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Primärbericht

MUPHOCOR, a Fortran Program to Determine
the Phonon Density of States from Neutron
Scattering Experiments

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1. INTRODUCTION

It has been demonstrated first by Oskotskii (1) that also for coherent scatterers the phonon density of states (PDOS) can be determined by an inelastic neutron scattering experiment with a polycrystalline sample if the scattering cross-section is integrated over a large range of momentum transfers Q . This special kind of incoherent approximation reads:

$$\int_{Q_{\min}}^{Q_{\max}} \left(\frac{d^2\sigma}{d(\hbar\omega) d\Omega} \right)_{\text{coh}} Q dQ \cong \int_{Q_{\min}}^{Q_{\max}} \left(\frac{d^2\sigma}{d(\hbar\omega) d\Omega} \right)_{\text{inc}} Q dQ \quad (1.1)$$

It is valid if

$$(Q_{\max} - Q_{\min}) \gg \frac{2\pi}{d} \quad (1.2)$$

d is the distance between nearest neighbors in the sample and Q_{\max} and Q_{\min} are the maximum and minimum momentum transfers in the experiment.

For a direct geometry time-of-flight (TOF) experiment with a multidetector between the scattering angles θ_{\min} and θ_{\max} Eq. 1.1 is equivalent to

$$\int_{\theta_{\min}}^{\theta_{\max}} \left(\frac{d^2\sigma}{d(\hbar\omega) d\Omega} \right)_{\text{coh}} \sin\theta d\theta \cong \int_{\theta_{\min}}^{\theta_{\max}} \left(\frac{d^2\sigma}{d(\hbar\omega) d\Omega} \right)_{\text{inc}} \sin\theta d\theta \quad (1.3)$$

Thus, the TOF-spectra for coherent scatterers weighted by $\sin\theta$ and integrated over all scattering angles can be treated to a good approximation with the theory of incoherent scattering.

The Fortran program MUPHOCOR extracts the PDOS (for polyatomic sample the generalized phonon density of states GPDOS) from the $\sin\theta$ -weighted, angle integrated TOF spectrum. As the PDOS must be derived from the one-phonon part of the inelastic scattering cross-section corrections for multi-phonon processes are applied in a self-consistent way.

1 Ph.

$$\frac{\partial \sigma}{\partial \omega} =$$

$$d_i =$$

This report describes the performance of MUPHOCOR and provides a listing of the input data.

$$\bar{G} =$$

2. BASIC FORMALISM

$$\bar{\Pi} =$$

We shall deal first with the case of a monatomic system and discuss afterwards the extension to systems with several atomic species. The phonon expansion of the incoherent scattering cross-section has been treated extensively by Sjölander (2). We use his results for the symmetric formulation in a slightly rearranged form:

F(t)

S(t)

$$\left(\frac{d^2 \sigma}{d(\hbar\omega) d\Omega} \right)_{inc} = \frac{\sigma}{4\pi} \frac{k_1'}{k_0} e^{-\hbar\omega/2k_B T} e^{-\gamma Q^2} \sum_{n=1}^{\infty} \left(\frac{\hbar^2 Q^2}{2M} \right)^n \frac{T_n(\hbar\omega)}{n!} \quad (2.1)$$

- k_0, k_1 : wave number of the neutron before and after the scattering
- M : atomic mass
- σ : bound neutron cross-section (in case of the incoherent approximation σ is the total cross-section)

$$Q^2 = k_0^2 + k_1^2 - 2k_0 k_1 \cos\theta$$

$$\gamma = \frac{\hbar^2}{2M} \int_0^{\infty} \frac{F(\hbar\omega)}{\hbar\omega} \cosh \frac{\hbar\omega}{2k_B T} d(\hbar\omega) \quad \text{Debye-Waller coefficient}$$

