cdot\frac{\Gamma/2}{E - E_i - i\Gamma/2}$$

$$h(E) = \underline{1}\cdot\sum_i \frac{1}{2}Tr(r_i)\cdot\frac{\Gamma/2}{E - E_i - i\Gamma/2}$$

Since the unit matrix commutes with all matrices $-ih(E) + ih^\dagger(E) = D(E)$ can be taken out

$$\rho(E,z) = e^{-\frac{1}{2}tzD(E)}e^{-\frac{i}{2}tzA(E)}\rho_r(E)e^{\frac{i}{2}tzA^\dagger(E)} \tag{6}$$

D(E), a real 2x2 unit matrix,

$$D(E) = \underline{1}\cdot\sum_i \frac{1}{2}Tr(r_i)\cdot\left(-i\frac{\Gamma/2}{E - E_i - i\Gamma/2} + i\frac{\Gamma/2}{E - E_i + i\Gamma/2} \right) \tag{7}$$

$$= \underline{1}\cdot\sum_i Tr(r_i)\cdot\frac{(\Gamma/2)^2}{(E - E_i)^2 + (\Gamma/2)^2}$$

The product td is the effective thickness of the absorber of thickness d.

$$td = \sigma_0 f(\mathbf{k})\mathbf{N}\mathbf{d} \tag{8}$$
$$N = 6.022\cdot 10^{23}/atomic\_weight\cdot density\cdot abundance$$
$$t = 0.465\,\mu^{-1}\cdot f(\mathbf{k})$$

The density matrix of the source radiation in case a) with all ^{57}Co at a depth of z=d in α-iron changes from $\rho_r(E)$ to $\rho(E,d)$. The Lamb-Mossbauer factor f for the source function $\rho_r(E)$ appears to be reduced by th efact that the resonanz part f of radiation is absorpt more strongly than the non-resonat part (1-f) with is only attenuated by electronic absorption exp(-$\mu_e \cdot z$) (absorption coeffizient μ_e). I_r shall denote the fraction of resonant and I_{nr} of non-resonant γ's

$$I_r = e^{-\mu_e \cdot d} \int_{-\infty}^{\infty} Tr(\rho(E,d)) dE \qquad (9)$$

$$I_{nr} = e^{-\mu_e \cdot d}$$

then the effective Lamb-Mossbauer factor is the ratio

$$f_{eff} = \frac{f \cdot I_r}{f \cdot I_r + (1 - f) \cdot I_{nr}} \qquad (10)$$

3 Constant concentration

The concentration ^{57}Co is taken constant fom the surface to a depth d.
Each layer at z is an independent source.
The integral over z from the surface z=0 to the depth z=d is replace by
a sum with weights/concentrations c and thickness δ.

$$\delta = d/N \qquad c = 1/N \qquad (11)$$

$$\sum_{j=1}^{N} c = 1$$

ρ from Eq. 6 multiplied by the attenuation factor of electronic absorption

$$\rho(E,z) = e^{-\mu_e \cdot d} e^{-\frac{1}{2} tz D(E)} e^{-\frac{i}{2} tz A(E)} \rho_r(E) e^{\frac{i}{2} tz A^{\dagger}(E)} \qquad (12)$$

is sumed over N layers of thichness δ.

$$\rho(E) = \sum_{k=1}^{N} c \cdot \rho(E, k \cdot \delta) \qquad (13)$$

The attennuation factors are

$$I_r = \int_{-\infty}^{\infty} Tr(\rho(E)) dE \qquad (14)$$

$$I_{nr} = \sum_{k=1}^{N} c e^{-\mu_e \cdot k \delta}$$

4 Concentration profile

The preparation of the source by diffusion of the Co atoms deposited on the surface leads to an diffusion profile with decreasing concentration. The solution for the situation of a fixed number of atoms N/area deposited at the surface, which diffuse into the bulk for some time t can be found in the lecture about Fick's law
http://www.eng.utah.edu/ lzang/images/lecture-4.pdf The solution for the 1-dimensional problem is given by

$$c(z,t) = \frac{1}{\sqrt{\pi Dt}} exp \left(-\frac{z^2}{4Dt} \right) \tag{15}$$

$$1 = \int_0^\infty c(x,t)dx$$

The length $2\sqrt{Dt}$ is called the diffusion length (dependent on time t), which will be a fit parameter. It is no problem to insert the function $c(z = k\delta)$ instead of a constant c in Eq. 13 for $\rho(E)$ and in Eq. 14 for the attenuation coefficients.

5 Theory function of an absorption spectrum

If $\mathbf{n}(E(v))$ is the index of refraction of a moving absorber and d_A the thickness of the absorber the convolution integral

$$I(v) = \int_{-\infty}^{\infty} Tr\left(\rho(E, v, d_A) \right) dE \tag{16}$$

with

$$\rho(E, v, d_A) = e^{i\mathbf{n}(\mathbf{E},\mathbf{v})kd_A} \rho(E) e^{-i\mathbf{n}(\mathbf{E},\mathbf{v})^\dagger kd_A} \tag{17}$$

$I(v)$ concerns the fraction fC_M of reonant γ's. At $v = \pm\infty$ only the fraction $I(\pm\infty) = I_r$ of fC_M comes out of the source. The total counts of the baseline C_{base} are therefore the sum

$$C_{base} = C_B + I_r f C_M + I_{nr}(1 - f)C_M \tag{18}$$

At velocity v the number of counts are

$$\begin{aligned} C &= C_B + I(v)fC_M + I_{nr}(1 - f)C_M \tag{19}\\ &= C_B + I_r f C_M + I_{nr}(1 - f)C_M - I_r f C_M + I(v)fC_M \\ &= C_{base} - fC_M I_r(1 - I(v)/I_r) \end{aligned}$$

Factoring out C_{base}

$$C = C_{base}\left(1 - (1 - I(v)/I_r)\frac{fC_M I_r}{C_B + I_r f C_M + I_{nr}(1 - f)C_M}\right) \quad (20)$$

For an infinite thin source ($I_r = I_{nr} = 1$) the usual equation

$$
\begin{aligned}
C &= C_{base}\left(1 - (1 - I(v))f(1 - bf)\right) & (21)\\
bf &= \frac{C_B}{C_M + C_B}
\end{aligned}
$$

is obtained. The following equality should hold if the theory is correct:

$$
\begin{aligned}
f_{eff} &= \frac{I_r f}{I_r f + I_{nr}(1 - f)} & (22)\\
f(1 - bf) &= f_{eff}(1 - b)
\end{aligned}
$$

where f is the true f factor, bf the fitted background fraction and b the measured one. Inserting b the expected value for bf can be calculated with f_{eff}.

6 Concentration profile in a source

The selfabsorption in a source is caused by the same distribution of absorbing and the emitting nulei. The number of absorbing nuclei at depth $d = k\delta$ is then given by the sum

$$c(d) = \sum_{n=1}^{k} c(n) \quad (23)$$

An array $intc(k)$ with $intc(N) = 1$ is used in the program code.

References

[1] W. Sturhahn and A. Chumakov, Hyperfine Interactions **123/124**, 809824 (1999).