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THRUSH ; A CODE FOR CALCULATING THERMAL NEUTRON SCATTERING KERNEL

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THRUSH; A Code for Calculating Thermal Neutron Scattering Kernel

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THRUSH is a code for computing the thermal neutron scattering kernel by phonon expansion method for both coherent and incoherent scattering processes. To evaluate the scattering kernel from the double differential scattering cross section, it is necessary to perform angular integration over scattering angle. Existing codes utilize, for this purpose, the numerical integration of the scattering law. So as to improve the accuracy and reduce the computing time, this integration is performed analytically in the THRUSH code. Another feature of THRUSH is that this code can calculate the coherent part of the scattering kernel as well as the incoherent part, which is suitable for calculating the scattering kernel for heavy water.

Keywords: Thermal Neutron, Scattering Kernel, Phonon Expansion, Coherent Scattering, Incoherent Scattering, Computer Code

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This manual is the English version of THRUSH code manual by H. Kadotani, JAERI-memo 4211, November 1970, in Japanese.

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THRUSH；熱中性子散乱カーネル計算コード

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THRUSHは干渉性および非干渉性散乱について，フオノン展開の方法で熱中性子の散乱カーネルを計算するコードであり，重水の散乱カーネルの計算に適している。

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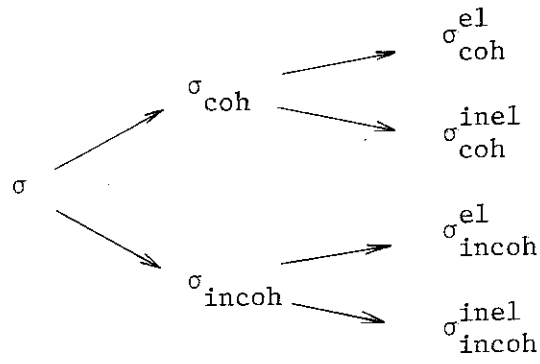
Contents

1. Introduction

Thermal neutron scattering cross section is customarily divided into following four categories.



In this diagram, suffixes coh and incoh correspond to the coherent and incoherent scattering of neutrons, and el and inel to the elastic and inelastic scattering. Analysis of so-called thermalization problems or design of thermal neutron reactors have been generally performed within the approximation of incoherent scattering. The coherent inelastic scattering kernel has been obtained only for few crystal materials.

The approximation, in which the contribution from the coherent scattering is neglected, is appropriate for hydrogeneous moderator, since the incoherent scattering length is very large for hydrogen atoms. For crystalline moderator which does not contain hydrogen atom, the coherent scattering is evaluated only for the elastic scattering (Bragg diffraction), and is neglected for the inelastic scattering part. The above approximation is widely accepted at least from the standpoint of reactor physics. Heavy water is probably only one non-crystalline moderator whose coherent scattering cross section can not be neglected.

The incoherent inelastic scattering cross section can be calculated from the generalized frequency distribution, or the spectral density function. We proposed more "generalized" spectral density which may have negative value for the calculation of the coherent scattering cross section.[1] By the use of this "generalized" spectral density the scattering law with the coherent scattering effect was successfully calculated for heavy water.

THRUSH is the code to calculate the coherent and incoherent scattering cross sections from the above "generalized" spectral density. We assumed that the calculational method of the coherent scattering cross

section is applicable to heavy water.

There exist many computer codes for calculation of the scattering cross section in the incoherent scattering approximation.[2),(3)] Most of the codes utilize the following procedure for cross section calculation. Firstly, the scattering law which is related to the double differential scattering cross section is calculated,

$$\sigma(E_0 \to E,\mu) = \frac{\sigma_b}{4\pi}\frac{1}{T}\sqrt{\frac{E}{E_0}}\, e^{-\beta/2}\, S(\alpha,\beta) \ . \tag{1}$$

where

$$\alpha = \frac{\kappa^2}{2MT} = \frac{m}{MT}\,(E_0 + E - 2\sqrt{E_0 E}\mu) \ , \tag{2}$$

$$\beta = -\frac{\omega}{T} = \frac{1}{T}\,(E - E_0) \ , \tag{3}$$

and E and E_0 : neutron energy before and after scattering, μ : cosine of scattering angle, κ, ω : momentum and energy change of neutron before and after scattering, M : mass of scattering atom, m : neutron mass, T : temperature of scattering system in energy unit and σ_b : bound atom scattering cross section. The scattering kernel is defined as the Legendre moment of double differential scattering cross section, $\sigma(E_0 \to E,\mu)$.

$$\sigma_\ell(E_0 \to E) = 2\pi \int_{-1}^{1} \sigma(E_0 \to E,\mu)\, P_\ell(\mu)\, d\mu \ , \tag{4}$$

where $P_\ell(x)$ is the ℓ-th order Legendre function.

The scattering law is calculated in the Gaussian approximation,

$$S(\alpha,\beta) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{i\beta t}\, e^{-\alpha w(t)}\, dt \ . \tag{5}$$

and

$$W(t) = \int_0^\infty \rho(\beta)\, \frac{\cosh(\frac{\beta}{2}) - \cos(\beta t)}{\beta \sinh(\frac{\beta}{2})}\, dt \ , \tag{6}$$

where $\rho(\beta)$ is the generalized phonon frequency distribution or the spectral density.[4] Except the over-simplified model like Einstein crystal in which $\rho(\beta)$ is given as $\delta(\beta - \beta_E)$, where β_E is Einstein's frequency of crystal, $\rho(\beta)$ is given only numerically. Therefore, the scattering law is obtained only numerically and as the result, the angular integration of Eq. (4) is performed only numerically.

If the scattering law is expressed in the phonon expansion, the angular integration in Eq. (4) can be performed analytically, even with numerical $\rho(\beta)$. THRUSH utilizes this procedure to increase the accuracy of the calculated scattering kernel and to reduce computer time.

As the mathematical procedure is based on the phonon expansion in THRUSH, the convergence worsens for high incident energy of neutrons or at high temperature. This is overcome by using Sjölander expansion or short time expansion in the region where the phonon expansion converges slowly.

The present version of THRUSH accepts only isotropic "generalized" spectral density. The improvement of THRUSH is desirable to accept δ-function type and anisotropic spectral density in the near future.