$F(\hbar\omega)$: Phonon density of states

The functions $T_n(\hbar\omega)$ in the expansion series can be calculated by a recursion formula

$$T_n(\hbar\omega) = \int_0^{\hbar\omega} T_1(\hbar\omega - \hbar\omega') T_{n-1}(\hbar\omega') d(\hbar\omega') \quad (2.2)$$

with the one phonon term

$$q^2 = k_i^2 + k_f^2 - 2k_i k_f \cos \Theta$$

$$q = \sqrt{\dots}$$

$$\frac{dq}{d\Theta} = \frac{1}{2} \frac{1}{\sqrt{\dots}} \cdot 2k_i k_f \sin \Theta$$

$$T_1(\hbar\omega) = \frac{F(\hbar\omega)}{2\hbar\omega \sinh \frac{\hbar\omega}{2k_B T}} = \frac{1}{f(\omega)} n_B(\omega) \cdot g(\omega) \cdot e^{\frac{\hbar\omega}{2k_B T}} \quad (2.3)$$

$n_B(\omega)$ - Bose-Faktor

As was explained in the introduction we are interested in a special angle integrated cross-section $\frac{d\sigma}{d(\hbar\omega)}$, which is exact for the incoherent case and a very good approximation also for the coherent case

$$\frac{d\sigma}{d(\hbar\omega)} = \int_{\Theta_{\min}}^{\Theta_{\max}} \left(\frac{d^2\sigma}{d(\hbar\omega) d\Omega} \right) \sin\Theta d\Theta = \int_{Q_{\min}}^{Q_{\max}} \left(\frac{d^2\sigma}{d(\hbar\omega) d\Omega} \right) \frac{Q dQ}{k_o k_i}$$

$$= \frac{\sigma}{8\pi} \frac{e^{-\hbar\omega/2k_B T}}{k_o^2} \sum_{n=1}^{\infty} \frac{T_n(\hbar\omega)}{n!} \left(\frac{\hbar^2}{2M} \right)^n \frac{1}{Y^{n+1}} (I_n(\gamma Q_{\max}^2) - I_n(\gamma Q_{\min}^2))$$

(2.4)

$I_n(x)$ is defined by

$$I_n(x) = \int_0^x u^n e^{-u} du$$

$$\frac{dQ^2}{dQ} = 2Q \quad \rightarrow \quad Q dQ = \frac{1}{2} dQ^2$$

$$\tau Q^2 := \bar{Q}^2 \quad \rightarrow \quad \frac{d\bar{Q}^2}{dQ^2} = \tau \quad \Rightarrow \quad \frac{1}{\bar{Q}^{n+1}}$$

(2.5)

For example:

$$I_1 = -(x+1)e^{-x}$$

$$I_2 = -(x^2 + 2x + 2)e^{-x} = -x^2 - 2 \cdot I_1$$

$$I_3 = -(x^3 + 3x^2 + 6x + 6)e^{-x} = -x^3 e^{-x} - 3 \cdot I_2$$

For $\gamma Q_{\max}^2 \ll 1$ and $\gamma Q_{\min}^2 \ll 1$ (low temperatures and large M) we can expand the exponential and omit the higher order terms which leads to the one phonon approximation

$$\left(\frac{d\sigma}{d(\hbar\omega)} \right) (1) = \frac{\hbar^2}{8\pi} \frac{\sigma}{k_i^2} \frac{1}{e^{\hbar\omega/k_B T} - 1} \frac{1}{M} \frac{F(\hbar\omega)}{\hbar\omega} (Q_{\max}^4 - Q_{\min}^4) \quad (2.6)$$

$$= h(k_i, \hbar\omega) F(\hbar\omega) \quad (2.7)$$

$$e^{-u} = \sum_{j=0}^{\infty} \frac{1}{j!} (-u)^j$$

$$\rightarrow \int_0^x u^n e^{-u} du \approx \int_0^x u^n (1 - u + \frac{1}{2}u^2 - \dots) du = \left[u^{n+1} - \dots \right]_0^x$$

$$n=1 \rightarrow u^2 \Big|_0^x = \frac{1}{2} x^2$$

$$\text{where } h(k_i, \hbar\omega) = \frac{\hbar^2}{8} \frac{\sigma}{k_i^2} \frac{1}{\hbar\omega (e^{\hbar\omega/k_B T} - 1)} \frac{1}{M} (Q_{\max}^4 - Q_{\min}^4)$$

Eq. 4 is the basis for determining the phonon density of states with MUPHOCOR for a monatomic system. It will be shown below it may be applied also to samples containing several atomic species if suitable average properties of the system are used.

