Contents

1 Intoduction

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
$1\mu\cdot7.8748$g/cm$^3 \cdot \sigma_0 \cdot 6.022 \cdot 10^{23}$/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 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 simulated.

2 Emission

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

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

$$
\begin{aligned}
1 &= Tr\left(\sum_i \frac{1}{2} r_i\right) \\
\begin{pmatrix} 1/2 & 0 \\ 0 & 1/2 \end{pmatrix} &= \int_{-\infty}^{\infty} \rho_r(E) dE
\end{aligned}
$$

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

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

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

$$
\rho(E, z) = e^{i\mathbf{n}kz} \rho_r(E) e^{-i\mathbf{n}^\dagger kz} \tag{3}
$$

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 an exponential distribution exp(-γd) with increasing depths d from the surface of the foil (see section 3.3). These are the cases which can be easily integrated.
The case a) is already described by eq. 2 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.2 is rewritten as

$$
\begin{aligned}
\rho(E, z) &= e^{-itz(A(E)+h(E))} \rho_r(E) e^{itz\left(A^\dagger(E)+h^\dagger(E)\right)} \qquad (4) \\
A(E) &= \sum_i \left(r_i - \frac{1}{2} Tr(r_i) \cdot \underline{1}\right) \cdot \frac{\Gamma/2}{E - E_i - i\Gamma/2} \\
h(E) &= \underline{1} \cdot \sum_i \frac{1}{2} Tr(r_i) \cdot \frac{\Gamma/2}{E - E_i - i\Gamma/2}
\end{aligned}
$$

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

$$\rho(E,z) = e^{-tzD(E)}e^{-itzA(E)}\rho_r(E)e^{itzA^\dagger(E)} \tag{5}$$

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

$$\begin{aligned} D(E) &= \underline{1} \cdot \sum_i \frac{1}{2} Tr(r_i) \cdot \left(-i \frac{\Gamma/2}{E - E_i - i\Gamma/2} + i \frac{\Gamma/2}{E - E_i + i\Gamma/2} \right) \\ &= \underline{1} \cdot \sum_i Tr(r_i) \cdot \frac{(\Gamma/2)^2}{(E-E_i)^2 + (\Gamma/2)^2} \end{aligned} \tag{6}$$

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 as the integral of trace $Tr(\rho_r(E))$ will be less then 1.

$$\begin{aligned} f_{eff} &= f \cdot \int_{-\infty}^{\infty} Tr(\rho(E,z))dE \\ &= f \cdot \int_{-\infty}^{\infty} Tr\left(e^{-tzD(E)}e^{-itzA(E)}\rho_r(E)e^{itzA^\dagger(E)} \right) dE \end{aligned} \tag{7}$$

f_{eff} gives an idea of the selfabsortion effect when comparing with the decrease of f-factors with the age of conventional sources.

3 Distribution

3.1 Constant concentration

The concentration N of ^{57}Co is constant fom the surface to a depth d.

$$N_t = \int_0^d N(z) * F dz \tag{8}$$

The total number is $N_t = N \cdot F \cdot d$ for the constant distribution such that $N(z) = N_t/(Fd)$. Each layer at z is an independent source the scattering spectra of which are added up. The declaration of several sources at increasing depths $\rho(E,d_j)$ weighted by w_j which can be chosen as fit parameters (effi alows for such a structure) would be a straightforward method to correct for selfabsorption.
The integral over z from the surface z=0 to the depth z=d can be partially integrated

$$
\begin{aligned}
N_t \cdot \rho_t(E,d) &= \int_0^d N(z) * F dz e^{-tzD(E)} e^{-itzA(E)} \rho_r(E) e^{itzA^\dagger(E)} \quad (9)\\
&= \frac{N_t}{d} \int_0^d dz e^{-tzD(E)} e^{-itzA(E)} \rho_r(E) e^{itzA^\dagger(E)}
\end{aligned}
$$

