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A Computational Method of Thermal Neutron Scattering Kernels for High Temperature Crystals

April 1972

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編集兼発行　日本原子力研究所
印　　刷　科学図書印刷株式会社

A Computational Method of Thermal Neutron Scattering Kernels for High Temperature Crystals

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Received December 9, 1971

Summary

Ae efficient treatment of thermal neutron scattering kernels for high temperature crystals has been established and a new computer code HIKER based our treatment has been developed.

Characteristic points in our treatment which are important for taking the high temperature characteristics of crystals into consideration are the following two approximations: 1) The Debye model is used for the low frequency part of the frequency distribution of crystal lattice vibrations. This makes it possible to perform the analytical computation of the scattering law or the dynamical structure factor S_1 (κ, ε) for the low frequency lattice modes: 2) The Doppler approximation is used when the Debye-Waller factor, for the high frequency part of the frequency distribution, exceeds a certain limit (above which a good convergence of Edgeworth series is violated).

When the Debye-Waller factor is below the limit, the scattering law S_2 (κ, ε) for the high frequency lattice modes is computed by the phonon expansion and Edgeworth series methods as usual. The total scattering law S (κ, ε) is obtained by convolution of the two partial scattering laws for the low and high frequency lattice modes. The scattering kernel σ (E_0, E) is obtained from S (κ, ε) by the interpolation over (κ, ε) and the Gaussian integration over the scattering angle.

Characteristics of the code HIKER and guides for users are given. Results of our calculation for $ZrH_{1.5}$ at 1000°C are also illustrated. Efficiency and accuracy of our method are discussed in comparison with the conventional method.

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* Century Research Center Corp.

高温結晶の熱中性子散乱核の一計算法

日本原子力研究所　東海研究所

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1971 年 12 月 9 日　受理

要　　旨

高温の結晶状減速材の熱中性子散乱核の効果的な計算法を案出し，さらに新しい計算コード HIKER を作成した．

結晶の高温特性を考慮した我々の方法における主要な計算法は次の 2 つである：
1)　結晶の格子振動の振動数分布の振動数の低い部分にはデバイ模型を用いる．さらに高温近似を適用すると，散乱則または動的構造因子の計算を解析的に行なうことができるようになる．2)　振動数分布の高振動数部に対するデバイ・ワラー因子がある極限の値（この値より大きくなるとエッジワース級数の収束が悪くなる）を越えた場合には，ドップラー近似を用いる．デバイ・ワラー因子の値が極限の値より小さい時には，高振動数モードに対する動的構造因子の計算は通常の音量子展開法及びエッジワース級数法を用いて行なう．全体の動的構造因子は高及び低振動数モードに対する動的構造因子を重ね合せて求める．散乱核は動的構造因子 $S(\kappa, \varepsilon)$ から (κ, ε) 空間での内挿及び散乱角についてのガウス積分という手続きを経て得られる．

HIKER コードの説明及び使用法の解説を行なった．1000°C の $ZrH_{1.5}$ についての計算結果を図示し，従来の方法による結果と比較を行ない，我々の方法の適用性及び精度についての議論を行なった．

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Contents

1. Introduction 1
2. Computational method 3
2. 1 Introduction 3
2. 2 Debye approximation for low frequency modes 4
2. 3 Phonon expansion and Doppler approximation for high frequency modes 5
2. 4 Convolution of dynamical structure factors 7
2. 5 Scattering kernels 7
3. Descriptions of computer code HIKER 9
3. 1 General description 9
3. 2 Input form 13
3. 3 Output form 16
4. Application to zirconium hydride 17
Acknowledgements 21
References 21

目　　次

1. 序　　論…… 1
2. 計　算　法…… 3
2. 1 序　　論…… 3
2. 2 低振動数モードに対するデバイ近似…… 4
2. 3 高振動数モードに対する音量子展開及びドップラー近似…… 5
2. 4 動的構造因子の重ね合せ…… 7
2. 5 散　乱　核…… 7
3. HIKER コードの解説…… 9
3. 1 一 般 的 説 明…… 9
3. 2 入 力 形 式…… 13
3. 3 出 力 形 式…… 16
4. ジルコニウム・ハイドライドへの適用…… 17
謝　　辞…… 21
引 用 文 献…… 21

1. Introduction

A method which has been used generally to evaluate scattering kernels for crystalline moderators is Parks' method[1], which was programmed for computer by J. BELL. Bell's program is the well known SUMMIT[2]. We have also the UNCLE program which is a version of SUMMIT revised by Japanese Nuclear Data Committee with permission of PARKS and US AEC[3].

In the Parks' method the frequency distribution of crystal lattice vibrations is divided into the low and high frequency parts, $f_1(\omega)$ and $f_2(\omega)$, respectively. The phonon expansion method[4] and the short time approximation[4] are used to evaluate the scattering kernel. The calculation for the high frequency modes is performed by means of the phonon expansion method only. The phonon expansion method involves two different kind of expansions. Which expansion must be used is determined by the value of the Debye-Waller factor for the low frequency part. If this factor is smaller than a certain value which is controlled by input data, each of the first n_{pho} terms in the phonon expansion is computed numerically performing the convolution, which determines the cross section for the n-phonon process ($n \leq n_{\text{pho}}$, where n_{pho} is an integer given as input). The phonon terms of order $n(>n_{\text{pho}})$ are approximated by means of the centrallimit theorem of statistics. This approximated expansion is called the Edgeworth series[3]. For larger values of the Debye-Waller factor, the short time approximation is used for the low frequency modes. For high frequency modes the phonon expansion is made even in this case. The central limit theorem is applied to the contributions from high frequency modes for all values of order n. The Parks' method has been proved very useful for the evaluation of the scattering kernels for crystalline moderators at relatively low temperature ($<1000°C$) and for neutrons with relatively low incident energy ($<$leV). For crystals at relatively high temperature ($\gtrsim 1000°C$) and for hot neutrons*) the number of phonons excited becomes very large and much more computational time is required to obtain reasonable values of the scattering kernel. Moreover, for some types of crystals the convergence of the Edgeworth series becomes violated, so that it can happen that we get meaningless values of scattering kernels for some incident and final energies.

The purpose of our peresent work is to establish a computational method effective in such a case, i. e., a method with which we can get reasonable values of scattering kernels for crystals at high temperature with a good accuracy without spending much computer time. We also divide the frequency distribution into the low and high frequency parts. We approximate the low frequency part by the Debye distribution with a suitable Debye temperature, which is to be determined appropriately from the shape of the original low frequency part of the frequency distribution. Using the Debye model, we can perform analytically the calculation of the scattering kernel for the low frequency modes. For high frequency modes we use the phonon expansion method formulated by PARKS and the Doppler approximation. If the Debye-Waller factor for the high frequency modes is smaller than a values which is controlled by input data and if $n \leq n_{\text{pho}}$, each of n-phonon terms in the phonon expansion is computed rigorously. If $n > n_{\text{pho}}$, the phonon terms are approximated by the Edgeworth series. When the Debye-Waller factor is lager then the control value, the scattering kernel is computed by means of the Doppler approximation.

*) We call neutrons with energies between 1 and 2 or 3 eV hot neutrons.

Generally speaking, low frequency acoustic modes have the Debye type frequency distribution. The contribution of the low frequency modes is relatively unimportant at high temperature, since the mean energy of thermalized neutrons becomes larger as the temperature of a crystal rises. For these reasons, it is reasonable to use the Debye model for the low frequency modes. On the other hand, the expression of the scattering kernel in the Doppler approximation becomes identical with that for the free gas in the high temperature limit. We can expect that the Doppler approximation holds quite good for the scattering of hot neutrons by high temperature crystals.

In the range of temperature of several thousands degrees it would be very difficult to investigate atomic motions of crystals. Anharmonic vibrations may have important effects on the scattering of neutrons. Since we have not enough data on the frequency distributions for the real materials at high temperature and it is very difficult to perform the theoretical evaluation of the frequency distribution taking into consideration of the anharmonic effects, we are obliged to use the frequency ditribution at the room temperature even in the case of high temperature. But this causes no serious errors for neutron moderators used in thermal reactors.

At much more higher temperature, the computational technique of the scattering kernel may be simplified for scattering with relatively small energy transfer because the expansion in T^{-1} may be effective in such a case.

2. Computational Method

2. 1 Introduction

The general expression of the differential scattering cross section for thermal neutrons is as follows :

$$\frac{\sigma(E_0 \to E, \mu)}{\sigma_{\text{free}}} = \frac{1}{4\pi}\left(1+\frac{1}{M}\right)^2 \sqrt{\frac{E}{E_0}} \int_{-\infty}^{\infty} dt\, e^{i\varepsilon t} X(\kappa, t), \tag{2.1}$$

where

$$\varepsilon = E - E_0,$$

$$\kappa^2/_2 = E + E_0 - 2\sqrt{EE_0}\,\mu,$$

$$X(\kappa, t) = \exp\left\{\frac{\kappa^2}{2M}[\gamma(t)-\gamma(0)]\right\}, \tag{2.2}$$

$$\gamma(t) = \int_0^{\infty} d\omega \frac{f(\omega)}{\omega}\left[\coth\left(\frac{\omega}{2T}\right)\cos(\omega t) + i\sin(\omega t)\right]. \tag{2.3}$$

The function $X(\kappa, t)$ is the so-called intermediate scattering function. The meaning of physical quantities in Eqs. (2.1)~(2.3) is given below :

σ_{free} free atom scatterimg cross section,
E_0, E energies of incident and scattered neutrons, respectively, (eV),
M atomic mass (in the unit of neutron mass to be 1.0).
μ cosine of the scattering angle,
t time,
ω frequency of the crystal lattice vibration, (eV),
$f(\omega)$ frequency distribution of the crystal lattice vibrations,
T temperature of crystal, (eV).

