DETERMINATION OF DEBYE TEMPERATURE FROM MÖSSBAUER DATA.

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ABSTRACT

The temperature dependence of Lamb-Mössbauer factor (W) from Mössbauer data has been fitted using numerical calculation in C-language. It is common ground, that the absorption area of the Mössbauer spectrum is proportional to recoilless fraction of Mössbauer atoms (f). In order to study the dynamical lattice properties of the solid is common to use the Debye model. This program allow us to estimate the Debye temperature (θ_D). In spite, the Debye model may be a poor description, particularly for complicated solids or systems with high impurity concentrations, we had perform it in some diluted sample. It is open the possibility to introduce the anharmonicity of the lattice vibrations in order to improve the model.

Key-words: Mössbauer; Debye temperature in diluted alloy; C-language.

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1. INTRODUCTION.

It is common ground that the Mössbauer Effect is related to nuclear resonant absorption and emission process of γ radiation in a recoil-free, i.e., without any loss energy to the lattice The ***f factor*** measures the probability no phonons are created or annihilated in connection with the γ decay. The temperature dependence of ***f factor*** is related to the lattice dynamics of the solids. The lattice vibration behavior can be studied by Mössbauer spectroscopy [Ref. 1] through the temperature (T) dependence of absorption areas of the Mössbauer spectrum. By assuming the harmonic oscillators model for solids, the ***f factor*** is often written as $f = exp(-2W)$. The Debye model leads to:

$$2W = [\frac{-6E_R}{k\theta_D}\{\frac{1}{4} + (\frac{T}{\theta_D})^2 \int_0^{\theta_D/T} (\frac{x dx}{e^x - 1})\}], \qquad (1)$$

where E_R is a recoil energy of Mössbauer atom and k is Boltzmann constant. This expression takes no account anharmonicity of the lattice vibrations. The integral in the expression (1) has not analytical value and in order to solve it, we used a subroutine in C-language that use the optimized trapezium method to calculation it [ref. 2].

We use C-language in order to build a program for fit the experimental data from the area of the Mössbauer spectra using the expression (1). This fit allow us to get the Debye temperature. The C-language has been used because the run time is faster than the other one. On the other hand, C-language is a structure language and give us possibility to use functions already known. The idea of this work was to fit the experimental data of Mössbauer measurements with the expression (1), obtaining the Debye temperature correspondent. Usually the results of Debye temperature are obtained by fit of the Mössbauer data using the expression (1) in two limit values ($T \rightarrow 0$, $T > \theta_D/2$).

2 - THEORY AND METHOD OF CALCULATION.

The Fig. 1 show the flux diagram of main program, and it was built in three steps. ***In the first part***, the experimental data are read from the hard disk. To run of the program, it needs the values of the areas of the spectra for each temperature, the initial value (θ_D^0) and the step ($\Delta\theta$) for the change of the Debye temperature. The

areas are normalized respect to median value of the area of the three firsts spectra in low temperature. ***In the second step***, it makes the calculation of the normalized function $F_t[T,K]$, from eq. (1), where K is a parameter, such as:

$$\theta_D[K] = \theta_D^0 + (K-1)*\Delta\theta, \quad K \leq \text{NTHETA}, \tag{2}$$

this part will be explain with more detail in the next point. ***On the end step***, the theoretical graphics, superimposed by the experimental data, and the relevant numerical parameters in the evolution of fits for the different values of the Debye temperature are shown on the screen and are salve in the output file.

The fit calculation have two parts:

(a) The evaluation of the integral in expression (1). This integral show a divergence problem at T = 0. In order to solve this problem, we divide the integral in two parts, for one assumed value of θ_D. The algorithm is the same for two parts. The Fig. 2 shows the flux diagram for the calculation of the integral and for the ***f factor*** theoretical normalized: $F_{theo}[T,K]$. The part about T = 0 is developed using power series.

