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Scattering Laws and Cross Sections for Moderators and Structure Materials for Calculation of Production and Transport of Cold and Ultracold Neutrons

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For calculation of generation and transport of cold and ultracold neutrons scattering law data for gaseous, liquid and solid H_2 and D_2 as well as for liquid He and some structure materials were derived and applied for transport calculations. The data format of generated scattering laws is ENDF-6. The transport calculations can be performed by both multigroup programs (S_N or Monte Carlo) and with the continuous energy Monte Carlo program MCNP. In case of MCNP the production term of ultra cold neutrons is calculated externally to get sufficient statistical accuracy for UCN transport. Reflection in storage of UCN or in neutron guides is treated by a modified reflection routine. Validation is in progress by comparison of evaluated and measured cross sections and -so far available- calculated and measured neutron spectra and gain factors.

KEYWORDS: Scattering Law, solid deuterium, liquid deuterium, cold neutrons, ultracold neutrons, UCN, MCNP, neutron transport

I. Introduction

Sources of cold or ultracold neutrons (UCN) based on supercritical, liquid or solid H_2 or D_2 or liquid ^4He are important facilities for neutron research. Optimisation of such sources which may be installed in fission reactors or near spallation targets can be based on both experience from existing experiments and neutron transport calculations using adequate scattering laws for neutrons in cold moderators and structure materials. Since several years we derive scattering laws for these applications, especially for liquid H_2 and D_2 and ^4He as well. New are scattering laws for solid H_2 and D_2. Our library includes now scattering laws for moderators: gaseous, liquid and solid H_2 and D_2 from 5K to 25K in ortho and para modification and ^4He at 1K; structure materials: Al at 20K; shields and filters: Pb or Bi at 77K or room temperature. Data for alternative temperatures can be generated by a limited effort. Additionally, scattering laws for D bound in (liquid) D_2O taking into account coherent scattering were generated, too. For liquid hydrogen and deuterium we have derived scattering law data which consider both the intramolecular and intermolecular interference. For supercritical H_2 and D_2 the scattering laws are according to the Young-Koppel model. For solid H_2 and D_2 the coherent elastic scattering corresponds to the hexagonal close packed (hcp) lattice, the inelastic and incoherent elastic scattering are derived from a frequency distribution. The model regards free rotation of H_2 or D_2 molecules on the corresponding lattice positions like in the liquid phase. For liquid helium at 1K we connected the atomic neutron scattering with the interatomic interference scattering by a static structure factor. For the coherent scattering for Bi the rhomboedric crystal structure, for Pb and Al the face-centered cubic (fcc) structure of the lattice is taken into account. The scattering laws $S(\alpha,\beta)$ are stored in ENDF-6 format and can be processed to multigroup scattering matrices or thermal data sets for the Monte Carlo code MCNP[1] by means of the NJOY[2)] modules THERMR, GROUPR and ACER, respectively. The energy range for the application of MCNP for UCN transport calculations was extended to 10^{-9} eV. To simulate reflection of neutrons with large wave lengths on mirror materials the reflect routine of MCNP was extended to account for this effect. For calculation of UCN source rate a special procedure is applied derived from $S(\alpha,\beta)$ directly to get the UCN source distribution for MCNP with sufficient statistical accuracy and spectral resolution. As far as available, processed data were validated by comparison of calculated and measured differential and integral cross sections and neutron flux spectra or gain factors.

II. Scattering Law for Solid Deuterium and Solid Hydrogen

The molecular dynamics of hydrogen and deuterium is determined by the motion of the either free H_2 or D_2 molecules (gaseous phase) or the bound state (condensed phase). Solid hydrogen and deuterium have a polycrystalline hcp lattice like metallic Be. The translatoric motion in the lattice is well known[3-6)]. The frequency distribution (**Figs. 1** and **2**) of the acoustical modes is pronounced by lattice-forces like van der Waals and quadrupole-quadrupole. The acoustical motion of the moderator atoms can be get from Nielsen, Bjerrum Møller[4)] or Yu *et al.*[3)] or Biem, Mertens[5)] (central force dynamical model). The Yu model leads to good agreement of the specific heat capacity for both H_2 and

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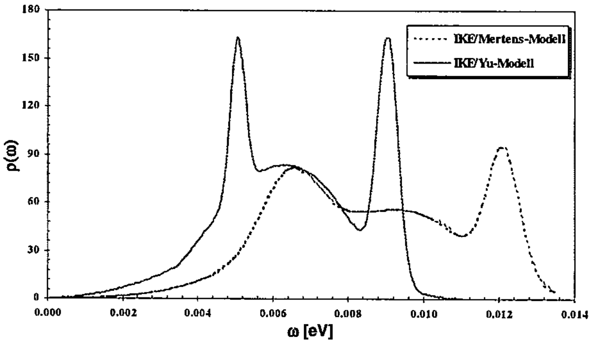