Since three dimensional quantities such as $\sigma(E_0, E, \mu)$ require very large core memory of computer, it is desirable to use two dimensional quantities. The differential scattering cross section can be written in terms of the dynamical structure factor $S(\kappa, \varepsilon)$ as follows ;

$$\frac{\sigma(E_0 \to E, \mu)}{\sigma_{\text{free}}} = \frac{1}{4\pi}\left(1+\frac{1}{M}\right)^2 \sqrt{\frac{E}{E_0}}\, S(\kappa, \varepsilon). \tag{2.4}$$

From $S(\kappa, \varepsilon)$ we evaluate the Legendre moments $\sigma_l(E_0 \to E)$ by means of the Gaussian integration over μ. The definition of the scattering kernal of order l is given by

$$\frac{\sigma_l(E_0 \to E, \mu)}{\sigma_{\text{free}}} = \frac{1}{2}\left(1+\frac{1}{M}\right)^2 \sqrt{\frac{E}{E_0}} \int_{-1}^{1} S(\kappa, \varepsilon) P_l(\mu) d\mu. \tag{2.5}$$

The value of $S(\kappa, \varepsilon)$ for given initial and final energies and for the scattering angle corresponding to the Gaussian mesh μ_i is obtained by interpolating the values of $S(\kappa, \varepsilon)$ which have been calculated beforehand for input (κ, ε) values. In Eq. (2.5) $P_l(\mu)$ is the Legendre polynomials.

The relation between $S(\kappa, \varepsilon)$ and the so called scattering law $S(\alpha, \beta)$ is given by

$$S(\alpha, \beta) = Te^{\beta/2} S(\kappa, \varepsilon), \tag{2.6}$$

where

$$\alpha=\frac{\kappa^2}{2MT}=\frac{1}{MT}(E_0+E-2\sqrt{E_0E}\,\mu),$$

$$\beta=\frac{\varepsilon}{T}=\frac{1}{T}(E-E_0).$$

We divide the frequency distribution of the crystal lattice vibrations into low and high frequency parts;

$$f(\omega)=f_1(\omega)+f_2(\omega). \tag{2.7}$$

As can be easily seen from Eqs. (2.2) and (2.3), dividing $f(\omega)$ as in Eq. (2.7), we can write the intermediate scattering function in the form of product of partial ones:

$$X(\kappa,t)=X_1(\kappa,t)X_2(\kappa,t), \tag{2.8}$$

where indices 1 and 2 refer to the low and high frequency modes, respectively.

We begin our calculation with partial dynamical structure factors, $S_1'(\kappa,\varepsilon)$ and $S_2'(\kappa,\varepsilon)$, which correspond to the low and high frequency modes, respectively. We apply our method mentioned above to the calculation of them. Total $S(\kappa,\varepsilon)$ is obtained by convolving the partial $S_1'(\kappa,\varepsilon)$ and $S_2'(\kappa,\varepsilon)$;

$$S(\kappa,\varepsilon)=\int_{-\infty}^{\infty}d\varepsilon' S_1'(\kappa,\varepsilon-\varepsilon')S_2'(\kappa,\varepsilon'). \tag{2.9}$$

2.2 Debye Approximation for Low Frequensy Modes

We apply the Debye model to the low frequency modes. The Debye frequency distribution is

$$f_1(\omega)=C(3/\omega_D{}^3)\omega^2, \tag{2.10}$$

where $f_1(\omega)$ is normalized to C. The parameter C is a weight factor for the low frequency modes and ω_D is the Debye cut-off frequency. The phonon expansion method writes $S_1'(\kappa,\varepsilon)$ in the form[1),4)]

$$S_1'(\kappa,\varepsilon)=e^{-2W_1-\beta\varepsilon}\sum_{n=0}^{NPl}\frac{(2W_1)^n}{n!}G_n(\varepsilon), \tag{2.11}$$

where β is $(2T)^{-1}$ and $2W_1$ is the Debye-Waller factor for the low frequency modes defined as

$$2W_1=\frac{\kappa^2}{2M}\gamma_1(0), \tag{2.12}$$

$$\gamma_1(0)=\int_0^{\omega_D}d\omega\frac{f_1(\omega)}{\omega}\coth(\beta\omega). \tag{2.13}$$

The quantity NPl is an intput which gives the number of phonon terms to be calculated. The functions $G_n(\varepsilon)$ are given in the form of successive convolution

$$\left.\begin{aligned}&G_0(\varepsilon)=\delta(\varepsilon),\\&G_1(\varepsilon)=g(\varepsilon)=\frac{f_1(\varepsilon)}{2\varepsilon\gamma_1(0)\sinh(\beta\varepsilon)},\\&G_n(\varepsilon)=\int_{-\infty}^{\infty}d\varepsilon' g(\varepsilon')G_{n-1}(\varepsilon-\varepsilon').\end{aligned}\right\} \tag{2.14}$$

When $\beta\ll1$, i.e., when temperature is sufficiently high, Eqs. (2.13) and (2.14) can be considerably simplified. Using Eq. (2.10) in Eq. (2.13) and the condition $\beta\ll1$, we get

$$\gamma_1(0)=C\frac{3}{\beta\omega_D{}^2}, \tag{2.15}$$

$$G_1(\varepsilon)=\begin{cases}\dfrac{1}{2\omega_D}, & \text{if } |\varepsilon|\leq\omega_D,\\ 0\ , & \text{if } |\varepsilon|>\omega_D,\end{cases} \tag{2.16}$$

$$G_n(\varepsilon)=\begin{cases}\dfrac{n}{(2\omega_D)^n}\sum_{\nu=0}^{N_D}(-1)^\nu\dfrac{\{(n-2\nu)\omega_D-|\varepsilon|\}^{n-1}}{\nu!\,(n-\nu)!}, & \\ \qquad\qquad \text{if } |\varepsilon|\leq n\omega_D, & \\ 0, \qquad\qquad \text{if } |\varepsilon|>n\omega_D, & \end{cases} \tag{2.17}$$

where

$$N_D=\left[\frac{1}{2}\left(n-\frac{|\varepsilon|}{\omega_D}\right)\right].$$

The bracket [A] means the largest integer which is smaller than A.

Since a computer can not deal with the delta-function, at first we do not calculate zero phonon term and we take the summation in Eq. (2.11) from $n=1$. We redefine $S_1(\kappa,\varepsilon)$ here:

$$S_1(\kappa,\varepsilon)=e^{-2W_1-\beta\varepsilon}\sum_{n=1}^{NP1}\frac{(2W_1)^n}{n!}G_n(\varepsilon).$$

The contribution of the zero phonon term is evaluated as the elastic scattering cross section in the later stage of our calculation.

2. 3 Phonon Expansion and Doppler Approximation for High Frequency Modes

We use phonon expansion method when the condition $2W_2\leq\overline{N}$ is satisfied, where $2W_2$ is the Debye-Waller factor for the high frequency modes:

$$2W_2=\frac{\kappa^2}{2M}\gamma_2(0), \tag{2.18}$$

$$\gamma_2(0)=\int_{\omega_1}^{\omega_2}d\omega\frac{f_2(\omega)}{\omega}\coth(\beta\omega). \tag{2.19}$$

$\overline{N}$ is an input number, ω_1 and ω_2 being the lower and higher boundaries of $f_2(\omega)$, respectively. The normalization factor for $f_2(\omega)$ is (1-C).

1) The first method. When $2W_2\leq\overline{N}$ and $0\leq n\leq NP2$, we use the exact phonon expansion[3]

$$S_2(\kappa,\varepsilon)=\sum_{n=1}^{NP2}S_2{}^{(1)}(\kappa,\varepsilon)_n, \tag{2.20}$$

where $NP2$ is an input number and

$$S_2{}^{(1)}(\kappa,\varepsilon)_n=e^{-2W_2-\beta\varepsilon}\frac{(2W_2)^n}{n!}H_n(\varepsilon), \tag{2.21}$$

$$\left.\begin{aligned}H_1(\varepsilon)=h(\varepsilon)&\equiv\frac{f_2(\varepsilon)}{2\varepsilon\gamma_2(0)\sinh(\beta\varepsilon)},\\ H_n(\varepsilon)&=\int_{-\infty}^{\infty}d\varepsilon' h(\varepsilon')H_{n-1}(\varepsilon-\varepsilon').\end{aligned}\right\} \tag{2.22}$$

As in the case of the calculation for low frequency modes, we do not include the zero phnonon term in the summation of Eq. (2.20).

