

INDC - 175

revised version

A DISCUSSION OF THE REQUESTS ON MODERATOR MATERIALS CONTAINED IN

EANDC 55"U"

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The following discussion on the scattering properties of different moderator materials is based on references contained in CINDA 1965/66, some information provided by CID Euratom and some additional references from NSA up to December 1966 but does not claim to be complete in the sense that all available experimental data are reviewed and critically discussed, but concentrates on a selection of papers from which the main developments in this field can be seen and from which most of the unmentioned references can be found.

1. Introduction

Neutrons are slowed down in a thermal nuclear reactor from fission energies around 1 MeV to thermal energies around 25 meV. Since the main contribution to the slowing down density stems from neutrons with an energy below 100 eV, it is this region for the scattering kernel which we will consider.

It is reasonable for a consideration of moderating properties, to neglect for a start nuclear reaction processes including absorption and discuss only the double-differential scattering cross section, introducing the absorption effects on the neutron energy spectrum in a reactor at a later point.

We write for the double-differential scattering cross section:

$$\frac{\partial^2 \sigma}{\partial \Omega \partial \omega} = a_{\text{coh}}^2 \frac{k'}{k} S(\underline{Q}, \omega) + a_{\text{inc}}^2 \frac{k'}{k} S_s(\underline{Q}, \omega)$$

define the slowing down density

$$\sigma_s(E_0) = 2\pi \int_0^\infty \int_{-1}^{+1} \frac{\partial^2 \sigma}{\partial E \partial \Omega} \ln \frac{E_0}{E} dE d(\cos \theta)$$

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the average cosine of the scattering angle

$$\overline{\mu(E_0)} = \frac{2\pi}{\sigma_s} \int_0^\infty \int_{-1}^{+1} \frac{d^2\sigma}{dE d\Omega} \cos \theta dE d(\cos \theta)$$

and finally the relation between the "scattering kernel" and the "double differential scattering cross-section"

$$\sigma(E_0 \rightarrow E) = \int \frac{d^2\sigma}{d\Omega dE} d\Omega$$

where we have used the following symbols

$a_{coh}, a_{inc} \dots$ coherent and incoherent scattering length

$$(\sigma_b^{coh} = 4\pi a_{coh}^2)$$

$\underline{k}_0, \underline{k}' \dots\dots$ initial and final neutron wave vector ($E_0 = \frac{h^2 k_0^2}{2m}$,
 $E = \frac{h^2 k'^2}{2m}$)

$\hbar\underline{Q}, \hbar\omega \dots\dots$ momentum and energy transfer in the scattering process

$S(\underline{Q}, \omega) \dots\dots$ scattering law

$S_s(\underline{Q}, \omega) \dots\dots$ self term of the scattering law

$\Omega \dots\dots\dots$ solid angle

$\sigma_s(E_0) \dots\dots$ total scattering cross section

It is obvious that whatever model one may use for $S(\underline{Q}, \omega)$ an accurate knowledge of the scattering length is necessary.

Since it is implicitly assumed in the derivation of the double differential scattering cross section that the scattering on a single free nucleus in the CM system is isotropic, one has to bear in mind that this assumption is valid only for neutron energies below about 100 keV (e.g. Weinberg and Wigner, 1958). We will restrict the main part of our discussion to this energy range.

While it is true that the equation for the double differential scattering cross section holds for neutrons $E \leq 100$ keV and the main part of the slowing down density stems from neutrons with energies < 100 eV it is important to have reliable knowledge of inelastic nuclear reactions thermalizing neutrons of energies $E > 100$ keV and consider this part of the slowing down density very carefully. It is this region where nuclear reactions play a major part in the neutron energy loss processes. Obviously these reaction rates will be of main importance in fast and intermediate reactors.

2. The Scattering Law

2.1 Generalities

While $S(\underline{Q}, \omega)$ describes the probability for the scattering system (the moderator) to take in a single interaction the energy $\hbar\omega$ from the neutron (or give it to this neutron) if the momentum $\hbar\underline{Q}$ is transferred, independently of the neutron energy before the collision, we have still to distinguish different energy groups of neutrons since we have neither a model which is equally valid for all values of \underline{Q} and ω , nor experimental results for $S(\underline{Q}, \omega)$ over the whole (\underline{Q}, ω) range.

