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## 1 Introduction

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

$1\mu \cdot 7.8748\text{g}/\text{cm}^3 \cdot \sigma_0 \cdot 6.022 \cdot 10^{23} / \text{atomic\_weight} \cdot \text{abundance} \cdot \text{f-factor} = 0.465 \cdot \text{f-factor}$ . W. Sturhahn and A. Chumakov measured the f-factor of polycrystalline iron foils [2] 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  $1\mu$  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  $\gamma$ -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  $\theta = 90^\circ$  with respect to the  $\gamma$ -direction. Calculating the source function with an angle less than  $\theta = 90^\circ$ , 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  $r_i$ :

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

The total intensity, sum over all Lorentzians, is normalized to 1.  $\Gamma$  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  $E_i^j$ .

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

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

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

with the unit 2x2 matrix  $\underline{1}$ , the cross section  $\sigma$ , 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

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

The electronic absorption  $\exp(-\mu_e z)$  shall be included later. In the following the double sum is written as a sum over  $i$  only for simplicity. Several simplifications for the selfabsorption of a  $^{57}\text{Co}$  in  $\alpha$ -iron are introduced. First of all the  $f$ -factor is taken to be isotropic. The profile of the distribution of the  $^{57}\text{Co}$  diffused into the  $\alpha$ -iron foil is simplified

to a) an  $\delta$ -function, b) uniform distribution, and a distribution given by some function  $C(z)$ , i.e a diffusion 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  $\alpha$ -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

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

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

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

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

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

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

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

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

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

$$td = \sigma_0 f(\mathbf{k}) N d \quad (8)$$

$$N = 6.022 \cdot 10^{23} / \text{atomic\_weight} \cdot \text{density} \cdot \text{abundance}$$

$$t = 0.465 \mu^{-1} \cdot f(\mathbf{k})$$

The density matrix of the source radiation in case a) with all  $^{57}\text{Co}$  at a depth of  $z=d$  in  $\alpha$ -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 the fact that the resonant part  $f$  of radiation is absorbed more strongly than the non-resonant part  $(1-f)$  which is only attenuated by electronic

absorption  $\exp(-\mu_e \cdot z)$  (absorption coefficient  $\mu_e$ ).  $I_r$  shall denote the fraction of resonant and  $I_{nr}$  of non-resonant  $\gamma$ 's

$$\begin{aligned} I_r &= e^{-\mu_e \cdot d} \int_{-\infty}^{\infty} Tr(\rho(E, d)) dE \\ I_{nr} &= e^{-\mu_e \cdot d} \end{aligned} \quad (9)$$

then the effective Lamb-Mossbauer factor is the ratio

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

### 3 Constant concentration

The concentration  $^{57}\text{Co}$  is taken constant from 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 replaced by a sum with weights/concentrations  $c$  and thickness  $\delta$ .

$$\begin{aligned} \delta &= d/N \quad c = 1/N \\ \sum_{j=1}^N c &= 1 \end{aligned} \quad (11)$$

$\rho$  from Eq. 6 multiplied by the attenuation factor of electronic absorption

$$\rho(E, z) = e^{-\mu_e \cdot d} e^{-\frac{1}{2}tzD(E)} e^{-\frac{i}{2}tzA(E)} \rho_r(E) e^{\frac{i}{2}tzA^\dagger(E)} \quad (12)$$

is summed over  $N$  layers of thickness  $\delta$ .

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

The attenuation factors are

$$\begin{aligned} I_r &= \int_{-\infty}^{\infty} Tr(\rho(E)) dE \\ I_{nr} &= \sum_{k=1}^N c e^{-\mu_e \cdot k\delta} \end{aligned} \quad (14)$$

## 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/~ljang/images/lecture-4.pdf> The solution for the 1-dimensional problem is given by

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

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

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  $n(E(v))$  is the index of refraction of a moving absorber and  $d_A$  the thickness of the absorber the convolution integral

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

with

$$\rho(E, v, d_A) = e^{in(\mathbf{E}, \mathbf{v})kd_A} \rho(E) e^{-in(\mathbf{E}, \mathbf{v})^\dagger kd_A} \quad (17)$$

$I(v)$  concerns the fraction  $fC_M$  of resonant  $\gamma$ '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

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

At velocity  $v$  the number of counts are

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

Factoring out  $C_{base}$

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

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

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

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

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

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 nuclei. 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.