2) The second method. When $2W_2 \leq \bar{N}$ and $NP2 < n \leq NT$, we apply the central limit theorem to each term of order n. Here NT is fixed at 30. The phonon expansion is then given in the form of the Edgeworth series, the n-th term in which is[3]

$$S_2^{(2)}(\kappa,\varepsilon)_n = e^{-2W_2}\left(\frac{\kappa^2}{2M}\right)^n f_1 f_2 f_3, \tag{2.23}$$

where

$$f_1 = \frac{[\gamma_2(0)]^n}{n!},$$

$$f_2 = \frac{e^{-v^2/2}}{\sqrt{2\pi b}},$$

$$v = \frac{-\varepsilon + a}{\sqrt{b}}, \qquad a = \frac{n}{\gamma_2(0)}, \qquad b = n\sigma^2,$$

$$\sigma^2 = \alpha_2 - (\alpha_1)^2, \qquad \alpha_1 = \frac{1}{\gamma_2(0)}, \qquad \alpha_2 = 2\bar{T}\alpha_1,$$

$$\bar{T} = \frac{1}{2}\int_{\omega_1}^{\omega_2} d\omega f_2(\omega)\omega \coth(\beta\omega),$$

$$f_3 = 1 - \frac{1}{3!}\left(\frac{c}{b^{3/2}}\right)H_3(v) + \frac{1}{4!}\left(\frac{d}{b^2}\right)H_4(v) + \frac{1}{2}\left(\frac{1}{3!}\right)^2\left(\frac{c}{b^{3/2}}\right)^2 H_6(v),$$

$$c = n\kappa_3,$$

$$\kappa_3 = \alpha_3 - 3\alpha_1\alpha_2 + 2(\alpha_1)^3,$$

$$\alpha_3 = \beta\alpha_1,$$

$$H_n(v) = \text{Hermite polynomials},$$

$$B = \int_{\omega_1}^{\omega_2} d\omega f_2(\omega)\omega^2,$$

$$d = n\kappa_4,$$

$$\kappa_4 = \alpha_4 - 3(\alpha_2)^2 - 4\alpha_1\alpha_2 + 12(\alpha_1)^2\alpha_2 - 6(\alpha_1)^2,$$

$$\alpha_4 = 2D,$$

$$D = \frac{1}{2}\int_{\omega_1}^{\omega_2} d\omega f_2(\omega)\omega^3 \coth(\beta\omega).$$

3) The third method[4]. When the condition $2W_2 > \bar{N}$ is satisfied, we use the Doppler approximation. If $2W_2$ is sufficiently large ($\gg 1$), we can expand $\gamma(t)$ in powers of t and take only two leading terms

$$\gamma(t) - \gamma(0) \simeq it - \frac{1}{3}E_c t^2, \tag{2.24}$$

where

$$E_c = 3\int_{\omega_1}^{\omega_2} d\omega f_2(\omega)\frac{\omega}{2}\coth(\beta\omega), \tag{2.25}$$

$E_c/2$ being the mean kinetic energy of atoms E_{kin}. In the high temperature limit E_{kin} approaches to $3T/2$ which is the mean kinetic energy of free atoms. In this case $S_2'(\kappa,\varepsilon)$ is given in the form of Doppler broadened function

$$S_2'(\kappa,\varepsilon) = \frac{1}{\sqrt{2\pi}\Delta}\exp\left[-\frac{\left(\varepsilon + \frac{\kappa^2}{2M}\right)^2}{2\Delta^2}\right], \tag{2.26}$$

where

$$\Delta^2=\frac{2}{3}\frac{\kappa^2}{2M}E_c.$$

2. 4 Convolution of Dynamical Structure Factors

The total dynamical structure factor is obtained by convolving the partial ones, $S_1(\kappa,\varepsilon)$ and $S_2(\kappa,\varepsilon)$. The zero-phonon contributions, which have been omitted from the phonon expansion series for $S_1(\kappa,\varepsilon)$ and $S_2(\kappa,\varepsilon)$, must be added to the partial dynamical factors to be convolved. The total (elastic+inelastic) dynamical structure factor for the low frequency modes is

$$S_1'(\kappa,\varepsilon)=e^{-2W_1}\delta(\varepsilon)+S_1(\kappa,\varepsilon). \tag{2.27}$$

Those for the high frequency modes is

$$S_2'(\kappa,\varepsilon)=e^{-2W_2}\delta(\varepsilon)+S_2(\kappa,\varepsilon). \tag{2.28}$$

When $2W_2\leq\bar{N}$, $S_2(\kappa,\varepsilon)$ is the sum of the values calculated by means of the first and second methods:

$$S_2(\kappa,\varepsilon)=\sum_{n=1}^{NP2}S_2^{(1)}(\kappa,\varepsilon)_n+\sum_{n=NP2+1}^{NT}S_2^{(2)}(\kappa,\varepsilon)_n. \tag{2.29}$$

When $2W_2>\bar{N}$, the Doppler expanion method was used. In this case the elastic contribution is included in $S_2'(\kappa,\varepsilon)$. We separate the contribution with $\varepsilon=0$ from $S_2'(\kappa,\varepsilon)$ in analogy with Eq. (2.28);

$$S_2'(\kappa,\varepsilon)=\frac{1}{\sqrt{2\pi}\Delta}\exp\left[-\frac{1}{2\Delta^2}\left(\frac{\kappa^2}{2M}\right)^2\right]\delta(\varepsilon)+S_2(\kappa,\varepsilon)\simeq e^{-2W_2}\delta(\varepsilon)+S_2(\kappa,\varepsilon). \tag{2.30}$$

The convolution of $S_1'(\kappa,\varepsilon)$ and $S_2'(\kappa,\varepsilon)$ gives the total dynamical structure factor $S(\kappa,\varepsilon)$:

$$S(\kappa,\varepsilon)=\int_{-\infty}^{\infty}S_1'(\kappa,\varepsilon')\,S_2'(\kappa,\varepsilon-\varepsilon')d\varepsilon'=e^{-2W_1-2W_2}\delta(\varepsilon)+S_{in}(\kappa,\varepsilon), \tag{2.31}$$

where the first term in the right hand side of Eq. (2.31) is the contribution from the elastic scattering and the second term is the inelastic part:

$$S_{in}(\kappa,\varepsilon)=e^{-2W_2}S_1(\kappa,\varepsilon)+e^{-2W_1}S_2(\kappa,\varepsilon)+\int_{-\infty}^{\infty}d\varepsilon'S_1(\kappa,\varepsilon')\,S_2(\kappa,\varepsilon-\varepsilon'). \tag{2.32}$$

2. 5 Scattering Kernels

Once we get the values of $S(\kappa,\varepsilon)$, we can obtain scattering kernels from Eq. (2.5) by performing the Gaussian integration over μ. Usually the elastic contributions are not includcd in the so-called scattering kernels. But when we use a code in which total, transport cross sections, $\bar{\mu}(E)$, etc., are to be computed from scattering kernels, the elastic contributions have to be included in the input kernels.

The elastic angular scattering cross section for crystals is

$$\frac{d\sigma_{el}}{d\Omega}=\frac{1}{4\pi}\sigma_{free}\left(1+\frac{1}{M}\right)^2e^{-2A(E_0)\sin^2(\theta/2)}, \tag{2.33}$$

where θ is the scattering angle and Ω is the solid angle.

$$A(E_0)\equiv 2\frac{E_0}{M}\gamma(0).$$

The elastic scattering cross sections are given by

$$\frac{\sigma_{\mathrm{el}}(E_0)}{\sigma_{\mathrm{free}}}=\frac{1}{2}\left(1+\frac{1}{M}\right)^2\int_{-1}^{1}e^{-A(E_0)(1-\mu)}d\mu=\frac{1}{2}\left(1+\frac{1}{M}\right)^2\frac{1}{A(E_0)}(1-e^{-2A(E_0)}) \tag{2·34}$$

and the Legendre moments of order 1 is

$$\begin{aligned}\frac{\sigma_{\mathrm{el},1}(E_0)}{\sigma_{\mathrm{free}}}&=\frac{1}{2}\left(1+\frac{1}{M}\right)^2\int_{-1}^{1}e^{-A(E_0)(1-\mu)}\mu d\mu\\&=\frac{1}{2}\left(1+\frac{1}{M}\right)^2\frac{1}{[A(E_0)]^2}e^{-2A(E_0)}\times\{e^{2A(E_0)}[A(E_0)-1]+[A(E_0)+1]\}.\end{aligned} \tag{2.35}$$

The contributions of the elastic scattering to the diagonal jj elements of thc scattering kernels are $\sigma_{\mathrm{el},l}(E)/\Delta E$, where ΔE is the input energy mesh size. Thus we have the following scattering kernels,

$$\sigma_l(E_{\mathrm{j}}, E_{\mathrm{i}})=\sigma_{\mathrm{in},l}(E_{\mathrm{j}}, E_{\mathrm{i}})+\frac{\sigma_{\mathrm{el},l}(E_{\mathrm{j}})}{\Delta E_{\mathrm{i}}} \tag{2.36}$$

where $l=0, 1$.

3. Description of Computer Code HIKER

3. 1 General Description

The computationl method described in Chapter 2 has been programmed using the FORTRAN-IV language. Our program is named HIKER, which means HI-gh temperature KER-nels. The physical quantities which can be obtained by HIKER are

1) the dynamical structure factor, $S(\kappa, \varepsilon)$,
2) the scattering law, $S(\alpha, \beta)$,
3) the scattering kernels, $\sigma_l(E_0, E)$, $l=0, 1$,
4) THERMOS kernels, $P_{ij,l}$, $l=0, 1$,
5) the total scattering cross section, $\sigma_s(E_0)$,
6) the transport cross section, $\sigma_{tr}(E_0)$,
7) the mean cosine of the scattering angle, $\bar{\mu}(E_0)$.