2. Theory

2.1 Incoherent scattering part

The scattering kernel $\sigma_\ell(E_0 \to E)$ can be calculated with the use of the scattering law of Eq. (1), as,

$$\sigma_\ell(E_0 \to E) = \frac{\sigma_b}{2T}\sqrt{\frac{E}{E_0}}\ e^{-\beta/2} \int_{-1}^{1} S(\alpha,\beta)\ P_\ell(\mu)\ d\mu\ . \tag{7}$$

Defining the asymmetric scattering law by,

$$S(|\vec{\kappa}|,\ \omega) = \frac{1}{T}\ e^{-\beta/2}\ S(\alpha,\beta)\ , \tag{8}$$

we can rewrite Eq. (7) as,

$$\sigma_\ell(E_0 \to E) = \frac{\sigma_b}{2}\sqrt{\frac{E}{E_0}} \int_{-1}^{1} S(|\vec{\kappa}|,\ \omega)\ P_\ell(\mu)\ d\mu\ , \tag{9}$$

where $\rho(\beta)$ is the generalized phonon frequency distribution or the spectral density.[4] Except the over-simplified model like Einstein crystal in which $\rho(\beta)$ is given as $\delta(\beta - \beta_E)$, where β_E is Einstein's frequency of crystal, $\rho(\beta)$ is given only numerically. Therefore, the scattering law is obtained only numerically and as the result, the angular integration of Eq. (4) is performed only numerically.

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where

$$\omega = E_0 - E \tag{10}$$

$$\vec{\kappa} = \vec{\kappa}_0 - \vec{\kappa} \tag{11}$$

and $\vec{\kappa}_0$, $\vec{\kappa}$ are the momenta for neutron before and after collision, respectively.

We now express $S(|\vec{\kappa}|, \omega)$ by the phonon expansion:[5]

$$S(|\vec{\kappa}|, \omega) = e^{-2W} \sum_{n=1}^{\infty} \frac{1}{n!} (2W)^n \phi_n(\omega) \ . \tag{12}$$

In this equation, 2W and $\phi_n(\omega)$ can be written with the spectral density function $\rho(\omega)$:

$$2W = \frac{\vec{\kappa}^2}{2M} \gamma(0) \ , \tag{13}$$

where

$$\gamma(0) = \int_0^{\infty} \frac{\rho(\omega)}{\omega} \coth(\frac{\omega}{2T}) \, d\omega \ . \tag{14}$$

And,

$$\phi_n(\omega) = \int_{-\infty}^{\infty} \phi_1(\omega - \omega') \, \phi_{n-1}(\omega') \, d\omega' \ , \tag{15}$$

$\phi_1(\omega)$ being defined as

$$\phi_1(\omega) = \frac{\rho(\omega)}{2W \ \gamma(0) \ \sinh(\frac{\omega}{2T})} e^{W/2T} \ . \tag{16}$$

Using Eq. (13), we can transform the integration of μ to the integration of 2W, since

$$\frac{\vec{\kappa}^2}{2M} = \frac{m}{M} (E_0 + E - 2 \sqrt{E_0 E} \, \mu) \ . \tag{17}$$

Substituting this equation into Eq. (13), we obtain

$$\mu = \frac{1}{2\sqrt{E_0 E}} \left(E_0 + E - \frac{M}{m} \frac{x}{\gamma(0)} \right) , \tag{18}$$

where $x = 2W$. Equation (12) becomes by this transformation

$$\sigma_\ell(E_0 \to E) = \frac{\sigma_b}{2} \sqrt{\frac{E}{E_0}} \sum_{n=1}^{\infty} \frac{1}{n!} \phi_n(\omega) \int_{-1}^{1} P_\ell(\mu)\, e^{-x}\, x^n\, d\mu$$

$$= \frac{\sigma_b}{4} \frac{1}{E_0} \frac{M}{m} \frac{1}{\gamma(0)} \sum_{n=1}^{\infty} \frac{1}{n!} \phi_n(\omega)$$

$$\times \int_{(\sqrt{E} - \sqrt{E_0})^2 \frac{m}{M} \gamma(0)}^{(\sqrt{E} + \sqrt{E_0})^2 \frac{m}{M} \gamma(0)} e^{-x}\, x^n\, P_\ell\left(\frac{1}{2\sqrt{E_0 E}} (E_0 + E - \frac{M}{m} \frac{x}{\gamma(0)}) \right) dx . \tag{19}$$

As $P_\ell(x)$ is a polynomial of ℓ-th order at most, the integration of Eq. (19) can be performed analytically.

The integration can be reduced as follows. We define

$$J_n(\ell) = \int_{a_-}^{a_+} e^{-x}\, x^n\, P_\ell(A - Bx)\, dx , \tag{20}$$

with

$$a_\pm = \frac{m}{M} \gamma(0) \left(\sqrt{E_0} \pm \sqrt{E} \right) , \tag{21}$$

$$A = \frac{1}{2\sqrt{E_0 E}} (E_0 + E) , \tag{22}$$

$$B = \frac{1}{2\sqrt{E_0 E}} \frac{M}{m} \frac{1}{\gamma(0)} . \tag{23}$$

Performing the integration, we get the following relations ;

$$\ell=0 \; ; \quad J_n(0) = \int_{a_-}^{a_+} e^{-x} x^n P_0(A - Bx)\, dx$$

$$= \int_{a_-}^{a_+} e^{-x} x^n\, dx = \left[- e^{-x} \sum_{i=1}^{n} \frac{n!}{(n-i)!} x^{n-i} \right]_{a_-}^{a_+}$$

$$\equiv I(n) \; . \tag{24}$$

$$\ell=1 : \quad J_n(1) = A\, I\,(n) - B\, I\,(n+1) \; . \tag{25}$$

$$\ell=2 : \quad J_n(2) = \frac{3A^2 - 1}{2} I(n) - 3ABI(n+1) + \frac{3}{2} B^2 I(n+2) \; . \tag{26}$$

$$\ell=3 : \quad J_n(3) = \frac{15A^3-9A}{6} I(n) - \frac{45A^2B-9B}{6} I(n+1)$$

$$+ \frac{45AB^2}{6} I(n+2) - \frac{15}{6} B^3 I(n+3) \; . \tag{27}$$

The scattering kernel can be written explicitly for $\ell=0$ and $\ell=1$ as follows,

$$\sigma_0(E_0 \to E) = \frac{\sigma_b}{4E_0} \frac{M}{m} \frac{1}{\gamma(0)} \sum_{n=1}^{\infty} \phi_n(\omega)\, I(n) \; , \tag{28}$$

$$\sigma_1(E_0 \to E) = \frac{\sigma_b}{4E_0} \frac{M}{m} \frac{1}{\gamma(0)} \sum_{n=1}^{\infty} \phi_n(\omega) \left\{ \frac{E_0 + E}{2\sqrt{E_0 E}} I(n) \right.$$

$$\left. + \frac{1}{2\sqrt{E_0 E}} \frac{M}{m} \frac{1}{\gamma(0)} I(n+1) \right\} \; . \tag{29}$$

As one can see from these equations, the scattering kernels are expressed in an analytical form except $\phi_n(\omega)$, which is evaluated numerically from $\rho(\omega)$.