The way one proceeds to overcome these difficulties is obvious. After a model has been found to fit experimental data over a certain energy range one hopefully extrapolates the theoretical calculations to regions where experimental data are either scarce or uncertain and adjusts or alters the model approximations on the ground of physical arguments related to the difference in energy of the moderator molecule (both kinetic and potential) and the energy group to which a neutron belongs.

It can be shown from a classical discussion of $S(\underline{Q}, \omega)$ and $S_s(\underline{Q}, \omega)$ that while the first term describes the scattering of a neutron by any two interacting atoms and in this way the coherence phenomena in the scattering system, describes the second term the scattering of neutrons by single atoms in interaction with their

neighbours. The scattering law is in this way related to the molecular dynamics of the moderator, and constructing models means solving the equations of motion, (Schrödinger-equation or classical equations of motion) in certain approximations. The difference in $S(\underline{Q}, \omega)$ and $S_s(\underline{Q}, \omega)$ is most pronounced for values of \underline{Q} of the order of the reciprocal lattice vectors. As we go to larger \underline{Q} values the coherence effects vanish and consequently $S(\underline{Q}, \omega)$ approaches $S_s(\underline{Q}, \omega)$.

Before discussing the individual moderator substances let us make a few general remarks. In calculating $S(\underline{Q}, \omega)$ three approximations are most frequently made which can be shown more easily when we look at the Fouriertransform of $S(\underline{Q}, \omega)$

$$F(\underline{Q}, t) = \int S(\underline{Q}, \omega) \exp \{ +i\omega t \} d\omega$$

2.1.1 Quasi Classical Approximation

If one calculates $S_s(\underline{Q}, \omega)$ in its classical limit $S_s^{cl}(\underline{Q}, \omega)$ one misses a few important points; detailed balance is not fulfilled, recoil effects are neglected, etc.

Schofield (1960) and Egelstaff and Schofield (1962) suggested to substitute complex times into the classical forms of $F_s^{cl}(\underline{Q}, t)$. This procedure gives the correct relation for the detailed balance relation and the first moment. The results are correct to first order in \hbar .

2.1.2 Gaussian Approximation

Since in most manageable calculations $F_s(\underline{Q}, t)$ turns out to be of Gaussian form (e.g. Rahman et al., 1962)

$$F_s(\underline{Q}, t) = \exp \{ -Q^2 \gamma(t) \}$$

one assumes that this should hold true for the center of mass motion of more general dynamical situations and all the physics lies then in the quantity $\gamma(t)$. Model calculations are therefore concerned with finding $\gamma(t)$.

Considering $\gamma(t)$ it turns out to be of the form

$$\gamma(t) = \int_{-\infty}^{+\infty} \frac{f(|\omega|) \exp\left\{\frac{\hbar\omega}{2kT} - i\omega t\right\}}{2\omega \operatorname{sh} \frac{\hbar\omega}{2kT}} d\omega$$

Where for a solid $f(\omega)$ is the frequency spectrum of the normal modes.

2.1.3 Incoherent Approximation

This approximation consists in neglecting terms in the multiphonon expansion of $S(\underline{Q}, \omega)$ different from $S_s(\underline{Q}, \omega)$ for $\omega \rightarrow 0$.

Marshall and Stuart (1959) find for Al and Mg that this approximation gives satisfactory total cross sections. For Be, BeO and C we will discuss its validity when considering the individual substances. Another discussion is given by Jankus (1962).

One can show (Sköld 1967) that for liquids the altered convolution approximation

$$F(\underline{Q}, t) = F(\underline{Q}, 0) \exp\left\{-Q^2 \gamma(t)/F(\underline{Q}, 0)\right\}$$

gives a good approximation to $F(\underline{Q}, t)$, but in general will be too tedious for reactor calculations.

2.2 Models for the Scattering Law

While for some time, as Egelstaff (1962) has pointed out, the scattering law was known to accurately for reactor calculations, and simple models like the perfect gas modes (e.g. Osborn, 1957) were sufficient, the situation has now changed in as far as details of the scattering law become more and more important to reactor calculations.