Now we explain the over-all structure of HIKER. The main program controls the over-all flow of the calculation and performs the calculation of quantities 1)~7) listed above, using subroutines and function routines for the detailed calculations. The main flow of the program is decribed in **Fig. 1**. The numbers in parentheses in the following explanation refer to the numbers on the flow chart of **Fig. 1**.

(1) Subroutine HIINP reads most of control and physical input data and performs preliminary calculations. Physical quantities which are calculated by HIINP are

CAPT=$\bar{T}$, CAPB=B, CAPC=D, GAMZ=$\gamma_2(0)$, ALP 1=α_1, ALP 2=α_2,
ALP 3=α_3, ALP 4=α_4, AKAP 3=κ_3, AKAP 4=κ_4, ENGC=E_c

The calculation of integrals

$$\int_{\omega_1}^{\omega_2} d\omega f_2(\omega)\omega^n \coth(\beta\omega), \quad n=\pm 1, 3, \quad \int_{\omega_1}^{\omega_2} d\omega f_2(\omega)\omega^2$$

is performed by Subroutine INTEG which uses the trapezoidal rule of integration.

(2) Subroutine EPSKAP is used to generate ε and κ meshes. The input numbers DEPS ($=\Delta\varepsilon$), EPSS ($=\varepsilon_c$), DXKAP ($=\Delta\kappa$) and XAPP ($=\kappa_c$) are used to generate uniform ε and κ meshes over the ranges:

$$\varepsilon=0, \Delta\varepsilon, 2\Delta\varepsilon, \cdots\cdots, \varepsilon_c,$$

$$\kappa=\Delta\kappa, 2\Delta\kappa, \cdots\cdots\cdots, \kappa_c.$$

In the remained range the ε, κ meshes are determined with geometrically increasing ε and κ intervals arranged to reach EMAX ($=\varepsilon_{max}$) and XMAX ($=\kappa_{max}$) with the number of meshes required in the input.

(3) When the several cases are to be calculated in a single run, the routine (2) is skipped in the case continued from the preceeding one.

(4) Subroutine CLEAR is used for zero clearance.

(5) IOPT controls the calculation in Subroutine CONGH.

(6) Subroutine COHGH calculates $H_1(\varepsilon)$ when IOPT=2 and $G_n(\varepsilon)$ ($n=1\sim$NP 1) when IOPT=1.

(7) Brock (7) performs the convolution calculation

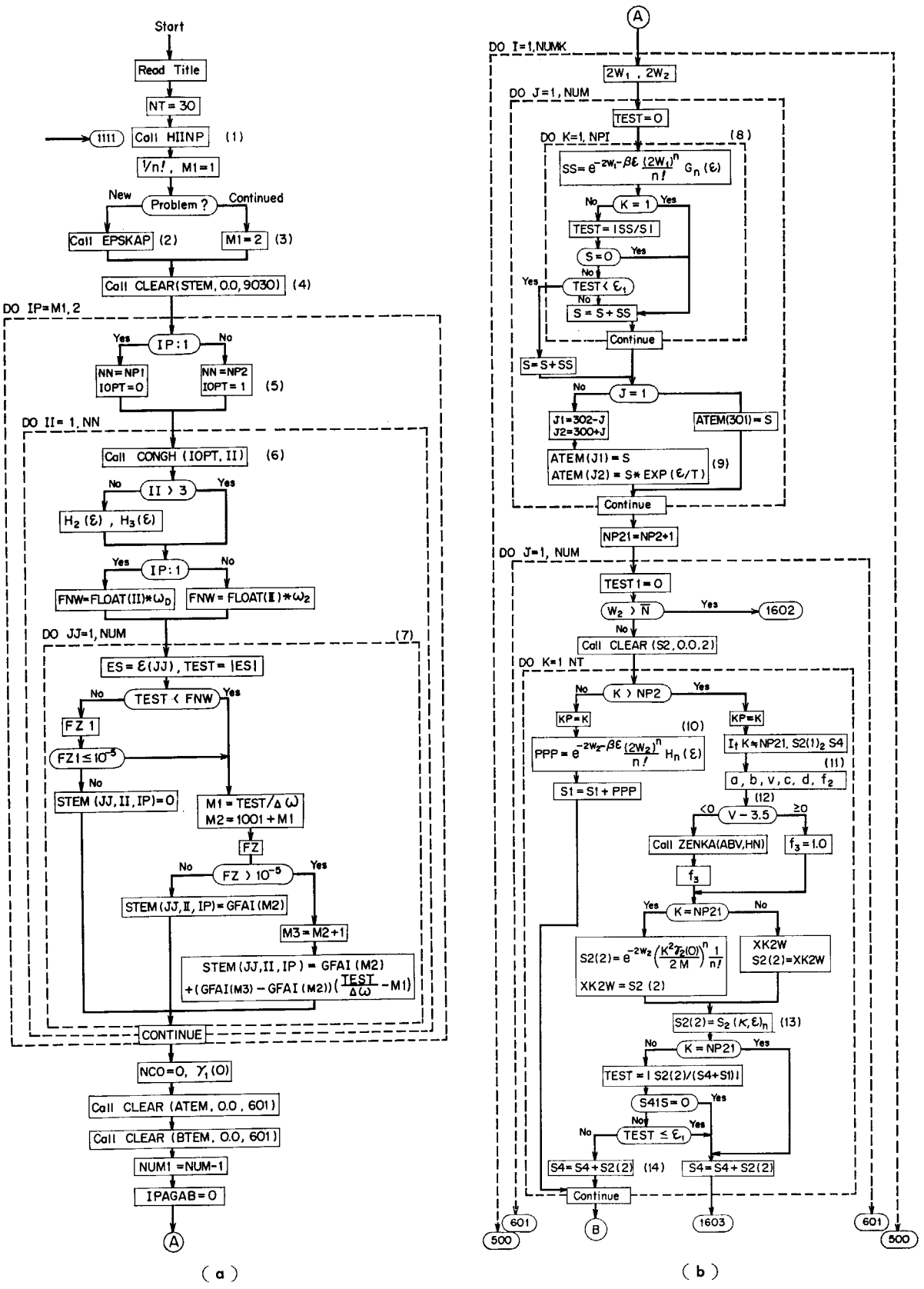


Fig. 1 Main flow of HIKER

The numbers in parentheses in the figure refer to the numbers of explanations in section 3.1.