The integrals are calculated by simple method of the trapezium sum. This method [ref. 2] is implemented in optimized form, such that increase the number of trapezium, utilizing the lowest interactions. Firstly, calculated the value of function in the extremes of interval, after take the value of integral in middle point. At second step, the values of integral will be calculated in 1/4 and 3/4; at third step 1/8, 3/8, 5/8 and 7/8 and go on. The numbers of trapezium for each step (interaction) increase with power of 2^n, and the number n of interactions increases until the value of the integral increase less than a ε value (ε = 0.001). This value is defined taking account the errors of approximation implicit on numerical calculation.

(b) Calculation of the end value of θ_D ***(fit parameter).*** It is determined by change θ_D^0 with step selected, and the error of numerical fit, obtained by least square method, is calculated for each situation and finally is selected the best θ_D.

3 - APPLICATIONS.

The absorption area of Mössbauer spectrum is related to the number of atoms that absorber γ-ray without loss energy to the lattice, i.e. proportional to ***f fator***. This program was applied on the Mössbauer data of thin film obtained from vapor quenching of Fe diluted in the matrix of Ho.

The temperature dependence Mössbauer spectra have been done ***IN SITU***, i.e. the measurements were done keeping the same conditions that were obtained

during the preparation of the films. The Mössbauer spectra as a function of temperature for $Fe_{0.05}Ho_{0.95}$ film is showed in the Fig.3. The spectra were fitted using a conventional program wrote by Brand et al [ref. 3]. The fits for the sample were made using a broad symmetric doublet, which was associated to quadrupole interactions at Fe nucleus. The line width of doublet decrease with increase of temperature, indicating that about 60 K there is a magnetic transition. This broadening can be interpreted by a continue distribution of Fe sites, characteristic of disordered systems. The fig. 3 shows the behavior of the normalized absorption area (normalized with respect average of the three firsts values at low temperature) obtained from the fits of the Mössbauer spectra as a function of temperature, and the correspondent theoretical function of ***f fator*** that gives us the best χ^2 . The values of Debye temperature obtained from the fit is 190(3) K for films. In general, the Debye temperature for pure Ho obtained by specific heat method is higher than that obtained from Mössbauer measurements.

In this report, we are not interested in details about physics of the problem, but we can say that the Debye temperature obtained from Mössbauer measurements is different than that obtained by specific heat or any other bulk techniques measurements for the matrix of Ho, because the Fe impurity, that is necessary to measure Mössbauer, has different mass of the atoms of the Matrix. On the other hand, in Debye model only harmonic term go in to the potential energy. To improve the values of Debye temperature obtained from the fit, we must use the anharmonicity terms in Debye model. The Debye temperature can also be obtained from linear equation obtained from the limit at high temperature ($T > \theta_D/2$).

Reference:

[1] E. Baggio-Saitovitch, R.B. Scorzelli, I. Souza Azevedo and F. J. Litterst, Hyperfine Interactions, 70 (1992) 1231.

[2]W.H. Press, B.P. Flannery, S.A. Teukolsky, W.T. Vetterling. Numerical Recipes in C. Cambridge University Press (1989).

[3] R. A. Brand, Duisburg University (1998).

Figures Captions:

Fig. 1 - Flux diagram of the main program for the calculation the Debye temperature using expression (1).

Fig. 2 - Flux diagram for the calculation of integral of the expression (1).

Fig. 3 - ^{57}Fe Mössbauer spectra obtained In Situ for the $Fe_{0.05}Ho_{0.95}$ film as a function of temperature.

Fig. 4 - f fator normalized as function of temperature for film of Fe diluted in matrix of Ho. The sinbols correspond to experimental data, while full line is the result of theoretical f fator obtained from the expression (1) for the best fit.