In general the energy interval can be divided naturally in three intervals when considering $S(\underline{Q}, \omega)$

- i) Chemical binding effects can be completely neglected. One has the simple case in which the moderator behaves gas-like. ($E_0 \gg$ molecular binding energy).

ii) The molecule as a whole occurs as an entity with internal modes of motion but still as a molecular gas. Now rotations and vibrations have to be considered.

(Molecular binding energy $> E_0 >$ lattice energy).

iii) The center of mass motion of the molecules plays an important part in the moderator process, and the complete dynamics of the moderator has to be considered.

($E_0 \sim$ lattice energy).

Obviously the boundaries between these regions are very interesting from a scientific point of view, but for reactor calculations of little importance.

Another distinction in our discussion will be made between liquid molecular moderators as e.g. H_2O , D_2O and polycrystalline moderators as e.g. Be, BeO, C.

3. The "scattering law" requirements from EANDC Request List 55 "U"

3.1 Light and Heavy Water-Theoretical Calculations

For a molecular liquid one makes the approximation that the Hamiltonian can be separated into a vibrational, rotational and translational (C.M.) part. Assuming no interactions between these different modes of motion, but allowing for unharmonic vibrations and hindered rotations.

Nelkin (1960) has given a treatment which takes into account vibrational motion as in a free gas (symmetric and antisymmetric change of the O-H bonds (0.48 eV), change of the angle between the bonds (0.20 eV)) hindered rotations approximated by one torsional oscillation (libration at 0.06 eV) while assuming for the C.M. motion that of a perfect molecular gas with a mass dependent on the energy range to which the incident neutron belongs (mass tensor concept).

In order to improve on the rotational motion one can follow Rahman (1961) and Yip (1962). The latter introduce a model in which the rotations are treated in the presence of an appreciable intermolecular force field.

A further improvement is the introduction of spatial anisotropy of the proton vibration in the H_2O molecule by Koppel and Young (1964). He postulates harmonic forces along the O-H bond, a force proportional to the angle between the O-H bonds and a harmonic potential for completely hindered rotation around the three principle axis of the molecule.

Honeck (1962) has adjusted the Nelkin kernel to D_2O , but it turns out that in order to fit double differential scattering cross section data a treatment of the coherence effects is needed.

Egelstaff and Schofield (1962) introduced a model which allows for inelastic scattering together with a realistic diffusion behaviour. By choosing a frequency spectrum, a diffusion constant and a parameter taking care of the fact that diffusion is only the long time limit of the dynamics of a liquid one is able to fit experimental scattering data in the quasielastic region reasonably well over a wide (Q, ω) range.

Having introduced inelastic scattering one choses to describe it for the liquid - in good agreement with experimental data - as a polycrystalline solid, using the multiphonon expansion. The important quantity being now the generalized frequency spectrum. The inelastic scattering is dealt with in programs called SUMMIT by Bell, LEAP by McLatchie and GASKET by Triplett. The last of these programs can deal with any shape of $f(\omega)$ while the two former are subject to convergence problems.

McMurry and Russel (1966) proposed a model for H_2O and D_2O calculating $S(Q, \omega)$ in which they assume the molecules to be distributed among single molecule states and two types of clusters containing bounded H_2O molecules in which the scattering masses for H atoms are 150 and 75 respectively.

While keeping the sizes of the clusters constant the distribution among them may change according to temperature. Leaving the internal vibrational modes unaltered by the clustering, McMurry and Russel introduce the motion of the clusters by assuming 17 properly weighted harmonic oscillators between 0 - 0.125 eV. While having to satisfy

a number of normalisation conditions - the frequency spectrum is chosen to give a good fit to Bruggers data (1966). The agreement between scattering data and theory is good for 293°K and 423°K - data by Haywood (1964) - and fair for 550°K - data by Page (1964) - but while always better than the Nelkin model it has the draw back to have the cluster sizes, the distribution among them, the frequency spectrum as rather artificial parameters, and neglects diffusion effects.

For D_2O the frequency spectrum is scaled appropriately ($1/\sqrt{2}$) and so are the cluster sizes (20/18). In order to fit Haywoods (1964) D_2O data it was necessary to adjust the amount of free molecules (17%) as compared to H_2O (10%) for room temperature. An investigation of clustering by small angle neutron scattering performed by Gissler (1964) has not shown any clustering within the accuracy of the experiment.