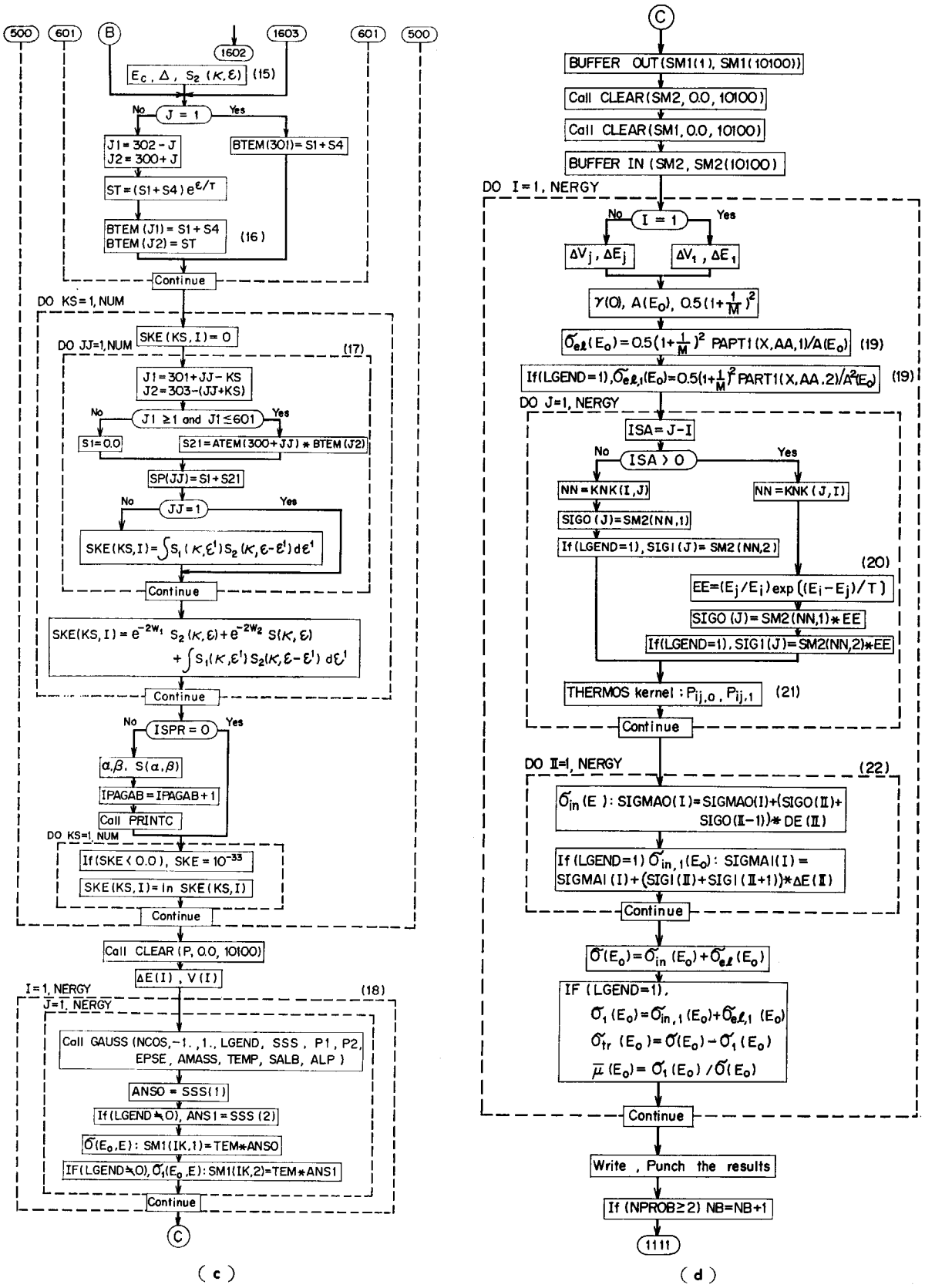


Fig. 1 Main flow of HIKER

The numbers in parentheses in the figure refer to the numbers of explanations in section 3.1.

$$H_n(\varepsilon)=\int_{-\infty}^{\infty} h(\varepsilon')H_{n-1}(\varepsilon-\varepsilon')d\varepsilon'.$$

The defining ε region for $H_n(\varepsilon)$ is given by

$$0\leq|\varepsilon|\leq n\cdot\mathrm{NOMG}\cdot\Delta\omega$$

where NOMG is the number of meshes for the frequency distribution and $\Delta\omega$ is its mesh size. We calculate $H_n(\varepsilon)$ for negative ε only. The FORTRAN symbol STEM (JJ, II, 1) refers to $G_n(\varepsilon)$ and STEM (JJ, II, 2) to $H_n(\varepsilon)$.

(8) In the block (8) the partial dynamical structure factor $S_1(\kappa,\varepsilon)$ is computed for the negative ε. As soon as the convergence criterion for the phonon expansion series controlled by input is satisfied, the calculation of $S_1(\kappa,\varepsilon)$ is terminated even if $n<$NP 1.

(9) Values of $S_1(\kappa,\varepsilon)$ for $-\varepsilon$ (ε negative) is obtained using the detailed balance relation

$$S_1(\kappa,-\varepsilon)=e^{\varepsilon/T}S_1(\kappa,\varepsilon).$$

(10) The dynamical structure factor for the high frequency modes, $S_2(\kappa,\varepsilon)$, is computed by means of the first method.

(11) The $K<$NP 2 calculation begins with the preliminary calculation of quantities necessary to perform the second method.

(12) When $v>3.5$, we approximate f_3 to be 1. For $v\leq3.5$, we calculate Hermite polynomials using the recurrence formula

$$H_0(v)=1,\qquad H_1(v)=v,$$

$$H_n(v)=H_1H_{n-1}-(n-1)H_{n-2}.$$

Subroutine ZENKA is used for the calculation of $H_n(v)$.

(13) The flow through (11), (12), (13), (14) is for the calculation of $S_2(\kappa,\varepsilon)$ by the second method. The calculation of $S_2(\kappa,\varepsilon)$ is terminated and skipped to the next step, as soon as the convergence criterion is satisfied.

(15) The computation of $S_2(\kappa,\varepsilon)$ is performed using the Doppler approximation when the Debye-Waller factor W_2 is larger than a value controlled by input.

(16) Values of $S_2(\kappa,\varepsilon)$ are obtained for all (positive and negative) meshes of using the detailed balance. BTEM refers to $S_2(\kappa,\varepsilon)$.

(17) Block (17) is for the convolution of $S_1(\kappa,\varepsilon)$ and $S_2(\kappa,\varepsilon)$.

(18) Subroutine GAUSS is for the intergration of $S(\kappa,\varepsilon)$ over μ. The 10 and 20 point Gauss integrations are available in our program. The value of $S(\kappa,\varepsilon)$ corresponding to the (κ,ε) point deterimened by input (E_i, E_j) and the Gaussian mesh μ_k is obtained by the Function routine FUN, which calls Subroutine TERP. Subroutine TERP is used to seek intermediate values of $S(\kappa,\varepsilon)$ by linear interpolation of ln S between successive values of κ or ε. The values of ε extend from 0 to ε_{max} but κ starts from a non zero value $\Delta\kappa$. For $\kappa<\Delta\kappa$, S is assumed to be proportional to κ^k. The value of k is determined form $S(\kappa_1,\varepsilon)$ and $S(\kappa_2,\varepsilon)$ using the relation

$$k=\frac{\ln\left[S(\kappa_2,\varepsilon)/S(\kappa_1,\varepsilon)\right]}{\ln(\kappa_2/\kappa_1)}.$$

This scheme of interpolation and extrapolation is used in FLANGE[5] which calculates scattering cross sections from the scattering law $S(\alpha,\beta)$.

In Block (18) half kernels $\sigma(E_i, E_j)$ and $\sigma_1(E_i, E_j)$ are determined.

(19) The calculation of elastic scattering cross sections is performed.

(20) The full kernels are obtained using the detailed balance relation

$$\sigma_l(E_0\rightarrow E)E_0e^{-E_0/T}=\sigma_l(E\rightarrow E_0)Ee^{-E/T}.$$

(21) THERMOS kernels defined by[6]

$$P_{ij,l}=0.0506 v_i v_j \Delta v_j \sigma_l(E_j \rightarrow E_i)$$

are calculated, if required, where v_i is the neutron velocity in units of 2200 m/sec and is calculated from E_i (eV);

$$v_i = 6.286944 \sqrt{E_i}.$$

(22) Integration over E is done by the formula

$$\sigma_l(E_j) = \sum_{i=1}^{NERGY-1} [\sigma_l(E_j \rightarrow E_i) + \sigma_l(E_j \rightarrow E_{i+1})] \Delta E_i$$

where

$$\Delta E_i = 0.5(E_{i+1} - E_i).$$

3. 2 Input Form

The form of input to HIKER is described on the following pages. Input data have to be prepared for items 1~3 in FORMAT (2I5, 6F10.0/(7F10.0)). The first integer indicates the relative location of the item and is fixed in our program. All numbers other than given on the following pages will result in an unexpected error. The second integer gives the number of data included in that item. For items 4~10 data should be given in FORMAT (2I5, 6E10.5/(7E10.5)).

Item	Columns	Program symbol	Physics symbol	Explanation
1	1~60			Title Card (A-Format).
2(1)	1~5			should be 1.
	6~10			should be 17.
	11~20	NPROB		Number of problems to be calculated.
	21~30	KERPR		Zero or non-zero. If non zero, the values of E_0, E and $\sigma_l(E_0, E)$ will be printed. If zero, this print is not given
	31~40	KERPC		Zero or non-zero. If non zero, half kernels will be punched in FORMAT (5E12.3) in the order σ (1→1), σ(2→1), σ(2→2), σ(3→1), σ(3→2), ……. If zero, no punched card will be obtained.
	41~50	KPIT		Zero or non zero. If non-rero, THERMOS kernels will be punched.
	51~60	ISPR		Zero or non zero. If non-zero, the Scattering Law $S(\alpha, \beta)$ will be printed. If zero, this print is not given.
	61~70	LGEND		Zero or 1. If zero, the calculation will be done only for $l=0$, where l is the order of Legendre moments. If 1, the calculation will be done up to $l=1$ and σ_{tr} and $\bar{\mu}$ will be obtained.
2(2)	1~10	NP 1		The number of phonon terms for the low frequency modes. $3 \leq NP\,1 \leq 15$.
	11~20	NP 2		The number of phonon terms for the high frequency modes. Terms of order $n < NP\,2$ are calculated by the second method. $3 \leq NP\,2 \leq 10$.
	21~30	NERGY		The number of energy points ≤ 110.