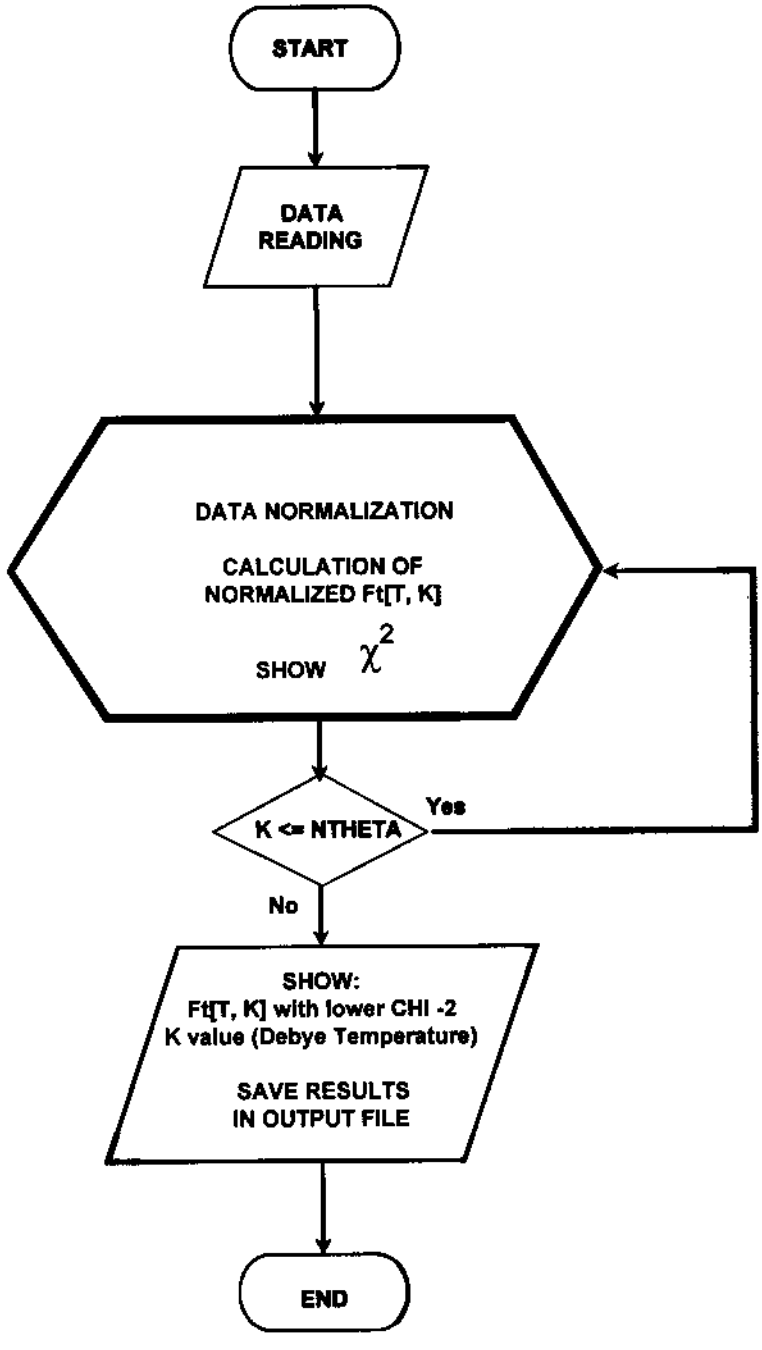
START
DATA READING
DATA NORMALIZATION
CALCULATION OF NORMALIZED Ft[T, K]
SHOW χ^2
K <= NTHETA
Yes
No
SHOW:
Ft[T, K] with lower CHI -2
K value (Debye Temperature)
SAVE RESULTS IN OUTPUT FILE
END