Fig. 1 Frequency distributions for solid deuterium

D_2 compared to measurements of Hill and Lounasmaa[7] (**Fig.3**). Therefore, the frequency distributions derived from the Yu model are used. For the optical modes, in the solid phase there are some uncertainties. Some authors[4,8] assume that due to the low temperature in the moderator some degrees of freedom are frozen and cause of the low energy neutron source spectra these modes must not be considered. Others[9] suppose, that the molecule at the lattice position can rotate relatively free and can also suffer excitation of the oscillation if the neutron energy is high enough (neutron downscattering). For the hcp-lattice the coherent elastic scattering cross-section must be taken into account. This part is based on the specific data of the lattice unit cell and atomic structure factor. The intramolecular scattering is calculated comparable to the liquid. Additionally, the elastic incoherent part is calculated separately as a function of the Debye Waller integral.

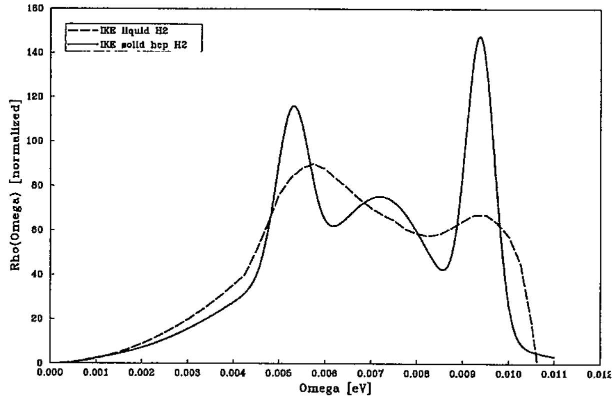

Fig. 2 Frequency distribution for liquid and solid hydrogen

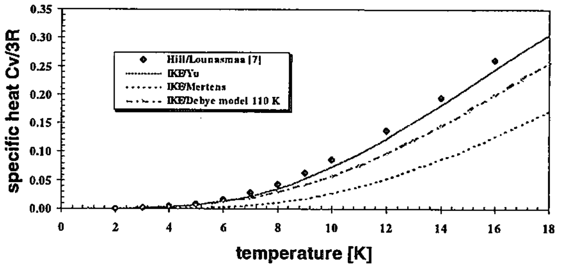

Fig. 3 Specific heat of solid deuterium

III. Cross Sections for H_2 and D_2

The evaluated cross sections for solid para-H_2 are compared with the measurement of Seiffert[10] in **Fig. 4**. The total cross section of solid ortho D_2 at 17K is compared with the measurements of Seiffert[10] in **Fig. 5.** Two calculated curves are shown in this figure, examining the excitation of the optical modes. The reason of discrepancies near 2.1 meV are not completely understood. One reason may be that the solid D_2 of the experiment was not pure polycrystalline.

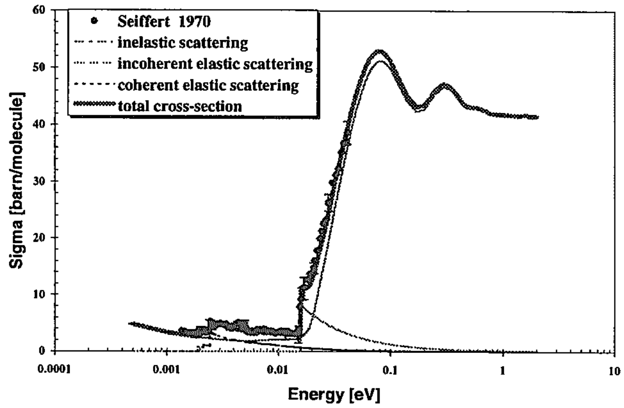

Fig. 4 Neutron cross sections for solid para H_2 at 6 K

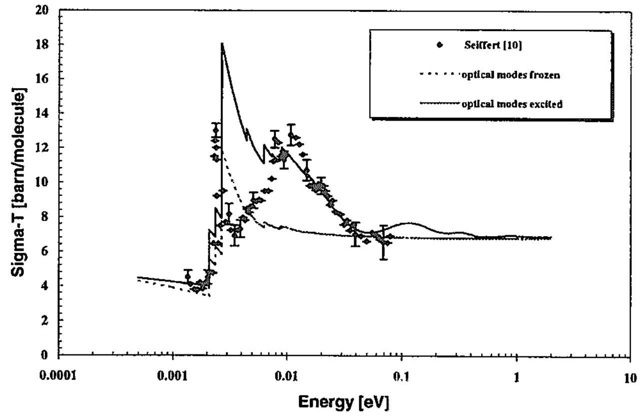

Fig. 5 Total neutron cross section for solid deuterium at 17 K

IV. Cross Sections for further Moderators and Structure Materials

For liquid H_2 and D_2 and superfluid He at 1K scattering law data were developed and used for cold neutron source optimisation calculations. The models for these moderators are discussed in ref.[11]. Additionally, for realistic transport calculations of cold neutron source designs also structure materials like Al or as shields and filters composed of Pb or Bi should be regarded at corresponding low temperatures. For these materials the scattering laws were developed, too. Examples for cross sections of these moderatos and structure materials are shown in **Figs. 6** to **8**. A comparison of calculated and measured spectra[12)] in a liquid D_2 source is shown in **Fig. 9**.