Item	Columns	Program symbol	Physics symbol	Explanation
	31～40	NOMG*)		The number of mesh points for $f_2(\omega) \leq 101$.
	41～50	NOMGL		The number of mesh points for the lower cut-off of ω value for $f_2(\omega) <$ NOMG. $\omega_1 = \Delta\omega$ *NOMGL.
	51～60	NRE		Zero or Nonzero. If zero, points are given with equal mesh size. If non-zero, ε will be given in uniform size up to ε_c, beyond which geometrically increasing mesh sizes will be used to generate ε points.
	61～70	NUM		The number ef ε points ≤ 301.
2(3)	1～10	NRK		The same explanation as for NRE is applied to κ.
	11～20	NUKK		The number of κ points $\leqq 100$.
	21～30	NBAR	$\bar{N}$	The control number to select methods in the calculation of $S_2(\kappa, \varepsilon)$. If $2W_2 \leq \bar{N}$, the first and second method are used, otherwise the third method is used.
	31～40	NCOS		The number of mesh points in Gauss integration over μ. Only 10 and 20 point values are stored in our program (should be 10 or 20).
3(1)	1～5			should be 31.
	6～10			should be 10.
	11～20	AMASS	M	Atomic mass.
	21～30	TEMP	T(eV)	Temperature of crystal.
	31～40	DOMG	ω_D(eV)	The Debye cut-off frequency for the low frequency part of the frequency distribution= $\Delta\omega$* NOMGD.
	41～50	OMGU	ω_2(eV)	The cut-off frequency for the high frequency part of the frequency distribution= $\Delta\omega$* (NOMG-1).
	51～60	CWEIT	C	Weight of the low frequency modes.
	61～70	SIGF	σ_{free} (barns)	Free atom scattering cross section.
3(2)	1～10	DEPS	$\Delta\varepsilon$	Interval for uniform ε meshes.
	11～20	EPSS	ε_c	ε value at which mesh interval begins increasing geometrically.
	21～30	EMAX	ε_{max}	Maximum ε value.
	31～40	EPS	ε_1	Convergence criterion for the phonon expansion series (The same value is used for the Debye approximation, the first and second method).
4	1～5			should be 751.
	6～10			should be 3.
	11～20	DXKAP	$\Delta\kappa$	Interval for uniform κ meshes.
	21～30	XKAP	κ_c	κ value at which mesh interval begins increasing geometrically.
	31～40	XMAX	κ_{max}	Maximum κ value.
5(1)	6～10	NERGY		The number of energy points ≤ 110.
	11～20	ENRGY (1)	E_i	Energy mesh.
	.....	.....		
	61～70	ENRGY (6)		
5(2)	1～10	ENRGY (7)		
	.....	.....		
6(1)	1～5			should be 151.
	6～10	NOMGD*)		The number of mesh points for $f_1(\omega) <$ NOMG.

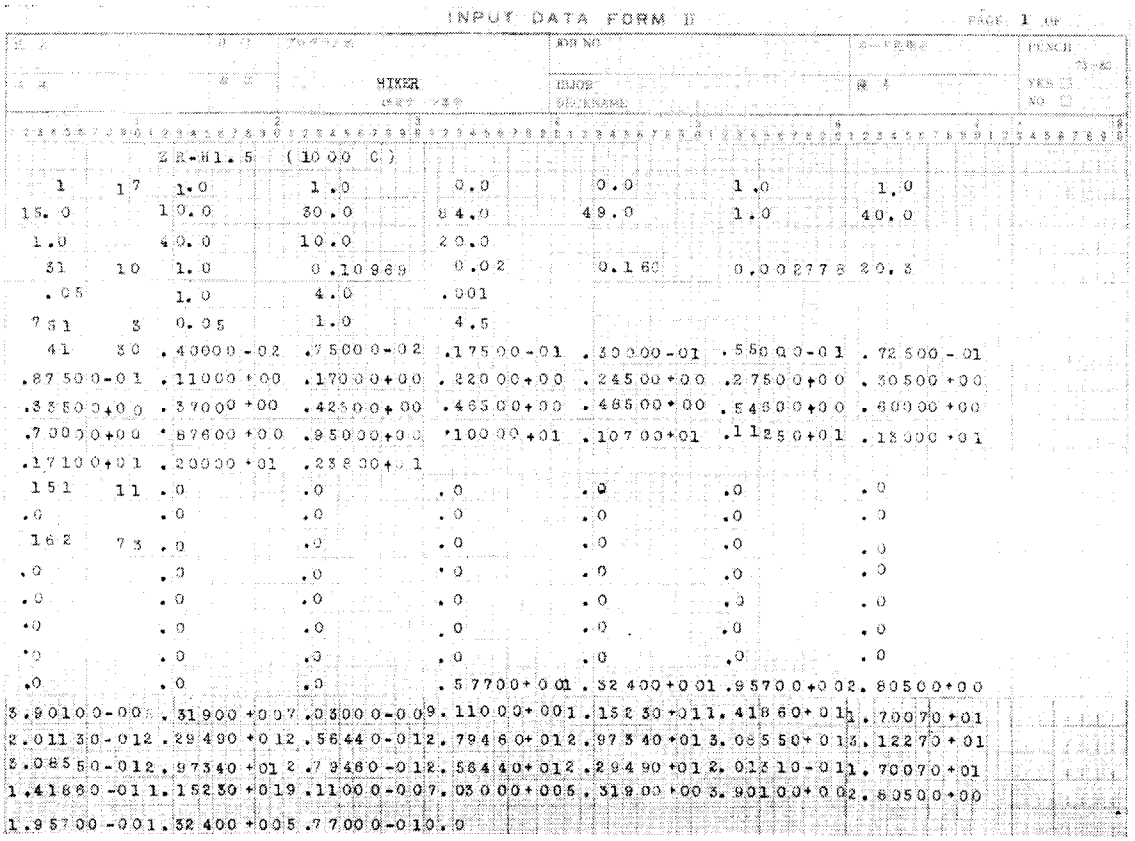
*) Values of NOMG and NOMGD should be chosen to generate the same $\Delta\omega$ for $f_1(\omega)$ and $f_2(\omega)$. $\Delta\omega = \omega_2/$(NOMG-1).

Item	Columns	Program symbol	Physics symbol	Explanation
	11～20	RHO (1)	$f_1(\omega)$	Values of $f_1(\omega_i)$ for $\omega_i=i*\Delta\omega$, $i=1\sim$NOMGD. When the Debye approximation is to be used, let $f_1(\omega)\equiv 0$. When non-zero values are given, the first method will be applied to $f_1(\omega)$.
	.....	.....		
	61～70	RHO (6)		
6(2)	1 ～10	RHO (7)		
	.....	.....		
7(1)	1 ～ 5			should be 151+NOMGL.
	6 ～10	NOMGU		The number of mesh points for $f_2(\omega)$ in the high frequency region=NOMG-NOMGD.
	11～20	RHO (1)	$f(\omega)_2$	Value of $f_2(\omega)$ in the high frequency frequency region. $i=$NOMGD+1～NOMG. Values of $f_2(\omega)$ for $\omega<\omega_1$ should be given. (Let $f_2(\omega)=0$ for $\omega<\omega_1$).
	21～30	.....		
7(2)	.....	.....		
	.....	.....		

Following cards are not necessary, if(κ, ε) meshes are to be generated as decribed above. If one wants to give (κ, ε) meshes arbitrarily, following cards are needed. When cards of item 8～10 are given, cards of item 2(2) and 3 should be omitted.

8	1 ～72			Blanck card.
9	1 ～ 5			should be 252.
	6 ～10			The number of ε_i points$\leq$301.
	11～20	ETS (1)	ε_i	Values of ε_i.
	.....	.....	.....	
10	1 ～ 5			should be 553.
	6 ～10			The number of κ_i points$\leq$100.
	11～20	XKAP (1)	κ_i	Values of κ_i.
	21～30	.....		
	.....	.....		

TABLE 1 Sample input data



3. 3 Output Form

1) Printed Output

The first section of output gives physical input data; E_i, M, $\overline{T}$, ω_D, ω_1, ω_2, C and unnormalized $f_2(\omega)$. The normalization of $f_2(\omega)$ is done in the program and the normalized $f_2(\omega)$ is also printed, which is followed by some quantities depending on $f_2(\omega)$: T, B, D, $\gamma_2(0)$, α_1, α_2, α_3, α_4, σ^2 κ_3, κ_4 and E_C.

Values of generated ε points are printed. The block is headed by ε_{max}, NUM, ε_C and the expansion factor for geometrically increasing series. Next, values of generated κ points are printed in the same form as for ε.

If ISPR$\neq$0, values of β, $S(\alpha, \beta)$ are printed for each α value.

If KERPR$\neq$0, values of E_i, $\sigma_l(E_j \rightarrow E_i)/\sigma_{free}$ are printed for each E_j.

If KPIT$\neq$0, values of E_i, $P(i \leftarrow j)$ are printed for each E_j.

The rest of output relates to $\sigma_s(E)$, $\sigma_{tr}(E)$ and $\overline{\mu}(E)$. When the whole calculation has been performed without any troubles, the phrase "SUCCESSFUL END" will be printed on the last page.

2) Punched Output

If KERPC$\neq$0, half kernels will be punched in the Format (5 E12. 3) with 5 data per card. The order is

$$\sigma_{1\rightarrow1},\ \sigma_{2\rightarrow1},\ \sigma_{2\rightarrow2},\ \sigma_{3\rightarrow1},\ \sigma_{3\rightarrow2},\ \sigma_{3\rightarrow3},\ \sigma_{4\rightarrow1},\ \sigma_{4\rightarrow2},\ \cdots\cdots.$$

If KPIT$\neq$0, THERMOS kernels are punched in the THERMOS-MUG Format (5 (2 I 2, E10. 3))[1]. The THERMOS kernels are given in the form of full matrix and the order is, for example, when NERGY=4,

1, 1, $P_{1\leftarrow1}$; 2, 1, $P_{2\rightarrow1}$; 3, 1, $P_{3\leftarrow1}$; 4, 1, $P_{4\leftarrow1}$; 1, 2, $P_{1\leftarrow2}$; 2, 2, $P_{2\leftarrow2}$;
3, 2, $P_{3\leftarrow2}$; 4, 2, $P_{4\leftarrow2}$;.....