## 7 Source localized in 3 dimension [1]

It is straightforward to verify that the product of three prototypical solutions, with spatial variables  $x$ ,  $y$  and  $z$ , respectively,

$$c(x, y, z, t) = \frac{M}{(\sqrt{4\pi Dt})^3} \exp\left(-\frac{x^2 + y^2 + z^2}{4Dt}\right) \quad (24)$$

is a solution to the 3D equation. Obviously, this is the solution to the case of a localized and instantaneous release, at location  $(0,0,0)$  and

at time  $t = 0$  of a quantity  $M$  of the substance. In contrast to the 1D situation, where  $M$  was expressed in units of substance per unit cross-section, the quantity  $M$  here is in units of substance (example: in grams). Since  $r = \sqrt{x^2 + y^2 + z^2}$  is the distance to the point of release, the concentration  $c$  depends on that distance and time only. It does not depend on the direction with respect to the coordinate axes. Physically, the spreading is identical in all directions of space; diffusion is said to be isotropic. The size of the 3D 'cloud' is measured by the diametrical span

$$4\sigma = 4\sqrt{2Dt} \quad (25)$$

### 7.1 Anisotropic medium

In most environmental systems (atmosphere, rivers, lakes and oceans), turbulence in the vertical direction differs greatly from that in the two horizontal directions, chiefly because of gravity. As a result, diffusion does not proceed at the same rates in the horizontal and vertical directions. If we generalize and imagine that all three directions are different from one another, then we are brought to define three distinct diffusion coefficients:

$$\begin{aligned} D_x \quad \text{diffusion in the } x - \text{direction} : q_x &= -D_x \frac{\partial c}{\partial x} \\ D_y \quad \text{diffusion in the } y - \text{direction} : q_y &= -D_y \frac{\partial c}{\partial y} \\ D_z \quad \text{diffusion in the } z - \text{direction} : q_z &= -D_z \frac{\partial c}{\partial z} \end{aligned} \quad (26)$$

the diffusion equation becomes

$$\frac{\partial c}{\partial t} = \frac{\partial}{\partial x} \left( D_x \frac{\partial c}{\partial x} \right) + \frac{\partial}{\partial y} \left( D_y \frac{\partial c}{\partial y} \right) + \frac{\partial}{\partial z} \left( D_z \frac{\partial c}{\partial z} \right) \quad (27)$$

and the solution to an instantaneous ( $t = 0$ ) and localized ( $x = y = z = 0$ ) release is:

$$c(x, y, z, t) = \frac{m}{(\sqrt{4\pi t})^3 \sqrt{D_x D_y D_z}} \exp \left( -\frac{x^2}{4D_x t} - \frac{y^2}{4D_y t} - \frac{z^2}{4D_z t} \right) \quad (28)$$

The spatial dimensions of the corresponding 3D cloud are measured by 3 equations of type Eq.25 with indices  $x, y, z$ .

## 7.2 Presence of a horizontal boundary

As for 1D problems, the preceding solution can serve as a building block for the construction of more realistic 3D applications. An important problem is that of a 3D instantaneous and punctual release near a boundary, such as an explosion in the air at some height (say  $z = H$ ) above the ground (say  $z = 0$ ). The ground, which we take to be flat and horizontal for simplification, acts as an impermeable horizontal boundary and requires that the vertical component of the diffusive flux be zero at that level ( $q_z = 0$  at  $z = 0$ ). This condition is accommodated by introducing a virtual release of the same amount at the same time and at a symmetric position below the ground ( $z = -H$ ). The solution then consists in the sum of two prototypical solutions, one caused by the actual release at ( $x = 0, y = 0, z = +H$ ) and the other due to the image at ( $x = 0, y = 0, z = -H$ ):