In the incoherent approximation, the cross-section of a compound is given by the sum of the partial cross-sections of the components weighted with their concentrations c_i

$$\frac{d^2\sigma}{d(\hbar\omega)} = \sum_i c_i \left(\frac{d\sigma}{d(\hbar\omega)} \right)_i, \quad \sum_i c_i = 1 \quad (2.8)$$

Each partial cross-section in the sum is an expression identical to Eq. (2.4) with σ , M and $F(\hbar\omega)$ replaced by the corresponding quantities σ_i , M_i and $F_i(\hbar\omega)$ where $F_i(\hbar\omega)$ is defined as

$$F_i(\hbar\omega) = \frac{1}{N} \sum_{j, \vec{q} < \text{BZ}} |\vec{p}_i^j|^2 \delta(\hbar\omega - \hbar\omega_j(\vec{q})) \quad (2.9)$$

Here \vec{p}_i^j is the polarization vector of atom i associated with the j^{th} phonon branch.

The total density of states is given by

$$F(\hbar\omega) = \sum_i c_i F_i(\hbar\omega) \quad (2.10)$$

The one phonon approximation (corresponding to Eq. 2.6) yields

$$\left(\frac{d\sigma}{d(\hbar\omega)} \right)^{(1)} = \frac{\hbar^2}{8\pi k_0^2} \frac{1}{\hbar\omega \cdot (e^{-\hbar\omega/k_B T} - 1)} (Q_{\max}^4 - Q_{\min}^4) \sum_i \frac{c_i \sigma_i}{M_i} F_i(\hbar\omega) \quad (2.11)$$

Introducing the generalized phonon density of states

$$G(\hbar\omega) = \sum_i \alpha_i F_i(\hbar\omega) \quad (2.12)$$

and average values for the cross-section and the mass defined by

$$\bar{\sigma} = \sum_i c_i \sigma_i \quad (2.13)$$

$$\bar{M} = \sum_i \alpha_i M_i \quad (2.14)$$

$$\text{with } \alpha_i = \frac{c_i \sigma_i / M_i}{\sum_j c_j \sigma_j / M_j} = \frac{c_i \sigma_i / M_i}{\frac{2 \cdot c_D \sigma_D}{M_D} + \frac{c_0 \sigma_0}{M_0}} = \frac{c_i \sigma_i / M_i}{\frac{1}{3} \sigma_D + \frac{1}{48} \sigma_0} \quad (2.15)$$

we arrive at

$$\left(\frac{d\sigma}{d(\hbar\omega)} \right)^{(1)} = \frac{\hbar^2 \bar{\sigma}}{8\pi k_0^2} \frac{1}{\hbar\omega (e^{-\hbar\omega/k_B T} - 1)} (Q_{\max}^4 - Q_{\min}^4) \frac{1}{\bar{M}} G(\hbar\omega) \quad (2.16)$$

This expression is identical to Eq. 2.6. An inspection of Eq. 2.4 shows that this equivalence does not hold for the higher phonon terms. Nevertheless, this relation, written in terms of $G(\hbar\omega)$, $\bar{\sigma}$ and \bar{M} as defined by Eqs. 2.13 - 2.14 often represents a rather good approximation as can be shown by a simple argument:

Calculating an effective Debye Waller coefficient γ_G using $G(\hbar)$ and \bar{M} we arrive at the following relation

$$\bar{M} \gamma_G = \gamma_G \sum_i \alpha_i M_i = \sum_i \alpha_i M_i \gamma_i \quad (2.17)$$

For equal γ_i 's, which is reasonably well fulfilled for many systems we obtain

$$\gamma_G = \gamma_i \quad (2.18)$$

Thus the magnitudes of the multiphonon terms, which are largely determined by γ are fairly well described.