Pelah and Surry (1966) assume an aggregat picture for the structure of the liquid caused by hydrogen bonding giving a polycrystalline behaviour together with a strong broadening of the rotational modes due to interactions, but do not actually write down the basic formulae of their calculations.

Haywood - Koppel (1966) Koppel (1966) obtained a slightly modified frequency spectrum from the data by Haywood and is able to obtain satisfactory agreement with experimental $S(\underline{Q},\omega)$ data over a wide energy range. Using GASKET this programme provides for the following dynamical situations in the incoherent approximation

- i) free translation
- ii) diffusive (Brownian) motion
- iii) harmonic isotropic vibrations with continuous frequency spectrum
- iv) harmonic anisotropic vibrations with continuous frequency spectrum
- v) harmonic isotropic vibrations with discrete frequency spectrum.

While the aim is to get more accurate $S(\underline{Q},\omega)$ data and construct models to fit them, much of the work done is concerned with fitting measured neutron spectra and compare transport theory parameters

(Beyster, (1966, 1967), Stamm'ler (1966), Green et al. (1967)), as the "thermal reproduction factor $\bar{\nu}$ ", and the "thermal utilisation factor f " with experimental results (e.g. by Worden et al. (1966)), for available core geometries. One dimensional transport calculations for these core lattices are subject to some uncertainties due to the necessary transformation of the real core into an equivalent core.

Beyster et al. find that neutron spectra in absorbing media are more sensitive to the scattering kernels used than spectra in non-absorbing media. For neutron spectra and transport parameters the general conclusion is that they cannot be fitted by a simple gas model. In particular Worden et al. found that the errors for these parameters lie in between 1 - 3%. For H_2O lattices $\bar{\nu}$, f can be fitted using the Nelkin model modified by Honeck (1964), the data for C-lattices can be fitted by a Parks-kernel discussed by Wilkner et al. (1964). For D_2O , f cannot be fitted by any of the currently available models (e.g. Honeck, 1964) this statement does not agree with the findings of Beyster et al. (1966), who conclude that neutron spectra can be fitted quite well using Nelkin-Honeck model and the incoherent approximation.

The group at General Atomics has made another calculation for D_2O using GASKET where the frequency spectrum used to generate $S(Q, \omega)$ consisted of:

- i) two discrete oscillators at 0.31, 0.145 eV with weights 1/3, 1/6 respectively
- ii) a rotational frequency band peaking at about 0.05 eV with a weight 9/20 obtained from Haywoods (1964) data
- iii) a δ -line at $\omega = 0$ (gas behaviour) weight 1/20; free translation of molecules with a mass 20.

While for neutron spectrum measurements in core lattices the coherence effects seem not to be of importance, these effects are of importance in $S(Q, \omega)$ and $S(Q)$. And the discussed models do not fit the data within experimental errors. Butler (1963) has treated coherence phenomena approximately. It is necessary to give a more realistic treatment of coherency since even the total cross section shows a

clear coherent effect around $E_0 < 0.002$ eV, as far as partial differential scattering data are concerned, strong coherence effects are observed.

3.2 Scattering Law Data for H_2O and D_2O

Most of the scattering law data have the drawback that no multiple-scattering corrections have been made until recently and little information on resolution is presented with the data.

Since deconvoluting the experimental data is, as yet, not done, one cannot plot all available data on to one and the same scale without comments, and it seems best to discuss every experiment on its own - performing a resolution broadening of the theoretical calculations relevant for this particular experiment before comparing it with the data.

As far as multiple scattering goes, it seems reasonable that experimentalists agree on certain types of set ups concerning sample geometry and transmission and use the same "multiple scattering correction program" (e.g. MUSE by Honeck (1964)) to make an easy comparison of different results possible.

3.2.1 Scattering Law $S(Q, \omega); \sigma_{n,n}(E_0, E'; \theta)$

For early reviews on various moderator materials see Egelstaff (1962), Brugger (1962) and Beckurts (1962). For more recent developments see Ghatak and Krieger (1965), McMurry et al. (1966) and the current series of Progress Reports by the group around Beyster, Koppel, Young etc. at General Atomics.