The shape of the function $\phi_n(\omega)$ for larger n tends to the Gaussian type function by the central limiting theorem. This property of $\phi_n(\omega)$ is well known as the Sjolander expansion. The THRUSH code employs the same method of Sjolander expansion[5] that is used in the SUMMIT[6]

(the equivalent japanese version is UNCLE.) to treat an anisotropic crystal like graphite. Although the present version of THRUSH does not treat an anisotropic crystal, this method is used for future modification, and the distinct term calculation described below.

The spectral density is divided, rather arbitrary, into two parts, a lower frequency part and higher frequency part. The n-th phonon term $\phi_n(\omega)$ in this expansion is given by

$$\phi_n(\omega) = \left(\frac{1}{\gamma(0)}\right)^n \sum_{r=0}^{n} f_1^{(r)} \cdot f_2^{(n,r)} \cdot f_3^{(n,r)} \quad , \tag{30}$$

where the Hermite correction is neglected and

$$f_1^{(r)} = \frac{1}{r!} \left(r^{(1)}(0)\right)^r \quad , \tag{31}$$

$$f_2^{(n,r)} = \frac{1}{(n-r)!} \left(r^{(2)}(0)\right)^{n-r} \quad , \tag{32}$$

$$f_3^{(n,r)} = \frac{1}{\sqrt{2\pi\ \kappa_2^{(n,r)}}}\ e^{-\frac{\left(\omega - \kappa_1^{(n,r)}\right)^2}{2\kappa_2^{(n,r)}}} \tag{33}$$

$$\kappa_\nu^{(n,r)} = r\ \kappa_\nu^{(1)} + (n - r)\ \kappa_\nu^{(2)} \quad , \qquad (\nu = 1,\ 2) \quad , \tag{34}$$

$$\kappa_1^{(i)} = \frac{\alpha_1^{(i)}}{\alpha_0^{(i)}} \quad , \tag{35}$$

$$\kappa_2^{(i)} = \frac{\alpha_2^{(i)}}{\alpha_0^{(i)}} - \left(\frac{\alpha_1^{(i)}}{\alpha_0^{(i)}}\right)^2 \quad . \tag{36}$$

$$\alpha_0^{(i)} = \int_0^\infty \frac{\rho^{(i)}(\omega)}{\omega} \coth\left(\frac{\omega}{2T}\right) d\omega \equiv \gamma^{(i)}(0) \quad , \tag{37}$$

$$\alpha_1^{(i)} = \int_0^\infty \rho^{(i)}(\omega)\ d\omega \equiv \delta^{(i)} \quad , \tag{38}$$

$$\alpha_2^{(i)} = \int_0^\infty \rho^{(i)}(\omega)\ \omega\ \coth\left(\frac{\omega}{2T}\right)\ d\omega\ , \tag{39}$$

and i = 1, or 2. In the above equations, $\rho^{(1)}(\omega)$ corresponds to the lower frequency part spectral density and $\rho^{(2)}(\omega)$ to the higher part.

When the convergence becomes slow for higher incident energy, we use the first term of short collision time expansion. In the approximation the scattering law is expressed as the free gas with effective temperature T_{eff},

$$S(\alpha,\beta) = e^{\frac{\beta}{2}(1-\gamma)} \frac{1}{\sqrt{4\pi\alpha}} e^{-\frac{\gamma}{4\alpha}(\alpha^2+\beta^2)} \tag{40}$$

where

$$\gamma = \frac{T_{eff}}{T}\ , \tag{41}$$

$$T_{eff} = \frac{1}{2}\int_0^\infty \rho(\omega)\ \omega\ \coth\left(\frac{\omega}{2T}\right)\ d\omega\ , \tag{42}$$

The scattering kernel is calculated directly from Eq. (40) by Gaussian integration.

2.2 Coherent scattering part

The coherent scattering calculation in the THRUSH code is based on the Butler's model for heavy water. The definition of the spectral density function for atom pair ν and ν', and its property are described and discussed in other place.[1] Here, we will briefly explain the calculational method of the scattering kernel. If we write the scattering law $S_{\nu\nu'}(|\vec{\kappa}|\ \omega)$ for a pair ν and ν' atoms in a molecule, this is given by,

$$S_{\nu\nu'}(\kappa,\omega) = \frac{\sin(|\vec{\kappa}|\ R_{\nu\nu'})}{|\vec{\kappa}|\ R_{\nu\nu'}}\ S_{\nu\nu'}(|\vec{\kappa}|,\omega)\ . \tag{43}$$

The reduced scattering law $\bar{S}_{\nu\nu'}(|\vec{\kappa}|,\omega)$ can be written in the usual phonon

expansion formulation. Here $R_{\nu\nu'}$ is the distance between atom pair ν and ν', and

$$\bar{S}_{\nu\nu'}(|\vec{\kappa}|,\omega) = \sum_{n=1}^{\infty} e^{-2W_{\nu\nu'}} \frac{1}{n!} (2W_{\nu\nu'})^n \phi_n^{\nu\nu'}(\omega) , \tag{44}$$

where

$$2W_{\nu\nu'} = \frac{|\vec{\kappa}|^2}{2M_{\nu\nu'}} \gamma_{\nu\nu'}(0) , \tag{45}$$

$$\gamma_{\nu\nu'}(0) = \frac{1}{2} \left(\frac{M_{\nu\nu'}}{M_{\nu}} \gamma_{\nu\nu'}(0) + \frac{M_{\nu\nu'}}{M_{\nu'}} \gamma_{\nu\nu'}(0)\right) . \tag{46}$$

$$\phi_n^{\nu\nu'}(\omega) = \int_{-\infty}^{\infty} \phi_1^{\nu\nu'}(\omega - \omega') \phi_{n-1}^{\nu\nu'}(\omega') \, d\omega' , \tag{47}$$

$$\phi_1^{\nu\nu'}(\omega) = \frac{\rho_{\nu\nu'}(\omega)}{2W \gamma_{\nu\nu'}(0) \sinh\left(\frac{\omega}{2T}\right)} e^{\omega/2T} \tag{48}$$

$$M_{\nu\nu'} = \sqrt{M_{\nu} M_{\nu'}} \tag{49}$$

$M_{\nu'}$: mass of the ν-th atom

The spectral density $\rho_{\nu\nu'}(\omega)$ is used in generalized meaning for the coherent scattering by ν and ν' atom pair. (See reference 1.)