Fig. 1

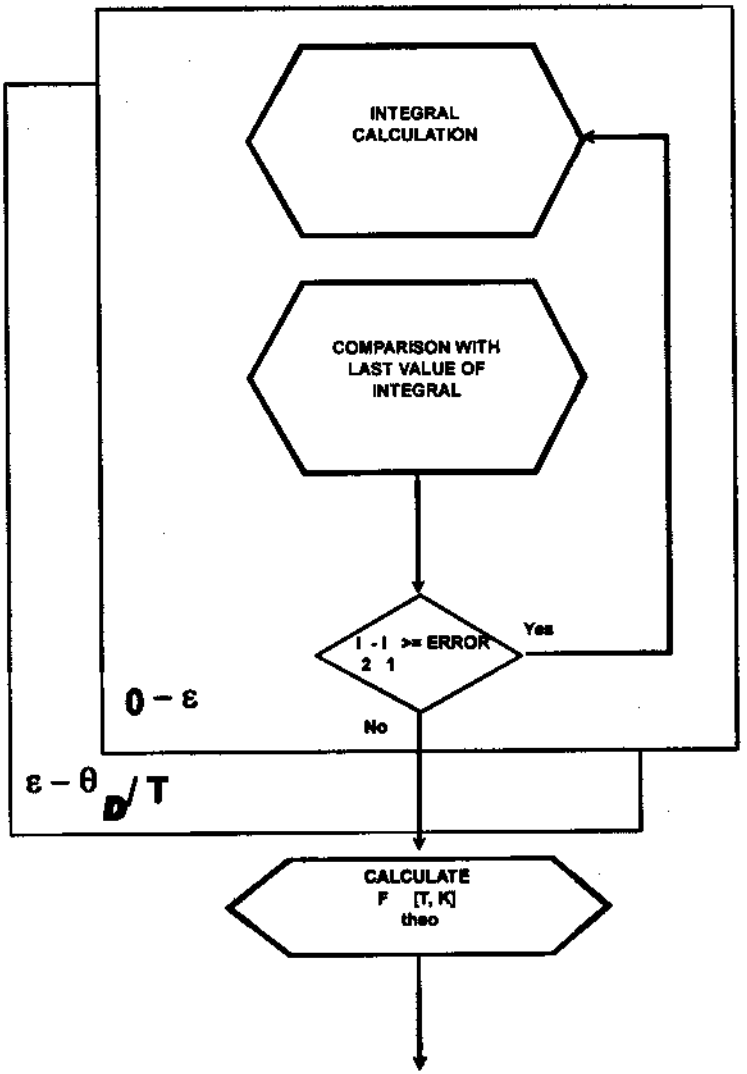
INTEGRAL CALCULATION
COMPARISON WITH LAST VALUE OF INTEGRAL
I - I >= ERROR
2 1
Yes
No
0 – ε
ε – θ D/T
CALCULATE F [T, K]
theo

Fig. 2

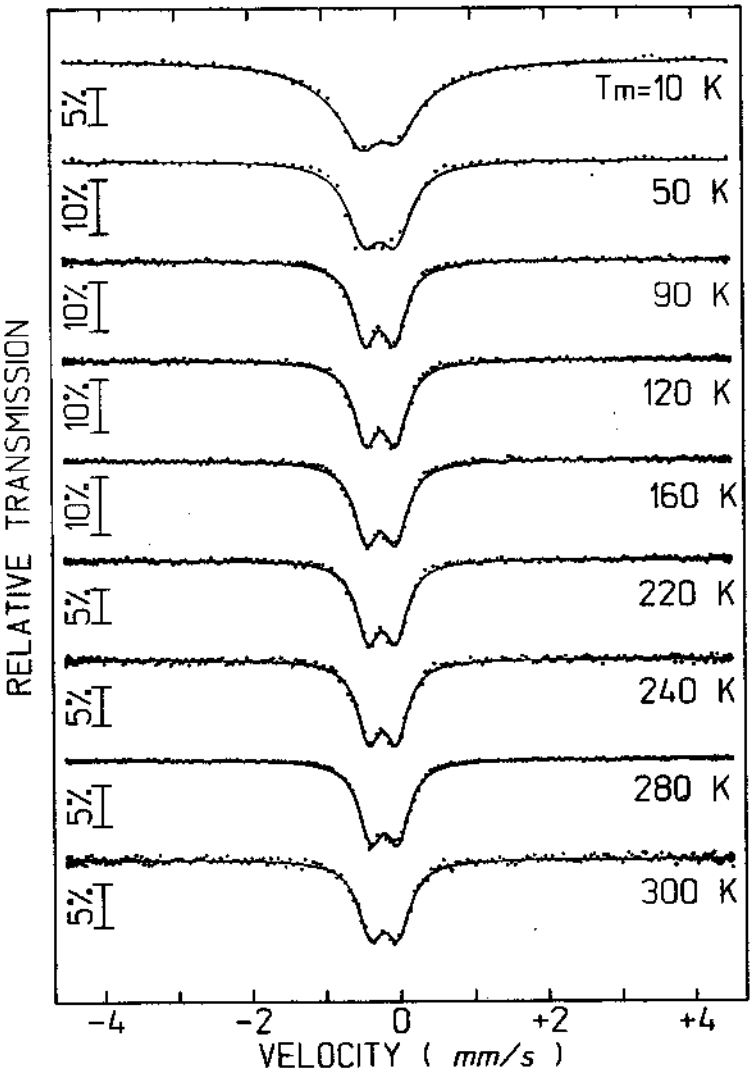
RELATIVE TRANSMISSION
5%
Tm=10 K
10%
50 K
10%
90 K
10%
120 K
10%
160 K
5%
220 K
5%
240 K
5%
280 K
5%
300 K
-4
-2
0
+2
+4
VELOCITY (mm/s)