The best data available are:

Kottwitz and Leonard (1962)

$E_0 = 0.147, 0.2, 0.3, 0.4$ eV; $T = 295^\circ K$

$0.050 < \hbar\omega < 0.250$ eV

$\hbar a < 14 \text{ \AA}^{-1}$

no correction for multiple scattering

Skoeld et al. (1964)

$E_0 = 0.005$ eV; room temperature

$0 < \hbar\omega < 0.013$ eV

$1 < Q < 3$ \AA^{-1}

No multiple scattering corrections.

The main emphasis lies on a check of the diffusion behaviour of H_2O , the authors conclude that the simple diffusion model fits within the experimental range of (Q, ω) the quasielastic scattering peaks.

Haywood (1964)

$E_0 = 0.039, 0.093, 0.256$ eV; $T = 295^\circ\text{K}, 323^\circ\text{K}$;

$-6 < \beta < 3.2$ $\beta = \hbar\omega/kT$

$0.44 < \alpha < 31.7$ $\alpha = \hbar^2 Q^2 / 2mkT$

These data have been corrected for multiple scattering by Antumez et al. (1966) and are the basis for the frequency spectrum for water by Koppel (1966).

Page (1964)

$E_0 = 0.107$ eV; $T = 550^\circ\text{K}$, $p = 1200$ psi;

$0.015 < \hbar\omega < 0.15$ eV

$2 < Q^2 < 300$ \AA^{-2}

no multiple scattering corrections

Mostovoy (1964)

$E_0 = 0.005$ eV; $T = 296^\circ\text{K}$,

$0.25 < \beta < 11.5$

$0.064 < \alpha < 34$

no corrections for multiple scattering

The calculated frequency spectrum exhibits fluctuations which have not been found by Haywood and are larger than errors on the data.

Kirouac et al. (1965)

$0.1 < E_0 < 1.81$; room temperature

$1 < \beta < 30$

$5 < \alpha < 80$

Multiple scattering corrections to these data are given in KAPL-P-3179 the original data are published in a thesis by Kirouac.

A comparison of the frequency spectrum with data by Kottwitz and Haywood is given in TID-22141.

Harker and Brugger (1965) $E_0 = 0.039, 0.050 \text{ eV}; T = 295^\circ\text{K};$
 $0 < \beta < 4$
 $1 < Q^2 < 110 \text{ \AA}^{-2}$

no multiple scattering corrections.

McMurry et al. fit their calculations to the measurements by Harker and Brugger. A comparison between these data and the data by Kirouac et al., Haywood, Kottwitz and Sakamoto (1962) et al. show some deviations larger than statistical errors quoted.

Harling (1967) $T = 268^\circ\text{K}, (\text{Ice}), 299^\circ\text{K}$
 $E_0 = 0.1515, 0.303, 0.404, 0.616 \text{ eV}$
 $-25.5 < \beta < 4$
 $0.4 < \alpha < 97.7$
 no multiple scattering correction.

Multiple scattering corrections to these data are given in KAPL-P-3179, the original data are published in a thesis by Kirouac.

A comparison of the frequency spectrum with data by Kottwitz and Haywood is given in TID-22141.

As for the errors in $S(Q, \omega)$ Kirouac has checked some of the experimental data available for H_2O . One can give limits for the errors looking at the data for other moderator materials discussed in the following sections.

Counting statistics, background uncertainty	$\sim 5 \%$
Normalisation of data by Vanadium	$< 5 \%$
Uncertainties due to flightpass, sample thickness	$< 5 \%$
Sensitivity of multiple scattering correction to the model	$< 10 \%$

These errors should be taken as an indication of their size to show that improvement is still desirable and indeed necessary for a more detailed check of advanced models.

In particular the error for the counting statistics in $S(Q, \omega)$ data show changes within the limits 1 - 10 %.

3.2.2 Angular Dependence of the Cross Section $\sigma_{n,n}(E_0; \theta)$

Beyster, Neill, Young (1966) $0.005 < E_0 < 10$ eV (55 values)
 room temperature
 $10^\circ < \theta < 160^\circ$
 experimental and theoretical studies
 of multiple scattering performed.