This expression is essentially same as the scattering law of the incoherent approximation except the term $\sin(\kappa R_{\nu\nu'})/\kappa R_{\nu\nu'}$. Due to this term, the integration of Eq. (43) with respect to ω (i.e. angle) could not be expressed by known functions. The formal expression for ℓ=0 and ℓ=1 kernels are

$$\sigma_0^{\nu\nu'}(E_0 \to E) = \frac{4\pi A_{\nu} A_{\nu'}}{2E_0} \frac{1}{F_{\nu\nu'} D_{\nu\nu'} R_{\nu\nu'}} \sum_{n=1}^{\infty} \frac{\phi_n^{\nu\nu'}(\omega)}{n!} I_{2n} , \tag{50}$$

$$\sigma_1^{\nu\nu'}(E_0 \to E) = \frac{E_0 + E}{2\sqrt{E_0 E}} \sigma_0^{\nu\nu'}(E_0 \to E)$$

$$- \frac{4\pi A_\nu A_{\nu'}}{4\sqrt{E_0^3 E}} \frac{1}{F_{\nu\nu'}^2 D_{\nu\nu'} R_{\nu\nu'}} \sum_{n=1}^{\infty} \frac{\phi_n^{\nu\nu'}(\omega)}{n!} I_{2n+2} \quad , \quad (51)$$

where

$$F_{\nu\nu'} = \frac{m \gamma_{\nu\nu'}(0)}{M_{\nu\nu'}} \quad (52)$$

$$D_{\nu\nu'} = \sqrt{\frac{2 M_{\nu\nu'}}{m \gamma_{\nu\nu'}(0)}} \quad , \quad (53)$$

$$I_n = \int_{a_-}^{a_+} \sin(D_{\nu\nu'} R_{\nu\nu'} t) \, e^{-t^2} \, t^n \, dt \quad , \quad (54)$$

$$a_\pm = \sqrt{F_{\nu\nu'}} \, | \sqrt{E_0} \pm \sqrt{E} \, | \quad , \quad (55)$$

A_ν : coherent scattering length of ν^{th} atom. (56)

The integral I_n is performed numerically and described in section 3.

The function $\phi_n^{\nu\nu'}(\omega)$ is calculated in the same manner as Eqs. (15), (16). The usual Sjölander expansion is, however, invalid for $\phi_n^{\nu\nu'}(\omega)$, since the spectral density function has negative and positive parts. This difficulty is overcome by utilizing the same formulation used in the coherent scattering approximation. In this case, we divide $\phi_n^{\nu\nu'}(\omega)$ into the sum of two parts, one positive and the other negative definite. We apply the Sjölander approximation separately to each part of the scattering law corresponding to the above division. The final result is obtained by the convolution integral of these two scattering law. The short collision time approximation also leads to a divergent results. This can be overcome by applying the short time expansion only to the scattering part corresponding to the positive definite spectral density, and the phonon expansion to the negative definite part. However, the

short collision expansion is not utilized for the coherent scattering calculation. Therefore, $\phi_n^{\nu\nu'}(\omega)$ in the Sjölander expansion is written as

$$\phi_n^{\nu\nu'}(\omega) = \left(\frac{1}{\gamma_{\nu\nu'}(0)}\right)^n \sum_{r=0}^{n} f_1^{(r)} \cdot f_2^{(n,r)} \cdot f_3^{(n,r)}, \tag{57}$$

with the definitions of Eqs. (31), (32) and (33) for $f_1^{(r)}$, $f_2^{(n,r)}$ and $f_3^{(n,r)}$, provided that $\rho^{(1)}(\omega)$ for lower frequency part spectral density is changed to $\rho_{\nu\nu'}^{(1)}(\omega)$ for positive spectral density and $\rho^{(2)}(\omega)$ for higher frequency part spectral density to $\rho_{\nu\nu'}^{(2)}(\omega)$ for negative definite. Accordingly $\delta^{(i)}$ should satisfy the following relation:

$$\delta^{(1)} > 0 , \qquad \delta^{(2)} < 0 , \tag{58}$$

$$\delta^{(1)} + \delta^{(2)} = 0 . \tag{59}$$

2.3 Elastic scattering cross section

The elastic scattering cross section or the zero phonon cross section is calculated by setting n=0 and $\phi_0(\omega) = \delta(\omega)$ in Eq. (19) for the incoherent scattering and in Eqs. (28), (29) for the coherent scattering. The integral I_0 for the coherent scattering is evaluated numerically also.

The coherent elastic scattering cross section calculated by the above method contains only the contribution from the intra-molecular scattering. The inter-molecular elastic scattering from the atom pair ν, ν' of a different molecule is generally difficult to evaluate. We incorporated the Butler's model[7] for this cross section into THRUSH. In this model, the coherent elastic scattering cross section $\sigma_\ell^{\text{inter}}(E)$ is given by

$$\sigma_\ell^{\text{inter}}(E) = \sigma_{\ell,OO'}^{\text{inter}}(E) + \sigma_{\ell,DD'}^{\text{inter}}(E) + \sigma_{\ell,OD'}^{\text{inter}}(E) , \quad \ell = 0, 1 , \tag{60}$$

where

$$\sigma_{0,\nu\nu'}^{\text{inter}}(E) = N_\nu n_{\nu'} A_\nu A_{\nu'} \frac{8\pi^2 S_{\nu\nu'}}{k^2} \left[j_0(2k S_{\nu\nu'}) - 1 \right] , \tag{61}$$

$$\sigma_{l,\nu\nu'}^{inter}(E) = - N_\nu n_{\nu'} A_\nu A_{\nu'} \frac{8\pi^2 S_{\nu\nu'}}{k^2} [1 + j_0(2k S_{\nu\nu'}) - 2 \{ j_0(k S_{\nu\nu'})\}^2] , \quad (62)$$

$$j_0(x) = \frac{\sin X}{x}$$

N_ν : number of ν^{th} atom per unit volume,

n_ν : number of ν^{th} atom in a molecule,

$S_{\nu\nu'}$: mean minimum distance between ν and ν' atom,

k : momentum of incident neutron.

For $S_{\nu\nu'}$, we used the numerical values due to Butler, i.e., $S_{OO'} = 2.9\mathring{A}$, $S_{DD'} = 1.9\mathring{A}$ and $S_{OD} = 1.9\mathring{A}$. The other parameter N_ν , n_ν , etc. are also set in the subroutine CSIM.