For a diatomic system an exact calculation of the multiphonon terms is only possible if the two partial densities of states $F_i(\hbar\omega)$ are known. These two functions can be determined, if in addition to $G(\hbar\omega)$ also the correction factor $S(\hbar\omega) = F(\hbar\omega) / G(\hbar\omega)$ is known. $S(\hbar\omega)$ is in general a much simpler function than the various densities of states. Using $G(\hbar\omega)$ and $S(\hbar\omega)$ the partial densities of states are obtained as follows:

$$F_1(\hbar\omega) = \frac{c_2 - \alpha_2 S(\hbar\omega)}{c_2 \alpha_1 - c_1 \alpha_2} G(\hbar\omega) \quad (2.19)$$

$$F_2(\hbar\omega) = - \frac{c_1 - \alpha_1 S(\hbar\omega)}{c_2 \alpha_1 - c_1 \alpha_2} G(\hbar\omega) \quad (2.20)$$

As $F_1(\hbar\omega)$ and $F_2(\hbar\omega)$ are only needed to correct for the higher order phonon terms, we need not know $S(\hbar\omega)$ very accurately. Often crude approximations are sufficient. A simple recipe to construct $S(\hbar\omega)$ for a system with very different atomic masses has been outlined in Ref. 3:

$$S(\hbar\omega) = S_0 + (S_1 - S_0) \left(\frac{\hbar\omega}{\hbar\omega_g}\right)^2 \quad \hbar\omega \leq \hbar\omega_g \quad (2.21)$$

$$S(\hbar\omega) = S_2 \quad \hbar\omega \geq \hbar\omega_g$$

where

$$S_0 = \frac{c_1 M_1 + c_2 M_2}{\alpha_1 M_1 + \alpha_2 M_2}, \quad S_1 = \frac{c_1}{\alpha_1} \quad (2.22)$$

$$S_2 = \frac{1 - \int_0^{\hbar\omega_g} S(\hbar\omega') G(\hbar\omega') d(\hbar\omega')}{1 - \int_0^{\hbar\omega_g} G(\hbar\omega') d(\hbar\omega')}$$

S_2 follows from the condition, that both $G(\hbar\omega)$ and $S(\hbar\omega) \cdot G(\hbar\omega)$ are normalized to unity.

3. GENERAL DESCRIPTION OF MUPHOCOR

The analysis performed by MUPHOCOR starts from the $\sin\theta$ -weighted angle integrated time-of-flight distribution $Z_0(t)$. After applying several experimental corrections to the input distribution as an option (see sections 4.1 and 4.2) $Z_0(t)$ is transformed to $Z_0(\hbar\omega)$, which is identical to $\frac{d\sigma}{d\hbar\omega}$ apart from a scaling factor A, as in general no absolute intensity measurements are performed.

For further treatment of $Z_0(\hbar\omega)$ an equidistant mesh in $\hbar\omega$ is produced by interpolation.

Deviding $Z_0(\hbar\omega)$ by $h(k_1, \hbar\omega)$ as defined in Eq. 2.7 a new function $Z'_0(\hbar\omega)$ is obtained which is already close to the phonon density of states apart from corrections due to the Debye Waller factor and the multi-phonon terms. In the low frequency region, where the TOF distribution is contaminated by elastic scattering $Z'_0(\hbar\omega)$ is quadratically extrapolated to $\hbar\omega=0$.

$Z'_0(\hbar\omega)$ is the starting distribution for the evaluation of $F(\hbar\omega)$ ($G(\hbar\omega)$) by an iteration procedure using Eq. 2.4 (see section 4.3). The final result of $F(\hbar\omega)$ ($G(\hbar\omega)$) is then transformed back to a mesh of $\hbar\omega$, which is given by the equidistant time-mesh of the experiment. As an option also energy loss spectra may be analyzed where due to a too low primary neutron energy only part of the spectrum could be measured (see section 4.5).

4. SOME DETAILS ABOUT MUPHOCOR

4.1 Corrections to the Input TOF-Distribution

In general, it is expected that the input TOF-spectrum has passed separate data reduction programs which perform those corrections, which are specific to the experiment, as for instance corrections for background, absorption losses in the sample or the flight path, detector efficiency and multiple scattering.

It is, however, possible to apply part of those corrections also in MUPHOCOR in a simplified way. There are the following options:

- a. Subtraction of a constant background
- b. Subtraction of a time-dependent background
- c. Absorption losses can be taken into account in the form $\exp(-\alpha \frac{v_0}{v_f})$, where $v_0 = 2200$ m/sec and v_f is the neutron velocity after scattering ($\alpha = ABK$ in the input data).
- d. The counter efficiency can be corrected for using the expression $1 - \exp(-\beta/\sqrt{E_f})$, where E_f is the secondary neutron energy. The parameter $\beta (=AEMP)$ can be read in. If $AEMP=0$ the program uses $AEMP=5.6$, which applies to a 4 atm He^3 counter with 1 inch diameter.
- e. Application of resolution corrections. This will be described in some details in the next section.