For the data integrated with respect to the energy transfer there is a clear need for an advanced model for $E_0 < 0.85$ eV.

A gas model with an effective temperature will reproduce the results for $E_0 > 0.85$ eV.

Springer et al. (1964) $E_0 = 0.0235, 0.044, 0.071, 0.105$ eV
 $T = 293^\circ\text{K}$
 $10^\circ < \theta < 170^\circ$

Multiple scattering corrections performed. There are discrepancies between these results and the data by Beyster et al. (1965) as large as 15 % for certain incident energies and momentum transfer. This may be caused by different correction procedures for multiple scattering and/or geometry effects, but needs investigation.

Whittemore and Reynolds (1961) $E_0 = 0.09, 0.05, 0.059, 0.109, 0.136,$
 0.170 eV
 room temperature
 $30^\circ < \theta < 140^\circ$

These data have not been corrected for multiple scattering, for a discussion see Beyster et al. (1965).

3.2.3 Total Cross Section $\sigma_{nT}(E_0)$

Dritsa and Kostikas (1967) room temperature, 473°K
 0.01 eV $< E_0 < 10$ eV
 The experimental error lies between
 0.5% - 1.1%.

Russel (1962)

The experimental error of these data lies between 0.3% and 0.8%. Showing a discrepancy with calculations of about 5% at 0.03 eV - see Beyster et al.(1966).

Heinloth and Springer (1961)

$$0.18 \times 10^{-3} < E_0 < 2.8 \times 10^{-3} \text{ eV}$$

$$123^\circ < T < 473^\circ \text{ K}$$

The statistical error of these data is <4%. They will be particularly important because of the structure influences exhibited in the total cross section at the phase transition points. A detailed check of theoretical models close to the melting and boiling point should help in constructing new models.

The experiments on $\sigma_{nT}(E)$ for light and heavy water should be extended to higher temperatures and energies (up to a few hundred meV with a hot source and even to 10 eV with a LINAC). The experiments by Wraight at AWRE cover this object partly. An accuracy of anything better than 1% should show a possible weak energy dependence.

As for the single and double differential scattering cross sections extension of the energy range, better statistical accuracy and higher resolution would be desirable. These requirements are, of course, interdependent. For model calculations the main problem for H_2O is still the need for a physical CM motion and a more realistic description of the hindered rotations.

3.2.4 The Scattering Law for D_2O ; $\sigma_{n,n}(E_0, E'; \theta)$

There are less data available for D_2O than for H_2O . None of the data have been corrected for multiple scattering:

Haywood (1964)

$$T = 295^\circ \text{ K}; \quad E_0 = 0.109, 0.039 \text{ eV}$$

$$-3 < \beta < -0.2$$

$$0.04 < \alpha < 6$$

$$T = 423^\circ \text{ K}$$

$$0.8 < \beta < 2.8$$

$$0.02 < \alpha < 6.0$$

<u>Whittemore (1966)</u>	$T = 297^{\circ}\text{K}$; $E_0 = 0.157, 0.206, 0.304 \text{ eV}$ $-6 < \beta < 0$
<u>Harling (1967)</u>	$T = 299^{\circ}\text{K}$; $E_0 = 0.101, 0.213$ $-7 < \beta < +2$ $0.1 < \alpha < 20$
<u>Page (1967)</u>	$T = 813^{\circ}\text{K}$; $p = 1200 \text{ psi}$ $E_0 = 107 \text{ eV}, 0.055 \text{ eV}$ $-1.85 < \beta < 4.08$ $0.02 < \alpha < 8$

Dahlberg et al. (1964)

These authors published extensive frequency spectra data on D_2O derived from inelastic scattering experiments using the incoherent approximation. A comparison between H_2O and D_2O frequency spectra is given.

3.2.5 The Partial Differential Scattering Cross-Section $\sigma_n(E_0; \theta)$

Beyster et al. (1965, 1966). The extensive data by these authors together with the scattering law data provide excellent material for a check of more advanced theoretical calculations.

The measurements have been performed for 55 incident energies between $0.006 < E_0 < 10 \text{ eV}$. The scattering angle was varied between $10^{\circ} < \theta < 160^{\circ}$.

Springer (1963, 1964) The data by Springer and Beyster et al. do not agree within the limits of the errors in the region where coherence effects are most pronounced. This point needs some further investigation.