3. Numerical Method

3.1 Energy Integration

The integration over energy (E) and frequency (ω) is performed by the trapezoidal rule. For example, an integration

$$\sigma_l(E_0) = \int_0^\infty \sigma_l(E_0 \to E)\, dE , \quad (63)$$

is performed, as

$$\sigma_l(E_I) = \sum_{k=1}^{IEX} \sigma_l(E_I \to E_K)\, DE(K) . \quad (64)$$

Here, DE(K) is defined as follows,

$$DE(1) = \{E(1) + E(2)\} , \quad (65)$$

$$DE(I) = \{E(I + 1) - E(I - 1)\}/2 , \quad I = 2, 3, \cdots IEX-1 , \quad (66)$$

$$DE(IEX) = \{E(IEX) - E(IEX - 1)\} , \quad (67)$$

$$\sigma_{l,\nu\nu'}^{inter}(E) = -N_\nu n_{\nu'} A_\nu A_{\nu'} \frac{8\pi^2 S_{\nu\nu'}}{k^2} [1 + j_0(2k S_{\nu\nu'}) - 2\{j_0(k S_{\nu\nu'})\}^2] , \quad (62)$$

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E(I) ; input energy mesh,

IEX ; number of energy mesh point.

3.2 Evaluation of I_{2n}

The integral of Eq. (54)

$$I_{2n} = \int_{a_-}^{a_+} \sin(at)\, e^{-t^2}\, t^{2n}\, dt \tag{68}$$

can be evaluated by using following recurrence formula:

$$I_{2n+2} = \left[e^{-t^2}\, t^{2n-1} \left\{ -\frac{a^2}{4} \cos(at)t + \frac{n}{2} \sin(at) - \frac{1}{2} \sin(at)t^2 \right\} \right]_{a_-}^{a_+}$$

$$- \frac{n(2n+1)}{2} I_{2n-2} + \left(\frac{4n+1}{2} - \frac{a^2}{4} \right) I_{2n} . \tag{69}$$

This equation is easily derived from Eq. (68) by the method of integration by part. Therefore, we should perform the numerical integrations:

$$I_0 = \int_{a_-}^{a_+} \sin(at)\, e^{-t^2}\, dt \tag{70}$$

$$I_2 = \int_{a_-}^{a_+} \sin(at)\, e^{-t^2}\, t^2\, dt \tag{71}$$

The integration for I_0 and I_2 is performed by Simpson's rule.

4. Input Quantities

The physical input data for THRUSH are the spectral density, mass of scatterer, free atom cross section (or coherent scattering length), temperature and energy mesh points. The simple flow chart for the input routine is shown in Appendix 1.

The main restriction of input data for the present version is

(1) Maximum number of frequency mesh points for spectral density (IMAX) : 400

(2) Maximum number of convolution integral for $\phi_n(\omega)$(NPX) :

E(I) ; input energy mesh,

IEX ; number of energy mesh point.

3.2 Evaluation of I_{2n}

The integral of Eq. (54)

$$I_{2n} = \int_{a_-}^{a_+} \sin(at)\, e^{-t^2}\, t^{2n}\, dt \tag{68}$$

can be evaluated by using following recurrence formula:

$$I_{2n+2} = \left[e^{-t^2}\, t^{2n-1} \left\{ -\frac{a^2}{4} \cos(at)t + \frac{n}{2} \sin(at) - \frac{1}{2} \sin(at)t^2 \right\} \right]_{a_-}^{a_+}$$

$$- \frac{n(2n+1)}{2} I_{2n-2} + \left(\frac{4n+1}{2} - \frac{a^2}{4} \right) I_{2n} . \tag{69}$$

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The physical input data for THRUSH are the spectral density, mass of scatterer, free atom cross section (or coherent scattering length), temperature and energy mesh points. The simple flow chart for the input routine is shown in Appendix 1.

The main restriction of input data for the present version is

(1) Maximum number of frequency mesh points for spectral density (IMAX) : 400

(2) Maximum number of convolution integral for $\phi_n(\omega)$(NPX) :

NPX $\leq$ 8000/IMAX

(3) Maximum number of energy mesh for scattering kernel (IEX) : 101

The THRUSH code uses only standard input output tape unit (tape 5 for input, tape 6 for output and tape 7 for card punch).

Item	Columns	Format	Code Symbol	Report Symbol	Description
1	1-72	18A4	TITLE		Title Card
2	1-5	I5	IAM		Number of spectral densities ($\leq$ 4).
	6-10	I5	ID		=0 : Incoherent scattering cross section calculation ≠0 : Coherent and Incoherent scattering cross sections calculation.
	11-15	I5	IDD		=0 : Calculate scattering kernels for all input spectral densities. ≠0 : Calculate scattering kernels for spectral densities between IDD and IAM (Note 1).
	16-20	I5	NPX		Number of phonons to be calculated by convolution integral (Note 2).
	21-25	I5	NGX		Maximum number of phonons to be treated in Sjölander expansion. If NGX=0, Sjölander expansion is not calculated. (Note 3).
	26-30	I5	IEX		Number of energy mesh points.
	31-35	I5	IMAX		Number of mesh points for spectral density.
	36-40	I5	INAX		Number of mesh points for positive spectral density for coherent scattering, if ID≠0 and NGX=0 ($\leq$ IMAX).
	41-45	I5	ID2OEL		Number of mesh points for lower frequency part of spectral density, if ID=0 and NGX≠0 ($\leq$ IMAX). ≠0 : Calculate inter-molecular coherent elastic scattering cross section for heavy water. =0 : Skip this calculation.

Item	Columns	Format	Code Symbol	Report Symbol	Description
	46-50	I5	NGP		Number of points for Gaussian integration for short time approximation ($\leq$ 10, Note 3).
3	1-5	I5	IP1		$\neq$0 : Print $\phi_n(\omega)$, for debugging purpose only. =0 : Skip printing.
	6-10	I5	IP2		=0 : Calculate ℓ=0 moment of kernel only. =1 : Calculate ℓ=0 and ℓ=1 moment of kernel.
	11-15	I5	IP3		=0 : Punch ℓ=0 moment of kernel. =1 : Punch ℓ=0 and ℓ=1 moment of kernel. =-1 : Skip punching
	16-20	I5	IP4		$\neq$0 : Print contribution from each phonon term, debugging purpose only. =0 : Skip printing.
	21-25	I5	IP5		=0 : Print ℓ=0 moment of kernel for whole molecule. =1 : Print ℓ=0 and ℓ=1 moment of kernel for whole molecule. =-1 : Skip printing.
	26-35	I5	IP6		Same as IP5 for punching option.
	26-30	I5	IP7		=0 : Print ℓ=0 moment without zero-phonon process (inelastic kernel only). =1 : Print ℓ=0 and ℓ=1 moment without zero-phonon process (inelastic kernel only). =-1 : Skip printing.