$$c(x, y, z, t) = \frac{m}{(\sqrt{4\pi t})^3 \sqrt{D_x D_y D_z}} \exp\left(-\frac{x^2}{4D_x t} - \frac{y^2}{4D_y t}\right) \cdot \left[ \exp\left(-\frac{(z-H)^2}{4D_z t}\right) + \exp\left(-\frac{(z+H)^2}{4D_z t}\right) \right] \quad (29)$$

where  $M$  is the amount released (e.g., mass) at time  $t = 0$ . The horizontal coordinates  $x$  and  $y$  are measured along the ground, with the origin at the vertical below the point of release. Of interest is the ground concentration,  $c_{ground} = c(x, y, z = 0, t)$ , which is:

$$c_{ground}(x, y, t) = \frac{m}{(\sqrt{4\pi t})^3 \sqrt{D_x D_y D_z}} \exp\left(-\frac{x^2}{4D_x t} - \frac{y^2}{4D_y t} - \frac{H^2}{4D_z t}\right) \quad (30)$$

The ground concentration is highest at the vertical below the release location ( $x = y = 0$ ) and decreases away with distance from there. Only when  $D_x$  and  $D_y$  are equal is this decrease 2D isotropic. At any time  $t$ , the maximum ground concentration is thus:

$$c_{ground}(t) = \frac{m}{(\sqrt{4\pi t})^3 \sqrt{D_x D_y D_z}} \exp\left(-\frac{H^2}{4D_z t}\right) \quad (31)$$

## 7.3 Source over a finite area

This problem can be solved by superposition of many prototypical solutions. If a localized release occurs not at  $r = 0$  but at  $x = \xi, y = \eta$ ,

then the solution is simply shifted by the distance  $\xi, \eta$ :

$$c(x, y, z, t) = \frac{M(\xi, \eta)}{(\sqrt{4\pi t})^3 \sqrt{D_x D_y D_z}} \exp\left(-\frac{(x - \xi)^2}{4D_x t} - \frac{(y - \eta)^2}{4D_y t}\right) \cdot 2 \left[ \exp\left(-\frac{(z)^2}{4D_z t}\right) \right] \quad (32)$$

The generalization to three and more punctual releases is straightforward. For a continuous release, we add an infinite number of tiny releases collectively covering a finite interval. If in 1 dimension the release the  $[\xi, \xi + d\xi]$  interval is  $dM(\xi) = c_0(\xi)d\xi$ , then

$$c(x, y, z, t) = \exp\left(-\frac{z^2}{4D_z t}\right) \int_{-\infty}^{+\infty} d\xi d\eta \frac{c_0(\xi, \eta)}{(\sqrt{4\pi t})^3 \sqrt{D_x D_y D_z}} \cdot \exp\left(-\frac{(x - \xi)^2}{4D_x t} - \frac{(y - \eta)^2}{4D_y t}\right) \quad (33)$$

The function  $c_0(\xi, \eta)$  is the initial concentration. The z- dependence is the same for any  $x, y$ .

#### 7.4 The real source

A conventional  $^{57}\text{Co}$  source diffused into Rh(Cu,...)-matrix has a diameter of ca. 5mm and a thickness of 6-7 $\mu$ . The typical diffusion length of 2-3 $\mu$  ; 6-7 $\mu$  is by a factor of 100 smaller than the diameter of the foil of the source. This means that the diffusion in the direction of the plane is negligible. If the initial concentration on the surface is homogeneous over some fraction of the foil the diffusion profile is essentially only dependent on z. A diffusion theory in 3-dimension is not necessary. If the active area is 3mm in diameter the area of the margin is about 4% where the activity will be less. Very likely the homogeneity over the 3mm is even worse.

## References

- [1] Benoit Cushman-Roisin, Engineering at Dartmouth, Hanover, New Hampshire 03755 USA.
- [2] W. Sturhahn and A. Chumakov, Hyperfine Interactions **123/124**, 809824 (1999).