4.2 Resolution Corrections

0.363 * 2
3 atm 1NG

In general, the resolution function $R(t, \tau)$ of a TOF-spectrometer is fairly well known. Therefore resolution corrections may be applied, if the data have a good statistical accuracy. This can be done by the subroutine RESCOR, which uses the following iteration prescription for a partial deconvolution of the TOF-distribution:

$$Z_n(z) = \frac{Z_{n-1}(z)}{\int Z_{n-1}(t-\tau)R(t,\tau) d\tau} Z_0(t) \quad (4.1)$$

Here $Z_n(t)$ is the TOF-distribution after the n -th iteration step and $Z_0(t)$ is the input distribution as determined by the experiment.

In order to prevent unphysical spikes caused by the statistical fluctuations in the measured data the iteration process is stopped, when the relative deviation between the reconstructed spectrum and the original spectrum is smaller than the relative statistical error $\rho(t)$ of the measurement.

$$\left| \frac{Z_0(t) - \int Z_n(t-\tau)R(t,\tau) d\tau}{Z_0(t)} \right| \leq \rho(t), \quad (4.2)$$

where $\rho(t)$ in general is given by

$$\rho(t) = \frac{\sqrt{Z_0(t) + 2U(t)}}{Z_0(t)} \quad (U(t) = \text{background}) \quad (4.3)$$

There may be straight forward modifications to Eq. 4.3, if background and sample measurements were not done over the same length of time or if during the process of data reduction scaling factors to $Z_0(t)$ or $U(t)$ have been introduced. In order to take this into account expression 4.3 can be multiplied in RESCOR by a correction factor FERR.

As both $\rho(t)$ and $R(t,\tau)$ vary across the TOF-spectrum, the number of iterations and hence the resolution achieved by this partial deconvolution procedure will fluctuate among the various time channels.

Instead of starting from the original $Z_0(t)$ a smoothed distribution $Z_0^{sm}(t)$ can be used in the iteration process. The final partially deconvoluted spectrum is then obtained as

$$Z_n(t) = Z_0(t) + (Z_n^{sm}(t) - Z_0^{sm}(t)). \quad (4.4)$$

$Z_n^{sm}(t)$ is determined from Eq. 4.1.

The resolution $(\Delta h\omega)_n$ after n iterations is given by

$$(\Delta h\omega)_n = \beta_n (\Delta h\omega)_0, \quad (4.5)$$

where $(\Delta h\omega)_0$ is the starting resolution, and β_n is determined from a recursion formula:

$$\beta_n^2 = \frac{\beta_{n-1}^2 + \beta_{n-1}^4}{1 + \beta_{n-1}^2 + \beta_{n-1}^4}, \quad \beta_0^2 = 1 \quad (4.6)$$

The first 10 values of the β sequence are as follows:

$$\{\beta_n\} = \{1, .817, .826, .667, .626, .594, .568, .547, .529, .514, .500, \dots\} \quad (4.7)$$

10 iterations are needed to reduce the original resolution by a factor of two.

The resolution function in RESCOR is a Gaussian distribution. The two partial time-widths in the input TAUE and TAUT are the time spread for elastic scattering due to the primary energy resolution and the burst-width of the chopper, respectively.

4.3 Determination of $G(\hbar\omega)$ by Iteration

As $G(\hbar\omega)$ is the more general quantity - it reduces to $F(\hbar\omega)$ for a monoatomic system - we shall omit henceforth the distinction between $F(\hbar\omega)$ and $G(\hbar\omega)$ and always use $G(\hbar\omega)$.