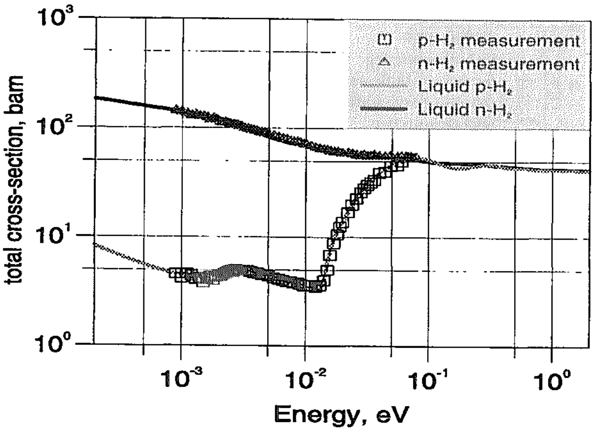

Fig. 6 Total cross sections for liquid n-H_2 and p-H_2

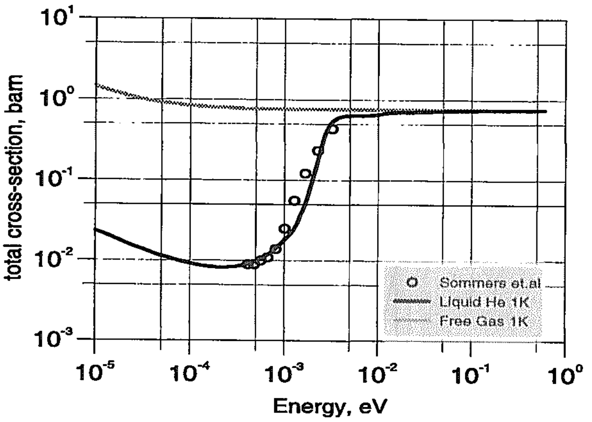

Fig. 7 Total cross section of liquid ^4He at 1K

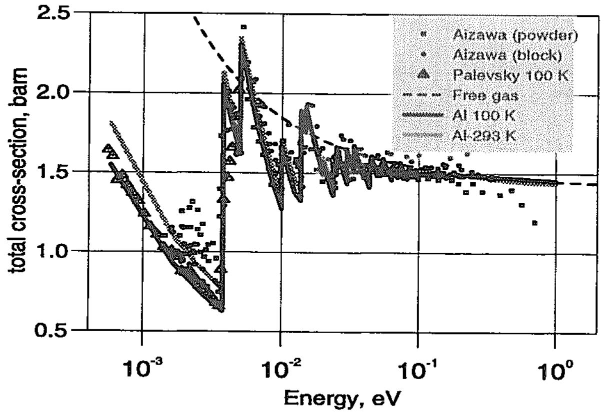

Fig. 8 Total cross sections for polycrystalline Al

V. Transport Calculations

The transport calculations based on the evaluated scattering laws can be performed with standard transport codes in multigroup approximation or by continuous Monte Carlo e.g. by the multigroup programs ANISN, DORT, TORT (S_N theory) or MORSE (Monte Carlo) and by continuous Monte Carlo codes like MCNP. The data processing for these codes can be performed by NJOY, if the scattering law data are available in corresponding ENDF-6 format. However, difficulties arise if the energy range of interest is lower than 10^{-5} eV. For the range of ultracold neutrons (some neV to about 500 neV) the present NJOY version cannot process data. Therefore, we tried to extend all corresponding limits in NJOY to produce cross section data for multigroup and continuous Monte Carlo applications for the UCN range. This attempt was quite successful, we could produce data for solid, liquid and gaseous D_2 for various temperatures. For multigroup calculations no further changes in transport programs are necessary. The generated 277 group data with 79 groups below 0.01 meV, 33 groups up to 3 eV and 165 groups above 3 eV can be applied directly in standard S_N codes like ANISN. Continuous Monte Carlo calculations e.g. by MCNP, however, must be splitted into two parts. First part treats the energy range above the standard cutoff of 0.01 meV. The spectrum calculated by this part is then used to calculate the scattering source for the UCN range. A direct approach in one calculation leads to completely insufficient statistical results for extreme low energies. The separate calculation of scattering source will be performed based on the S(α,β) scattering law data. This scattering source will be used then for a second run only for the UCN range. Using a biased source distribution the calculation for the UCN range results in spectra with sufficient statistical accuracy without extraordinary large computing time. As an example a simple model of a sphere was calculated to estimate the UCN production in a sphere filled by liquid and solid Deuterium of 20K and 10K, respectively. The sphere of 20 cm diameter was surrounded by a moderator of 293K. The outer diameter of the moderator was 150 cm. The problems were calculated by S_N code ANISN and MCNP (two parts, the space dependency of the scattering source in the inner sphere was regarded by