Fig. 3

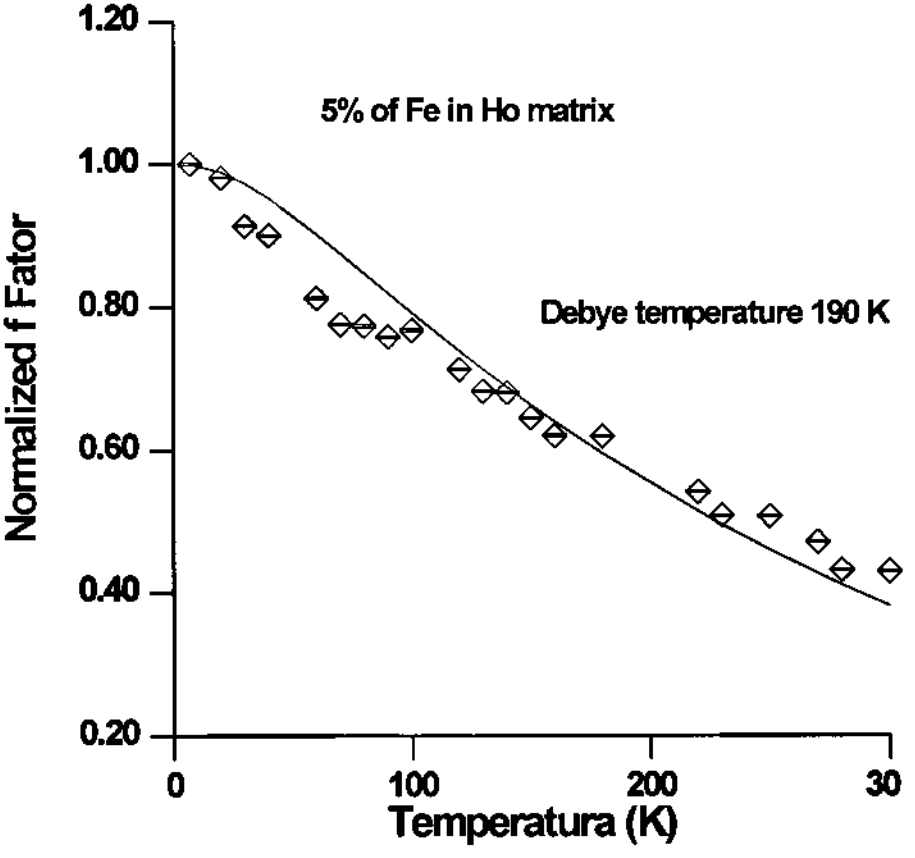
1.20
1.00
0.80
0.60
0.40
0.20
Normalized f Fator
5% of Fe in Ho matrix
Debye temperature 190 K
0
100
200
30
Temperatura (K)

Fig. 4