In order to determine $G(\hbar\omega)$ from the one-phonon part of the cross-section we have to correct for the higher phonon contribution, which itself depends in a complex way on $G(\hbar\omega)$. Therefore Eq. 2.4 has to be solved in a self-consistent manner by iteration. Starting from a first guess of $G(\hbar\omega)$ obtained from the one-phonon approximation (Eq. 2.6), $(\frac{d\sigma}{d\hbar\omega})_0$ is calculated with Eq. 2.4 and then compared to the $Z_0(\hbar\omega)$. From this comparison a corrected $G_{(1)}(\hbar\omega)$ is derived. This process is repeated until full consistency is obtained. Two prescriptions for correcting $G_{(n)}(\hbar\omega)$ can be chosen.

a. Quotient method:

$$G_n(\hbar\omega) = G_{(n-1)}(\hbar\omega) \cdot R_{(n-1)}(\hbar\omega) \tag{4.8}$$

$$\tag{4.8}$$

$$\text{where } R_{(n-1)}(\hbar\omega) = \frac{Z'_0(\hbar\omega) \int [(\frac{d\sigma}{d\hbar\omega})_{(n-1)} / h(k_0, \hbar\omega)] d\hbar\omega}{\int Z'_0(\hbar\omega) d\hbar\omega \cdot (\frac{d\sigma}{d\hbar\omega})_{n-1} / h(k_0, \hbar\omega)} \tag{4.9}$$

$h(k_0, \hbar\omega)$ is defined by Eq. 2.7).

b. Difference method:

$$G_{(n)}(\hbar\omega) = G_{(n-1)}(\hbar\omega) + \frac{(\frac{d\sigma}{d\hbar\omega})'_{(n-1)}}{h(k_0, \hbar\omega)} (R_{(n-1)}(\hbar\omega) - 1) \tag{4.10}$$

$(\frac{d\sigma}{d\hbar\omega})'$ is calculated in the same way as $(\frac{d\sigma}{d\hbar\omega})$ with $\gamma = 0$.

After each iteration step $G_{(n)}(\hbar\omega)$ is normalized to unity. Method b has several advantages compared to method a and therefore should be used as a rule. Above all it converges much faster.

Method b may be preferred, if the multiphonon corrections are very large (high temperatures and/or small atomic masses), because there is no danger, that the iteration process gets out of control. There is the option, that after a certain number of iterations one can switch over from the quotient method to the difference method.

4.4 Diatomic Systems

As has been discussed in section 2, a more accurate evaluation of the multi-phonon terms for diatomic systems is obtained if $G(\hbar\omega)$ is decomposed into $F_1(\hbar\omega)$ and $F_2(\hbar\omega)$ with the help of $S(\hbar\omega) = \frac{F(\hbar\omega)}{G(\hbar\omega)}$. This method of analysis has also been incorporated into MUPHOCOR. $S(\hbar\omega)$ is delivered by the subroutine CORRFA, where the relations 2.21 and 2.22 are programmed. The only free parameter is $\hbar\omega_g$, which is an input parameter (PARQ(1)). S_1 may be changed from the programmed value by PARQ(2) $\neq 0$. For IQUO=1 $S(\hbar\omega)$ is an input field (PARQ(L)).

4.5 Analysis of Incomplete Energy Loss Spectra

There may be cases, where the incident neutron energy E_0 is smaller than the maximum energy transfer of $G(\hbar\omega)$. As for the calculation of the multiphonon terms $G(\hbar\omega)$ must be known for all values of $\hbar\omega$ the normal evaluation method employed by MUPHOCOR breaks down, if one wants to analyze the neutron energy loss side of the time-of-flight spectrum.

This case can be treated by the subroutine INCOMP under the condition that as a first step an analysis of the neutron energy gain spectrum had been performed. The convolution integrals $T_n(\hbar\omega)$ and the scaling factor A between $Z_0(\hbar\omega)$ and $\frac{d\sigma}{d(\hbar\omega)}$ calculated during this step are stored and then used in INCOMP to calculate the multiphonon terms. $G(\hbar\omega)$ is then calculated in a straight forward manner from the one-phonon term which is obtained as

$$\text{one phonon term} = \frac{Z_0(\hbar\omega)}{A} - \text{multi-phonon contribution} \quad (4.11)$$