In $\int d(\varphi,\psi) = \int (d\varphi/dx)\psi dx + \int \varphi(d\psi/dx)dx$ the functions φ, ψ are chosen as

$$
\begin{aligned}
\varphi(z) &= \frac{-1}{tD} \cdot e^{-ztD} \quad (10)\\
\frac{d\varphi}{dz} &= e^{-ztD}\\
\psi(z) &= e^{-iztA(E)} \rho_r(E) e^{iztA^\dagger(E)} \quad (11)\\
\frac{d\psi}{dz} &= -itA(E)\psi + i\psi tA^\dagger(E) \quad (12)
\end{aligned}
$$

such that

$$
\begin{aligned}
-(tD)^{-1}\rho(E,z)|_0^d &= \int_0^d \rho(E,z)dz - \quad (13)\\
&\int_0^d \frac{-dz}{tD} \cdot e^{-ztD} \left(-itA(E)\psi + i\psi tA^\dagger(E)\right)
\end{aligned}
$$

since the diogonal matrix D commutes with A

$$
\begin{aligned}
-\rho(E,z)|_0^d &= tD \int_0^d \rho(E,z)dz \quad (14)\\
&\quad -itA(E) \int_0^d \rho(E,z)dz + i \int_0^d \rho(E,z)dz \cdot tA^\dagger(E)\\
I(E) &= \int_0^d \rho(E,z)dz
\end{aligned}
$$

Finally the integral I(E) is implicitly determined by a matrix equation

$$
(\rho(E,d) - \rho(E,0))/t = -D \cdot I(E) + iA(E) \cdot I(E) - iI(E) \cdot A^\dagger(E) \quad (15)
$$

The density matrix of the radiation of the source leaving the surface is according to eq.9 the matrix I(E) multiplied by N_t/d. For one ^{57}Co atom ($N_t = 1$ the equation for ρ_t reads

$$
(\rho(E,d) - \rho(E,0))/td = -D \cdot \rho_t(E) + iA(E) \cdot \rho_t(E) - i\rho_t(E) \cdot A^\dagger(E) \quad (16)
$$

3.2 Matrix equation

From the 2x2 matrix equation 16 an linear system of 4 equations are obtained. To be short $U = -(\rho(E,d) - \rho(E,0))/tdD$, $V = \rho_t(E)$ and $B = A/D$ (D was a real unit matrix) is defined

$$U = V - iB \cdot V + iV \cdot B^\dagger \tag{17}$$

The trace of matrix A is zero (see eq.4) so that $A_{22} = A_{11}$

$$U = \begin{pmatrix} 1 - i(B_{11} - B_{11}^*) & iB_{12}^* & -iB_{12} & 0 \\ iB_{21}^* & 1 - i(B_{11} + B_{11}^*) & 0 & -iB_{12} \\ -iB_{21} & 0 & 1 + i(B_{11} + B_{11}^*) & iB_{12}^* \\ 0 & -iB_{21} & iB_{21}^* & 1 + i(B_{11} - B_{11}^*) \end{pmatrix} \cdot V \tag{18}$$

The vectors of the linear equation are $U = (U_{11}, U_{12}, U_{21}, U_{22})$ and $V = (V_{11}, V_{12}, V_{21}, V_{22})$.

$$\begin{aligned} U &= (1 + iC) \cdot V \qquad (19) \\ V &= (1 + iC)^{-1} U \\ &= (1 - iC - C^2 - iC^3 - C^4 - ...)U \end{aligned}$$

If C is small the correction to $\rho_r(E)$ may obtained by the expansion series. If the source is not polarized the matrix A is zero, so that B=0 and U=V.

For $d \to \infty$ the matrix $\rho(E,d) \to 0$ such that for a constant density N $N_t/d = F$ (an infinite number of Co atoms $N_t = NFd$) the density matrix of the source multiplied by an effective number of atoms becomes $N_{eff}\rho_t(E) = NF/tD \cdot \rho(E,0)$ with $N_{eff} = NF/tD$. This result needs a further correction for electronic absorption which make the source atoms more and more invisible with increasing z.