3.4 Polycrystalline Moderators Be, BeO, C

The recent developments point toward a need for an improvement of calculations for the coherence effects in polycrystalline moderators. The data available are rather scarce, so one starts by calculating

frequency spectra and generates $S(Q, \omega)$ data.

3.5.1 Beryllium

Johnston (1966) discuss the theoretical calculations available and finds that after Schmunk et al. (1962) have extended a model by Slutsky and Garland (1957) to include fifth neighbour interaction their results fit the measured dispersion curves fairly well,

Young and Koppel (1964, 1965) obtain a frequency spectrum for Be following Schmunk. After calculating $S(Q, \omega)$ in the incoherent approximation they correct the one-phonon cross section for coherence effects and find that their calculation agrees well with measurements on polycrystalline Be by Schmunk (1964).

In general neutron spectra are difficult to predict in energy regions where the cross section undergoes violent changes or where there are spatial discontinuities like hot and cold source block etc. These problems need a separate discussion and are not yet fully in hand.

It is known for some time - see Gaerttner et al. - that Beryllium exhibits so called neutron trapping. This describes phenomena which occur in strongly coherent scattering materials and can be demonstrated by measuring the thermal spectrum very accurately and consider deviations from the Maxwellian distribution. The effect becomes pronounced in the region where the neutron wave interacts with an assembly of crystallites as a whole and is depended on the buckling. For further theoretical investigation the frequency spectrum for Be obtained by Young and Koppel (1964) is useful and should be tested on data for the scattering law, by Haywood and Sinclair (1964). The measurements were performed at 295⁰K the transmission of the sample was 0.87 but no corrections for multiple scattering were performed. The authors quote the accuracy of the results to be $\pm 10\%$.

3.5.2 Beryllium-Oxide

Since BeO seems to be the material which will be used in most "hot

sources" temperature dependent scattering law data are of importance. BeO will be used in the form of a sintered powder. In the work by Ottewitte (1965) the effects of temperature and microstructure are discussed. It is difficult to get a representative frequency spectrum for BeO, so one has to take either a Debye model or a measured spectrum for BeO - Sinclair (1962), for cross section calculations. A more recent measurement by Haywood and Sinclair (1964) for BeO at 22°C provides more extensive data with an accuracy quoted by the authors of $\pm 10\%$. Young and Koppel are investigating this problem and it seems that BeO is the substance where there is most need for theoretical and experimental investigations.

Calculations by Khubehandani and Sanatani (1963) show that only by considering coherence effects in one-, two-phonon cross-sections they are able to get results which compare with experiments by Begum et al. (1966) on inelastic spectra in BeO.

Total cross-section measurements are available for energies $0.0025 < E_0 < 10$ eV and temperatures of 290°, 800°, 1300°, 1500°K by Zhezherum and Chernyshov (1960).

3.5.3 Graphite

Yoshimari and Kitano (1956) calculated the frequency spectrum for graphite. Wilkner et al. (1964) used this spectrum for calculation of core parameters and $S(Q, \omega)$. While the integral parameters agree with experiments, show the scattering law calculation in the incoherent approximation no agreement for low Q data as expected.

An improvement of the frequency spectrum made by Young and Koppel still shows this shortcoming, when they compare their calculation with data by Whittemore (1966).

More data on graphite at high temperatures will be published soon by Page (1968).

4. Computer Codes

The following computer programmes are available.

<u>Shimada and Syoichiro (1964)</u>	Free gas model Nelkin model Egelstaff-Schofield model Anisotropic crystalline model
<u>Lawade (1966)</u>	Nelkin model Nelkin-Honeck model
<u>McMurry, Russel (1967)</u>	Murry-Russel model

The following authors have produced computer codes to generate $S(Q, \omega)$ starting from a frequency spectrum.

<u>Bell J.</u>	SUMMIT
<u>McLatchie R.C.F.</u>	LEAP
<u>Triplet J.R. et al.</u>	GASKET

5. Acknowledgement

The author wishes to thank Dr. Tisljar for letting him have a bibliography on neutron cross-section data for moderator materials, over the whole energy range interesting for nuclear reactors, prior to publication.

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