5. Input data for MUPHOCOR

- | | | | |
|----|--------|--------------------|--|
| 1. | (20A4) | (TITLE(I), I=1,20) | text to describe the scientific case |
| 2. | (8F10) | EO | incident energy (in meV) |
| | | FP | secondary flight path (in cm) |
| | | CW | channel width of the time-analyzer (in μ s) |
| | | XNEL | positions of the elastic line (channel number) |
| | | FIMA | maximum scattering angle |
| | | ABK | absorption coefficient |
| | | AEMP | coefficient for calculating the counter efficiency |
| 3. | (16I5) | LM | number of intervals for $\hbar\omega$ |
| | | NSPEC | number of different species in the sample (≤ 2) |
| | | IQUO | indicator to select model for $F(\hbar\omega)/G(\hbar\omega)$ |
| | | LPAR | number of parameters for the calculation of $F(\hbar\omega)/G(\hbar\omega)$
(INQUO and LPAR not necessary if NSPEC=1) |
| 4. | (8F10) | HOX | maximum energy of the phonon density of states (in meV) |
| | | TEMPO | temperature of the sample (in Kelvin) |
| | | DW | Debye Waller coefficient in [1 meV] (if available in units of [\AA^2] divide by 2.072). |

5. (3F10) AMASI(I) atomic mass (in A.U.)
 SIGI(I) scattering cross-section
 CONCI(I) concentration
 (input 5 NSPEC times)
6. (8F10) (PARQ(I), I=1, LPAR) parameters for the calculation
 of $F(\hbar\omega)/G(\hbar\omega)$
 (input 6 only if NSPEC=2)
7. (16I5) NPHO number of phonon terms
 ITM number of iterations
 IVIT =0: iteration by the difference
 method
 >0 iteration by the quotient
 method up to iteration number
 IVIT, afterwards application
 of the difference method
 IDW =0: Debye Waller coefficient
 is input value throughout the
 calculations
 =1: Debye Waller coefficient
 determined from the iterated
 distribution
 IEMP =0: no correction for counter
 efficiency
 =1: correction for counter-
 efficiency is done in the
 program
 IRES =0: no resolution correction
 =1: resolution correction is
 applied
 IPR =1: convolution integrals
 of the multiphonon terms are
 printed out
 IQUO indicator to select model
 for $F(\hbar\omega)/G(\hbar\omega)$
 ILOSS =1: analysis of incomplete
 energy loss spectrum will be
 done
 lower channel number of the TOF-
 spectrum
8. (16I5) NU upper channel number of the TOF-
 spectrum
 NO number of dummy data before the
 TOF-spectrum (≤ 8 , 0=8)
 NDUM Number of smoothing processes in
 case of a time-dependent
 background
 IGLU

- 9.. (8F10) (DUM(N),N=1,NDUM) dummy data in front of the TOF-spectrum
(ZO(N),N=1,NM) angle integrated TOF-spectrum (NM=NO-NU+1)
10. (8F10) UNT constant background
FUN scaling factor for a time-dependent background
11. (8F10) (DUM(N),N=1,NDUM) dummy data in front of the time-dependent background
(UN(N),N=1,NM) time-dependent angle-integrated background
- (input 10 only if FUN≠0)
12. (16I5) NUS first } time channel of the range,
NOS } where the resolution
IGL } corrections are applied
ITM }
number of smoothing processes
maximum number of iterations for the partial deconvolution
13. (8F10) TAUE primary time-width
TAUT secondary time-width
DFP average uncertainty of the flight path (in cm)
UNT average background
FERR scaling-factor between counting events and input TOF distribution ZO(N)
- (input 11 and 12 only if IRES = 1)
14. (16I5) LTEM number of temperature values for the calculation of the specific heat
15. (8F10) (TEMPUR(L),L=1,LTEM) temperatures (in Kelvin), at which the specific heat will be calculated

(input 14 only if LTEM ≠ 0)

If ILOSS=0 the data input is terminated

For ILOSS=1:

16. (16I5) IRES for explanation see 7.

Here follows 8,9,10,11,12,13 (12 and 13 only for IRES=1).