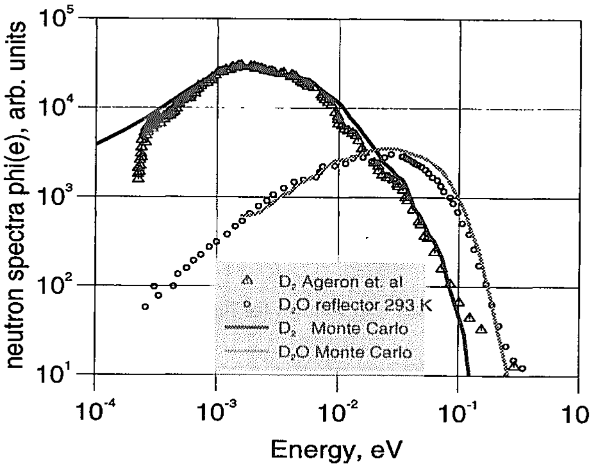

Fig. 9 Comparison of measured and calculated spectra in D_2 neutron source, and D_2O reflector (Ageron *et al.*[12)])

subdividing the sphere into 10 regions). The results are shown in **Fig. 10**. The ANISN and MCNP results are in good agreement. The only problem found for the first part of calculation was in the range from 0.01 to 0.1 meV. Here, probably the procedure for treating the thermal scattering based on S(α,β) tables should be improved. However, in the case of D_2 (liquid or solid) this range contributes not significantly to the UCN source.

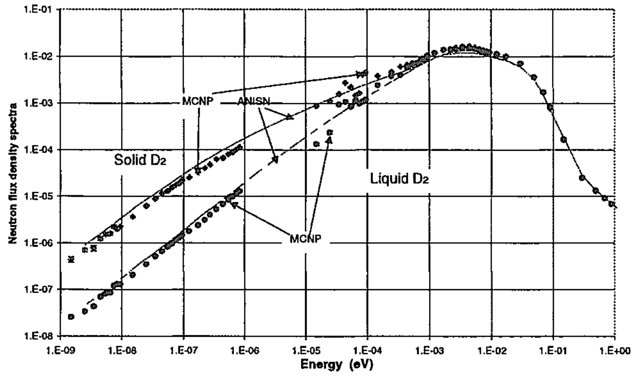

Fig. 10 Comparison of ANISN and MCNP calculations for solid and liquid D_2 in a spherical container

Since there is only a small gain of UCN per scattering UCN will be produced near neutron guides or storages with special treated surfaces to minimise their losses. In such regions total reflection must be regarded. This effect cannot be treated by the standard version of MCNP. Therefore, the reflection model for MCNP was extended to simulate reflection on mirrors or super mirrors by corresponding reflection law taking into account the losses at the walls of the guide tubes. The advantage of this application is that the geometry of the source and its environment can be treated for both spectrum calculation and UCN transport calculation by the same code. No special code for the UCN transport is necessary. All advantages of MCNP tally options for analysis of results can be used therefore. The only disadvantage is that gravity can only be regarded by further more complicated changes in reflection routine since the flight of neutrons in MCNP is simulated linearly. For calculation of neutron transport in storages the decay of neutrons can be regarded by a special tally or by changing the weight after every boundary crossing event.

VI. Conclusions

For a number of cold moderators for producing of cold or ultra cold neutrons scattering law data were evaluated and used in design and optimisation calculations for such sources. The cross section data were validated by comparison with measurements. The applicability of the data was proven by calculating spectra and gain factors for different experiments[8,12] with cold neutron sources or UCN sources. Furthermore, applications for the planned solid D_2 source for the FRM-2 reactor were performed[13]. The validation for solid cross sections for D_2 is not yet completed since we still see some discrepancies in relative gain factors for the gain of UCN cooling D_2 down from 20K to 10K corresponding to PNPI experiment[8]. The measured cross sections agree sufficiently good to very good for moderators and structure materials. Measured spectra in the energy range of cold neutrons can be reproduced well for both liquid and solid D_2.

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