Item	Columns	Format	Code Symbol	Report Symbol	Description
	36-40	I5	IP8		Same as IP7 for punching option.
4	1-10	E10.0	EPS1		Error criteria for truncation of phonon expansion (Note 3).
	11-20	E10.0	EPS2		Error criteria for truncation of scattering kernel (Note 4).
5		A5	XNAME(I)		Five characters for identification of spectral density and corresponding kernel (I=1, IAM).
6		I5	ISLF(I)		Define property of scattering for each spectral density. ≠0 : Coherent scattering. =0 : Incoherent scattering.
7					Card 7 is necessary for spectral density to be treated as coherent scattering.
	1-5	I5	IPA1(I)		No. of 1st atom for coherent scattering (1,2...IAM).
	6-10	I5	IPA2(I)		No. of 2nd atom for coherent scattering (1,2...IAM).
	11-20	E10.0	R(I)	$R_{\nu\nu'}$	Distance between IPA1(I) and IPA2(I) atoms.
8	1-10	E10.0	TEMP	T	Temperature in eV unit.
	11-20	E10.0	DLO	$\Delta\omega$	Width of frequency in eV unit for spectral density.
					Card 9 to Card 16 should be repeated IAM times (I=1, IAM). See Note 5.
9	1-10	E10.0	AMASS(I)	M_ν/m	Mass of ν^{th} atom in atomic mass unit for incoherent scattering calculation.

Item	Columns	Format	Code Symbols	Report Symbol	Description
				$\sqrt{\frac{M_\nu}{m}\frac{M_{\nu'}}{m}}$	$\sqrt{\frac{M_\nu}{m}\frac{M_{\nu'}}{m}}$, where M_ν and $M_{\nu'}$ are ν^{th} and ν'^{th} atomic mass in atomic mass unit for coherent scattering calculation.
	11-20	E10.0	SIGF(I)	σ_f	Free atom cross section in barn for incoherent scattering calculation.
				$4\pi A_\nu A_{\nu'}$	$4\pi A_\nu A_{\nu'}$ where A_ν is coherent scattering length of ν^{th} atom for coherent scattering calculation.
10	1-10	E10.0	RHOZ(I)		$\lim_{\omega\to 0}(\frac{\rho(\omega)}{\omega^2})$, where $\rho(\omega)$ is spectral density in eV^{-1} and ω is frequence in eV.
11		7E10.0	RHX(I,J,1)		ID=0 and IGX=0. Spectral density $\rho(\omega)$ (eV^{-1}), J=1, IMAX. Skip to card 17.
12		7E10.0	RHX(I,J,1)	$\rho^{(1)}(\omega)$	ID=0 and IGX≠0. Spectral density function for lower frequency part (eV^{-1}), J=1, INAX.
13		7E10.0	RHX(I,J,2)	$\rho^{(2)}(\omega)$	ID=0 and IGX≠0. Spectral density for higher frequency part (eV^{-1}) J=1, IMAX. Zoros should be input for lower frequence part. Skip to card 17.
14		7E10.0	RHX(I,J,1)	$\rho_{\nu\nu'}(\omega)$	ID≠0 and IGX=0. Spectral density for ν, ν' atom pair. Skip to card 17.

Item	Columns	Format	Code Symbol	Report Symbol	Description
15		7E10.0	RHX(I,J,1)	$\rho^{(1)}_{\nu\nu'}(\omega)$	ID≠0 and IGX≠0. Positive spectral density for ν, ν' atom pair, J=1, INAX.
16		7E10.0	RHX(I,J,2)	$\rho^{(2)}_{\nu\nu'}(\omega)$	Negative spectral density for ν, ν' atom pair, J=1, INAX.
17		7E10.0	E(I)		Energy mesh in eV, I=1, IEX.

Note 1

The scattering kernel of a heavy water molecule may be calculated corresponding to spectral densities of D_{self}, O_{self}, OD pair and D_1D_2 pairs with IAM=4 and ID≠0 option. If IDD is set to zero, the scattering kernels for each input spectral densities and the summed scattering kernel for a whole heavy water molecule will be calculated. If IDD is set to 3, the scattering kernels for OD and D_1D_2 pairs will be calculated. For the calculation of OD pair, one may input IPA1=1, IPA2=2 and R=1 Å and for D_1D_2 pair, IPA1=1, IPA2=1 and R=1.6 Å. The IDD option has no effect, when ID is set to zero.

Note 2

The maximum of NPX is limited by

$$NPX \leq 8000/IMAX.$$

Note 3

The phonon expansion is performed until expanded phonon numbers reach NPX without convergence check. The contribution of phonons from the series with the number greater than NPX is calculated in the Sjölander approximation. This expansion is terminated by the following conversion check. If Δ_n^{ℓ} is the scattering cross section (kernel) from the n-th phonon term,

$$\left| \frac{\Delta_n^{\ell}(E_i \to E)}{\sigma_{\ell}(E_i \to E)} \right| \leq EPS1 , \qquad \ell = 0, 1 . \tag{72}$$

If this inequality is not satisfied until n=NGX, $\sigma_{\ell}(E_i \to E)$ is evaluated by the short time approximation. In the THRUSH code the calculation of the scattering kernel continues to the whole down scattering. If the short time approximation is employed for a certain $E = E_{st}$, then the remaining $\sigma_{\ell}(E_i \to E_f)$ with $E_f < E_{st}$ is calculated in the short time approximation. The full scattering kernel matrix is constructed from the down scattering matrix by the detailed balance principle.

Note 4

If the inequality

$$\left| \frac{\sigma_\ell(E_i \to E_f)}{\sigma_\ell(E_i \to E_j)} \right| \leq \text{ESP } 2 \ , \qquad (\ell = 0, 1) \ , \tag{73}$$

is satisfied, $\sigma_\ell(E_i \to E)$ with $E < E_f$ is set to zero.

Note 5

The spectral density for the incoherent scattering calculation is not necessarily normalized to unity. The spectral density for the coherent scattering calculation, however, should obey Eqs. (58) and (59).