4. Application to Zirconium Hydride

What motivated us to develop our new program was the necessity of calculating scattering kernels for zirconium hydride at high temperature. When values of scattering kernels for crystalline moderators become necessary, we generally use UNCLE[3]. UNCLE is a very excellent and useful program, but is very time consuming at high temperature. For example, it took 1 hr 29 min sec to evaluate the 60 group THERMOS kernels for $ZrH_{1.5}$ at 1000°C on an electronic computer FACOM 230/60. On the other hand, HIKER can compute the same promblen in 1 min 49 sec on CDC-3600 computer. Morever, values of the scattering cross sections calculated with UNCLE for incident energies above 1 eV were found unreasonable (See **Fig. 2 e** and **Fig. 3**). The deviation of cross section values results from rapid increase of $\gamma_2(0)$ with temperature. The large $\gamma_2(0)$ at high temperature makes the Debye-Waller factor $2W_2$ too large for large momentum transfers (Remember the relation: $2W_2=(\kappa^2/2M)\gamma_2(0)$). The large Debye-Waller factor violates good convergence of the phonon expansion series and causes the deviation of cross section values at the relatively high energy range. The Doppler approximation used in HIKER has been found very effective in such a case.

In what follows, we show results of our computations for zirconium hydride $ZrH_{1.5}$. We calculated scattering cross sections by means of HIKER and UNCLE, using the same physical model. Some comparisons between HIKER and UNCLE results will be given in the following discussions.

1) Frequency Distribution of Lattice Vibrations for Hydrogen in Zirconium Hydride

Models to describe atomic motions of hydrogen in zirconium hydride were studied extensively at GGA in connection with the zirconium hydride moderated TRIGA reactor[8),9),10)]. The Doppler broadened Einstein oscillator model proposed by Nelkin and Rosenbluth has been found to give a good theoretical prediction as to thermal neutron scattering by hydrogen in zirconium hydride. We used this model in our calculations.

The frequency distribution $f(\omega)$ of lattice vibrations for hydrogen is divided into two parts: $f_1(\omega)$ for the low frequency acoustic modes and $f_2(\omega)$ for the high frequency optical modes;

$$f(\omega)=Cf_1(\omega)+(1-C)f_2(\omega), \tag{4.1}$$

where C is the weight associated with the low frequency modes. Since reliable experimental data on dynamical properties of hydrogen in zirconium hydride are rather scarce, simple models for $f_1(\omega)$ and $f_2(\omega)$ have been tried. The acoustic $f_1(\omega)$ is approximated by the Debye distribution

$$f_1(\omega)=\frac{3}{\omega_D{}^3}\omega^2 \tag{4.2}$$

with a cut-off $\omega_D=0.02$ eV and a weight $C=1/360$[9]. The optical $f_2(\omega)$ is taken as a Doppler broadened Einstein distribution given in the form of Gaussian distribution centered at $\omega_0=0.13$ eV with a full width at half maximum $\Delta\omega=0.03$ eV:

$$f_1(\omega)=\frac{2}{\sqrt{\pi}}\frac{\sqrt{\ln 2}}{\Delta\omega}\exp\left[-\frac{(4\ln 2)(\omega-\omega_0)^2}{(\Delta\omega)^2}\right]. \tag{4.3}$$

TABLE 2 Normalized $f_2(\omega)$ for $ZrH_{1.5}$

K	OMEG	RM	K	OMEG	RM
1	2.0000000-003	0.0000000+000	2	4.0000000-003	0.0000000+000
3	6.0000000-003	0.0000000+000	4	8.0000000-003	0.0000000+000
5	1.0000000-002	0.0000000+000	6	1.2000000-002	0.0000000+000
7	1.4000000-002	0.0000000+000	8	1.6000000-002	0.0000000+000
9	1.8000000-002	0.0000000+000	10	2.0000000-002	0.0000000+000
11	2.2000000-002	0.0000000+000	12	2.4000000-002	0.0000000+000
13	2.6000000-002	0.0000000+000	14	2.8000000-002	0.0000000+000
15	3.0000000-002	0.0000000+000	16	3.2000000-002	0.0000000+000
17	3.4000000-002	0.0000000+000	18	3.6000000-002	0.0000000+000
19	3.8000000-002	0.0000000+000	20	4.0000000-002	0.0000000+000
21	4.2000000-002	0.0000000+000	22	4.4000000-002	0.0000000+000
23	4.6000000-002	0.0000000+000	24	4.8000000-002	0.0000000+000
25	5.0000000-002	0.0000000+000	26	5.2000000-002	0.0000000+000
27	5.4000000-002	0.0000000+000	28	5.6000000-002	0.0000000+000
29	5.8000000-002	0.0000000+000	30	6.0000000-002	0.0000000+000
31	6.2000000-002	0.0000000+000	32	6.4000000-002	0.0000000+000
33	6.6000000-002	0.0000000+000	34	6.8000000-002	0.0000000+000
35	7.0000000-002	0.0000000+000	36	7.2000000-002	0.0000000+000
37	7.4000000-002	0.0000000+000	38	7.6000000-002	0.0000000+000
39	7.8000000-002	0.0000000+000	40	8.0000000-002	0.0000000+000
41	8.2000000-002	0.0000000+000	42	8.4000000-002	0.0000000+000
43	8.6000000-002	0.0000000+000	44	8.8000000-002	0.0000000+000
45	9.0000000-002	0.0000000+000	46	9.2000000-002	0.0000000+000
47	9.4000000-002	0.0000000+000	48	9.6000000-002	3.8256583-001
49	9.8000000-002	1.3567715+000	50	1.0000000-001	1.9758775+000
51	1.0200000-001	2.8520575+000	52	1.0400000-001	3.9386297+000
53	1.0600000-001	5.3730794+000	54	1.0800000-001	7.0973125+000
55	1.1000000-001	9.1978765+000	56	1.1200000-001	1.1634153+001
57	1.1400000-001	1.4322884+001	58	1.1600000-001	1.7170952+001
59	1.1800000-001	2.0525187+001	60	1.2000000-001	2.3178370+001
61	1.2200000-001	2.7891366+001	62	1.2400000-001	2.8215572+001
63	1.2600000-001	3.0020819+001	64	1.2800000-001	3.1152632+001
65	1.3000000-001	3.1526221+001	66	1.3200000-001	3.1152632+001
67	1.3400000-001	3.0020819+001	68	1.3600000-001	2.8215572+001
69	1.3800000-001	2.7891366+001	70	1.4000000-001	2.3178370+001
71	1.4200000-001	2.0525187+001	72	1.4400000-001	1.7171952+001
73	1.4600000-001	1.4322884+001	74	1.4800000-001	1.1634153+001
75	1.5000000-001	9.1978765+000	76	1.5200000-001	7.0973125+000
77	1.5400000-001	5.3730794+000	78	1.5600000-001	3.9386297+000
79	1.5800000-001	2.8520575+000	80	1.6000000-001	1.9758775+000
81	1.6200000-001	1.3567715+000	82	1.6400000-001	5.8256583-001
83	1.6600000-001	0.0000000+000	84	0.0000000+000	0.0000000+000

Both $f_1(\omega)$ and $f_2(\omega)$ are normalized to 1, respectively,

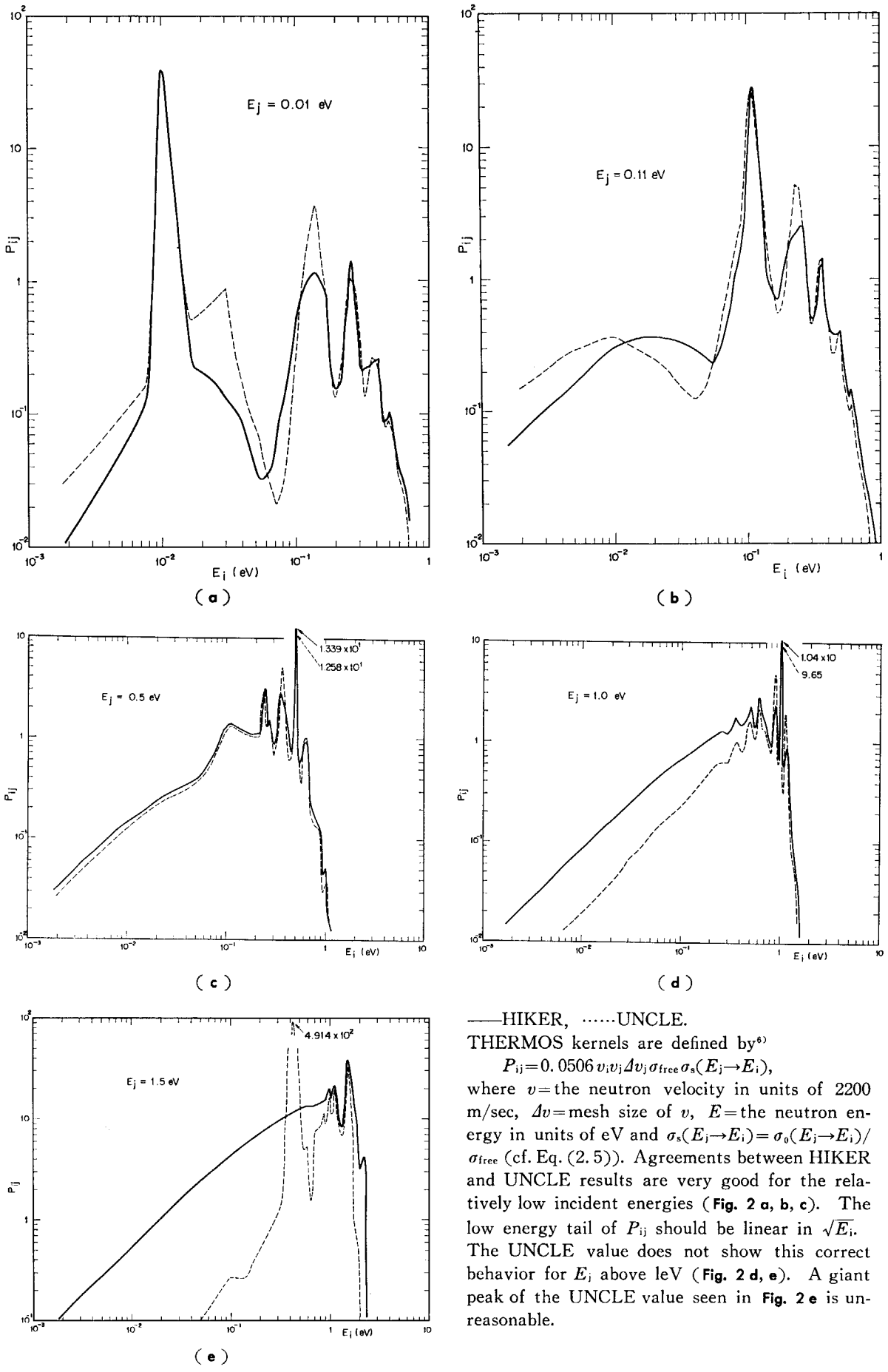
$$\int_0^{\omega_D} d\omega f_1(\omega)=1, \qquad \int_0^{\infty} d\omega f_2(\omega)=1.$$