At $d \to 0$ only the surface is aktiv. The expression $(\rho(E,d) - \rho(E,0))/d$ is the derivative $d\rho(E,z)7dz$ in the limit $d \to 0$. The derivation of the eq. 4 is just the right site of eq. 16 which is fulfilled for $\rho_t = \rho_r$.

3.3 Concentration profile

As already indicated above, the electronic absorption simulates a decreasing density of source atoms with increasing z. This can be taken

into account by an an exponential attenuation $exp(-\mu z)$ with the coefficient μ for electronic absorption.
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 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

$$c(z,t) = \frac{N}{\sqrt{\pi Dt}} exp\left(-\frac{z^2}{4Dt}\right) \tag{20}$$
$$N = \int_0^\infty c(x,t)dx$$

As shown in figure 1 the diffusion profile $\propto exp(-z^2)$ can be approximated by an exponemtial with 2 parameters $exp(-\alpha(z-z_d))$.

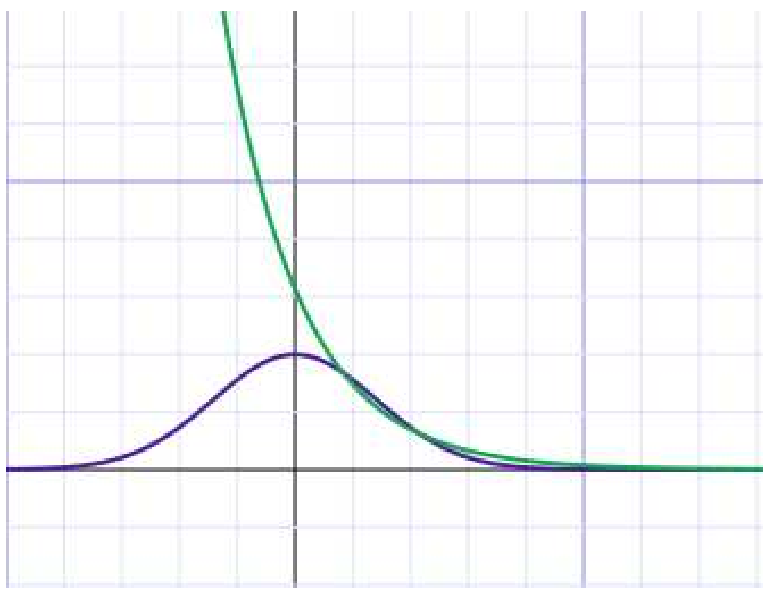

Figure 1: Comparison of $exp(-z^2)$ (blue) with $exp(-1.5 \cdot (z-0.3))$

Approximating the weight of the layer at z up to z=d by 1 and further by the function $exp(-\alpha(z-d))$ and over the whole range applying the attenuation $exp(-\mu z)$ for electronic absorption describes the self-absorption effect by 3 parameters $\alpha, d, and\, \mu$. μ can be considered as known from the electronic absorption of 14.4 keV of iron metal.

$$N_t \cdot \rho_t(E,d) = \int_0^d F dz \cdot e^{-\mu z} \cdot e^{-tzD(E)} e^{-itzA(E)} \rho_r(E) e^{itzA^{\dagger}(E)} + \tag{21}$$

$$\int_d^\infty F dz \cdot e^{-(\mu z+\alpha(z-d))} \cdot e^{-tzD(E)} e^{-itzA(E)} \rho_r(E) e^{itzA^\dagger(E)}$$

Since the unit matrix is just treated as a number, the exponential with with $(\mu+\alpha)z$ is added to D(E)z. The solution of the integral is given by the same routine.
The total number N_t is the integral

$$\begin{aligned} N_t &= N \int_0^d F dz + N \int_d^\infty F dz \cdot e^{-\alpha(z-d)} \\ &= NFd + NF/\alpha \end{aligned} \tag{22}$$

References

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