5. Output

The unit system in THRUSH is based on barn and eV, therefore, scattering kernels are in barn/eV unit. Punched output deck for a kernel is composed of one title card followed by a half kernel in the form,

$$((\sigma_\ell(K,J),\ J=1,K),\ K=1,\ IEX) \ ,$$

where K and J are the initial and final energy indexes, respectively. The structure of the card deck for scattering kernels with options, IP3=1, IP6=1 and IP8=1, is

1st atom inelastic kernel	1st atom total kernel	2nd atom inelastic kernel	...

...	IAM-th atom inelastic kernel	IAM-th atom total kernel	total kernel for whole molecule

Each kernel contains ℓ=0 and ℓ=1 moments. If one set -1 for punching option, corresponding the kernel punching will be deleted. Total scattering kernel is defined as

$$\sigma_\ell(E_0 \to E) = \sigma_\ell^{in}(E_0 \to E) + \frac{1}{\Delta E_0} \sigma_\ell^{el}(E_0)\delta(E_0, E) \tag{74}$$

where

$\sigma_\ell(E_0 \to E)$: total scattering kernel,

$$\left| \frac{\sigma_\ell(E_i \to E_f)}{\sigma_\ell(E_i \to E_j)} \right| \leq \text{ESP } 2 \ , \qquad (\ell = 0, 1) \ , \tag{73}$$

is satisfied, $\sigma_\ell(E_i \to E)$ with $E < E_f$ is set to zero.

Note 5

The spectral density for the incoherent scattering calculation is not necessarily normalized to unity. The spectral density for the coherent scattering calculation, however, should obey Eqs. (58) and (59).

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where K and J are the initial and final energy indexes, respectively. The structure of the card deck for scattering kernels with options, IP3=1, IP6=1 and IP8=1, is

1st atom inelastic kernel	1st atom total kernel	2nd atom inelastic kernel	...

...	IAM-th atom inelastic kernel	IAM-th atom total kernel	total kernel for whole molecule

Each kernel contains ℓ=0 and ℓ=1 moments. If one set -1 for punching option, corresponding the kernel punching will be deleted. Total scattering kernel is defined as

$$\sigma_\ell(E_0 \to E) = \sigma_\ell^{in}(E_0 \to E) + \frac{1}{\Delta E_0}\, \sigma_\ell^{el}(E_0)\delta(E_0, E) \tag{74}$$

where

$\sigma_\ell(E_0 \to E)$: total scattering kernel,

$\sigma_{\ell}^{in}(E_0 \rightarrow E)$: inelastic scattering kernel,

$\sigma_{\ell}^{el}(E)$: elastic cross section,

ΔE_0 : DE(I), with I for E_0,

$\delta(E_0, E)$: Kronecker's delta.

References

(1) Kadotani, H., Iijima, S.: J. Nucl. Sci. Tech. (Tokyo), 4, 37 (1967).

(2) Koppel, J. U. et al.: GA-7147 (rev.), (1967).

(3) Honeck, H. C., Naliboff, Y. D.: GA-6824 (1964).

(4) Egelstaff, P. A., Schofield, P.: Nucl. Sci. Eng. 12, 260 (1962).

(5) Sjölander, A.: Ark. Fis., 14, 315 (1958).

(6) Bell, J.: GA-2492 (1962).

(7) Butler, D.: Proc. Phys. Soc., London, 81, 276 (1963).

Acknowledgement

Author would like to thank S. Iijima of NAIG for his suggestion to initiate this work and his encouragement. The work was supported financially by Japanese Nuclear Data Committee.

$\sigma_{\ell}^{in}(E_0 \rightarrow E)$: inelastic scattering kernel,

$\sigma_{\ell}^{el}(E)$: elastic cross section,

ΔE_0 : DE(I), with I for E_0,

$\delta(E_0, E)$: Kronecker's delta.

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(3) Honeck, H. C., Naliboff, Y. D.: GA-6824 (1964).

(4) Egelstaff, P. A., Schofield, P.: Nucl. Sci. Eng. 12, 260 (1962).