Numerical values of $f_2(\omega)$ for 84 ω_i points are given in TABLE 2.

2) THERMOS Kernels

THERMOS kernels P_{ij} for $ZrH_{1.5}$ at 1000°C (0.1097 eV) are shown in **Fig. 2** in comparison with the UNCLE results for some typical incident neutron energies. The same physical parameters were used as input both to HIKER and UNCLE. In the relatively low energy region HIKER gives somewhat smaller values than UNCLE. The smaller HIKER values may be explained by the fact that in HIKER the calculation for the low frequency modes is performed throughout by means of the Debye phonon expansion method with phonon terms up to order 15. UNCLE uses the short collision time approximation when the Debye-Waller factor for the low energy modes exceeds a certain value. The maximum number 15 for the Debye phonons may be small and it may be desirable to take the larger number. The weight $C=1/360$ for acoustic modes may be too small at high temperature. Because the low energy scattering is not important in the high temperature crystal, the differences in the low energy P_{ij} may be expected to give almost no noticeable effects on integral reactor parameters.

In the intermediate energy region the agreement between HIKER and UNCLE results is excellent. A marked discrepancy between them is seen in the hot energy region. In this region we have to prefer HIKER values to UNCLE ones. In contrast to the case of low incident energies UNCLE uses the phonon expansion method only for the high frequency modes. This



——HIKER, ……UNCLE.

THERMOS kernels are defined by[6]

$$P_{ij}=0.0506\,v_i v_j \Delta v_j \sigma_{free}\sigma_s(E_j\to E_i),$$

where v=the neutron velocity in units of 2200 m/sec, Δv=mesh size of v, E=the neutron energy in units of eV and $\sigma_s(E_j\to E_i)=\sigma_0(E_j\to E_i)/\sigma_{free}$ (cf. Eq. (2.5)). Agreements between HIKER and UNCLE results are very good for the relatively low incident energies (**Fig. 2 a, b, c**). The low energy tail of P_{ij} should be linear in $\sqrt{E_i}$. The UNCLE value does not show this correct behavior for E_j above leV (**Fig. 2 d, e**). A giant peak of the UNCLE value seen in **Fig. 2 e** is unreasonable.

Fig. 2 THERMOS kernels for H in $ZrH_{1.5}$ at 1000°C.

is the reason why UNCLE gives too small values for large energy transfers, (i. e., large (E_j-E_i). Notice that E_j is the incident energy and E_i is the energy of scattered neutrons). As can be seen from **Fig. 2**, the UNCLE curve for $E_j=1.5$ eV has a giant peak in the neighborhood of $E_i=0.4$ eV. We are not clear about why this peak grows up as E_j becomes larger.

3) Total Scattering Cross Section and the Mean Cosine of Scattering Angle

The total scattering cross section $\sigma_s(E)$ per H for $ZrH_{1.5}$ at 1000°C is shown in **Fig. 3**. The unreasonable divergence of the UNCLE value in the hot energy region is due to the growing of a giant peak seen in P_{ij}. The causes leading to the difference between HIKER and UNCLE values are clear from the discussion on P_{ij}.

Fig. 4 shows the mean cosine of scattering angle $\bar{\mu}(E)$ for $ZrH_{1.5}$ at 1000°C. Making a comparison between UNCLE values and experimental data $ZrH_{1.5}$ at room temperature, we found that UNCLE values are systematically larger than experimental data. Morever $\bar{\mu}(E)$ should approach to the value of $2/(3M)$ at E increases. This is the value for a free atom and becomes 2/3 for a free hydrogen. As can be seen in **Fig. 4**, the UNCLE value becomes larger than this limiting value. From these facts it would appear that HIKER results is preferable to UNCLE ones at high temperature. Unfortunately we have no neutron experimental data on $ZrH_{1.5}$ at 1000°C. This fact prevents us from making detailed discussions further on the accuracy of the HIKER method.

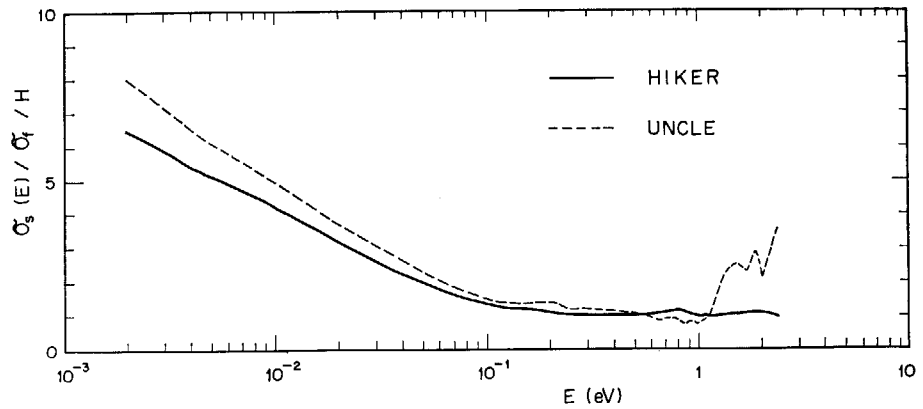


Fig. 3 Total scattering cross section per H in $ZrH_{1.5}$ at 1000°C
The divergence of the UNCLE value above 1 eV is unreasonable.

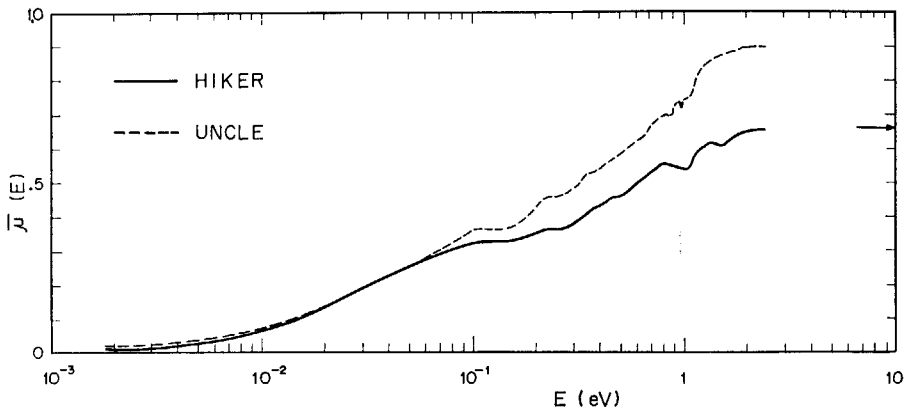


Fig. 4 Mean cosine of scattering angle for H in $ZrH_{1.5}$ at 1000°C
An arrow⟶indicates the value for a free hydrogen. The UNCLE value exceeds this limiting value. The result of HIKER calculation shows a reasonable behavior.

Acknowledgements

The Fortran IV program of HIKER was written by Miss H. ADACHIHARA and Mr H. IHARA of Century Research Center Corp. The authors would like to acknowledge their excellent works and express sincere thanks to them for their assistances. The authors are grateful to Dr. S. KATSURAGI for his encouragements. They are indebted to Mr. T. ISE, Mr. N. OHNISHI, Mr. H. TAKANO and Mr. A. HASEGAWA of JAERI for their assistances and arrangements in using UNCLE on electronic computer FACOM 230/60. Acknowledgement is further due to colleagues of the Thermal Neutron Scattering Group of Japanese Nuclear Data Committee for valuable discussions.

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