6. VARIOUS ITEMS

The method employed by MUPHOCOR is basically equivalent to the extrapolation method of Egelstaff and Schofield (4). However, there are some advantages:

The condensation of the spectra from all detectors into one input distribution leads to a rather easy and fast data handling. Furthermore, only a moderate amount of storage space is needed in the evaluation program. We have not exploited the latter advantage to the extreme in the version of the program, which is described in this report, however, there exists a version of MUPHOCOR, written by N. Nücker (5), for a small experiment computer of type NOVA2. Thus the evaluation of $G(\vec{n}, \omega)$ can be done directly at the experiment.

The good statistical accuracy of the sum spectra allows to apply resolution corrections. This can not be done with the spectra of the individual detectors.

A final remark concerns multiple scattering in the sample. This is a major problem for an accurate determination of the scattering law $S(Q, \omega)$, but is much less severe, if one is only interested in the phonon density of states. The dominant part of multiple scattering is caused by processes of the kind: elastic plus one phonon. As this contribution involves an integration over scattering angles similar to that described in section 2 it is not very detrimental. Nevertheless, strong multiple scattering contributions should be avoided in the experiment, because there is no easy way to correct for the higher order processes.

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Atomic Masses and Scattering Properties of Several Elements

Z	El.	M [A.U.]	b [10 ⁻¹² cm]	σ_{coh} [barn]	σ_{inc} [barn]	σ_b [barn]	$\frac{\sigma_b}{M}$
4	Be	9.01	.78	7.65	.005	7.65	.849
6	C	12.01	.6648	5.554	.008	5.562	.4631
7	N	14.01	.936	11.01	.46	11.47	.8187
8	O	16.00	.5803	4.23	-	4.23	.2644
12	Mg	24.31	.538	4.30	.06	4.36	.1794
13	Al	26.98	.3449	1.495	.008	1.503	.0557
14	Si	28.09	.4149	2.163	.010	2.173	.0774
15	P	30.97	.513	3.31	.06	3.37	.1088
16	S	32.06	.2847	1.019	.011	1.030	.0321
19	K	39.10	.371	1.730	.38	2.11	.0540
20	Ca	40.08	.490	3.017	0	3.02	.0753
22	Ti	47.90	-.337	1.428	2.79	4.22	.0881
23	V	50.94	-.041	.021	4.97	4.99	.0980
24	Cr	52.00	.3532	1.57	1.90	3.47	.0667
25	Mn	54.94	-.373	1.748	.55	2.30	.0419
26	Fe	55.85	.954	11.44	.30	11.74	.2102
27	Co	58.93	.278	.971	5.2	6.18	.1049
28	Ni	58.71	1.03	13.33	5.0	18.3	.3117
29	Cu	63.54	.7685	7.422	.501	7.923	.1247
30	Zn	65.37	.57	4.08	.05	4.13	.0632
31	Ga	69.72	.72	6.51	.2	6.71	.0962
32	Ge	72.59	.8186	8.42	.09	8.51	.1172
33	As	74.92	.673	5.69	.82	6.51	.0869
39	Y	88.91	.775	7.548	.135	7.68	.0864
40	Zr	91.22	.71	6.33	.11	6.44	.0707
41	Nb	92.91	.711	6.35	.004	6.36	.0685
42	Mo	95.94	.695	6.07	-	6.07	.0633
50	Sn	118.69	.622	4.86	.01	4.87	.0410
51	Sb	121.75	.5641	3.955	.17	4.05	.0333
57	La	138.91	.827	8.59	1.84(1.0)	10.43(9.6)	.0751(.069)
58	Ce	140.12	.483	2.93	-	2.93	.0209
59	Pr	140.91	.445	2.49	-	2.49	.0177
78	Pt	195.09	.95	11.34	.59	11.92	.0611
79	Au	196.97	.763	7.32	.37	7.69	.0390
81	Tl	204.37	.889	9.93	-	9.93	.0486
82	Pb	207.19	.940	11.10	.001	11.10	.0536
83	Bi	208.98	.8526	9.13	.008	9.14	.0437
90	Th	232.04	1.008	12.77	-	12.77	.0550
92	U	238.03	.861	9.32	-	9.32	.0392
38	ST	87.62	.688	6.09	-	6.09	.0695
37	PL	85.47				6.6	.0772
	CS					3.9	0.0293

$\frac{b}{M} = \frac{.3337 \text{ barn}}{.483} = 0.726$
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