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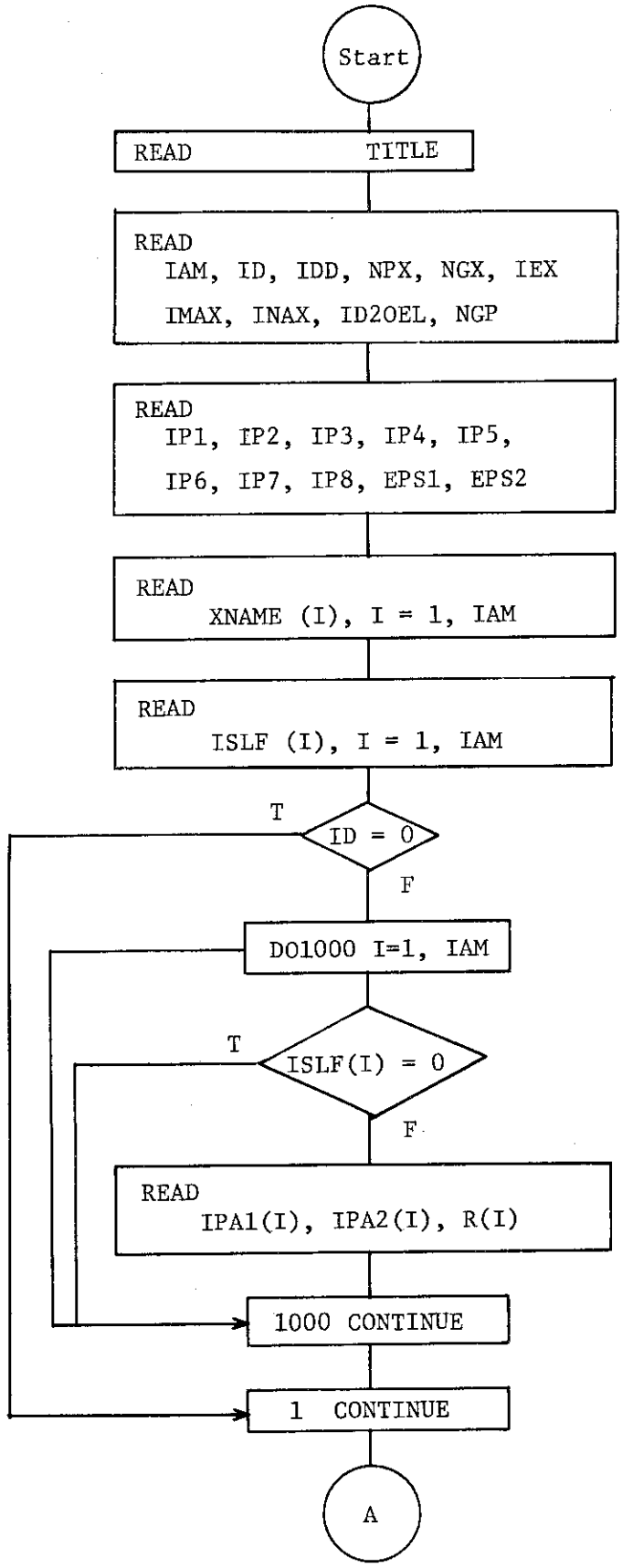
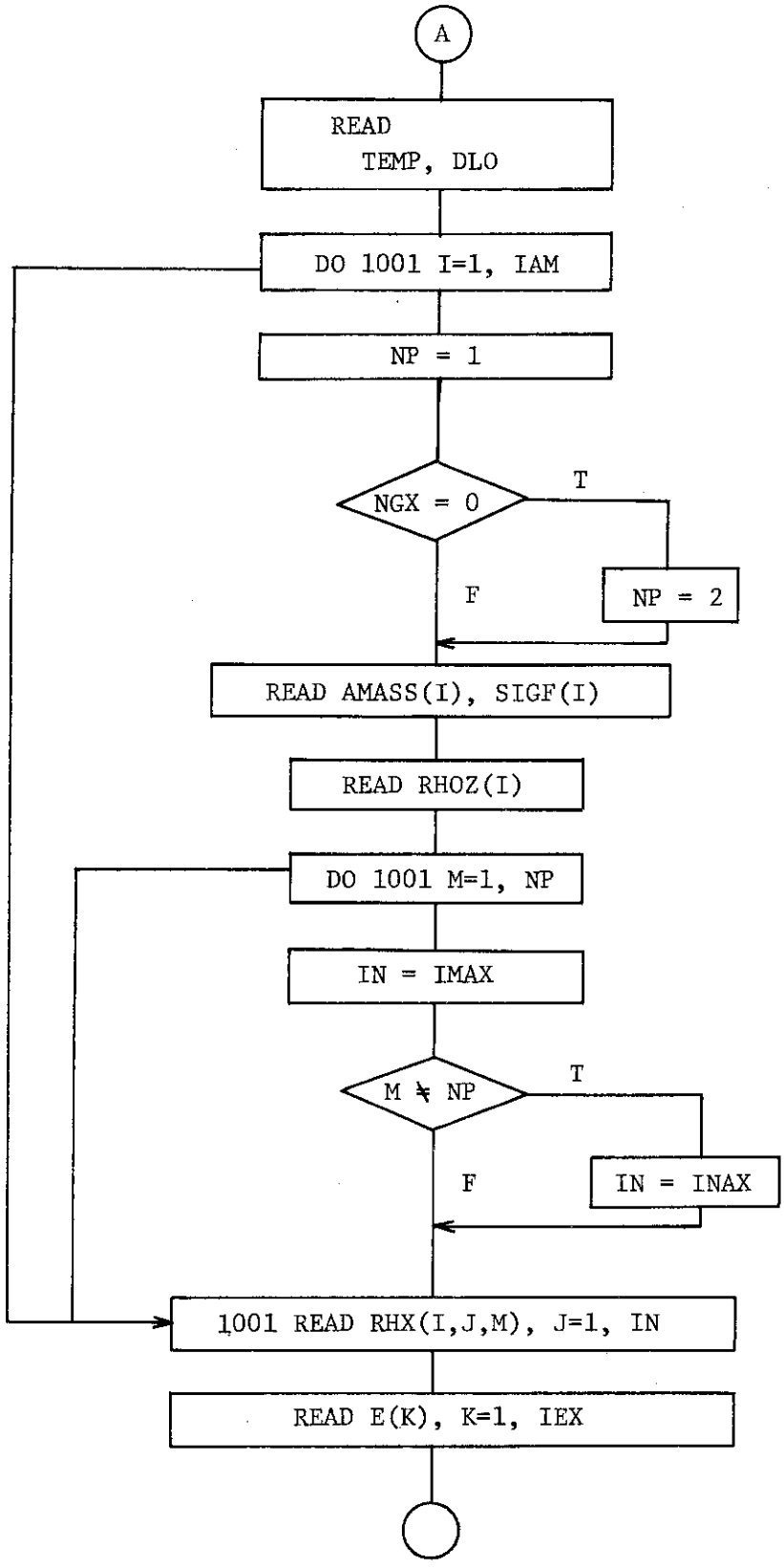
Appendix 1 Flow Chart for Input Routine




A
READ
TEMP, DLO
DO 1001 I=1, IAM
NP = 1
NGX = 0
T
F
NP = 2
READ AMASS(I), SIGF(I)
READ RHOZ(I)
DO 1001 M=1, NP
IN = IMAX
M ≠ NP
T
F
IN = INAX
1001 READ RHX(I,J,M), J=1, IN
READ E(K), K=1, IEX

Appendix 2: Sample input data for the calculation of scattering kernel of Hydrogen in Zirconium Hydride at room temperature.

客先名

作業名

作成者名

日付 / / ページ /

DATA

Line	1–10	11–20	21–30	31–40	41–50	51–60	61–70	71–80
1	H(ZR-H2)	AT ROOM TE	MPERATURE					
2	1 0	0 10	100 IEX*	84 10	0 10			
3	0 1	-1 0	-1 -1	1 -1				
4	0.000011	0.00001						
5	ZR-H2							
6	0							
7	0.0255	0.002						
8	1.0	20.4						
9	85.0							
10	0.00034	0.00141	0.0032	0.00568	0.00888	0.01275	0.01736	
11	0.02268	0.02873	0.03346					
12	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
13	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
14	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
15	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
16	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
17	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
18	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
19	0.0	0.0	0.0	0.00195	0.00437	0.00923	0.01845	
20	0.03492	0.06313	0.10584	0.116956	0.25702	0.368611	0.5	

CRC センチュリリサーチセンタ株式会社

様式番号B－001

客先名
作業名
作成者名

DATA

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1–10	11–20	21–30	31–40	41–50	51–60	61–70	71–80
0.64171	0.77917	0.89503	0.97265	1.0	0.97265	0.89503	
0.77917	0.64171	0.5	0.36861	0.25702	0.16956	0.10584	
0.06313	0.03492	0.01845	0.00923	0.00437	0.00195	0.0	
	[IEX/7] cards for Energy Meshes						
* IEX≦101	: No. of Energy Mesh Points						

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