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Generation of neutron multigroup constants in the energy range 0.1 μeV–10 MeV for light and heavy water at four different temperatures

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Abstract

On the basis of the cross section models of neutron scattering in liquid H_2O and D_2O, which have been developed in the previous papers, we have generated eight sets of multigroup constants (energy-averaged cross sections) for each liquid at 5, 27, 52 and 77 °C. The multigroup constants cover a wide energy range 0.1 μeV–10 MeV with 140 energy groups at equal logarithmic intervals and represent an angular scattering distribution by the Legendre polynomial expansion up to order 3. Major characteristics of neutron scattering inherent to liquid water are fully included in terms of coherent and incoherent properties and temperature-dependent quasi-elastic and inelastic scattering. These characteristics are assured by comparison with relevant experimental results of scattering cross section and also by neutron slowing-down and thermalization analysis in liquid H_2O and D_2O. It is shown that the present multigroup constants serve for analysis of neutron moderation from fission/spallation to ultra-cold energies, in combination with the already-generated ones for liquid ^4He, H_2, D_2 and CH_4 and solid CH_4.

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1. Introduction

During the past 3 years an extensive study of neutron scattering in liquid water has been carried out with a view to developing a cross section model [1–4].

- Cold and thermal neutron scattering in liquid H_2O has been studied in terms of a physical cross section model expressed basically by a velocity auto-correlation function and, equivalently, a generalized frequency distribution. The microscopic dynamics of water molecules is fully described from very general considerations connected with jump diffusion, intermolecular vibration, hindered rotation and intramolecular vibration at temperatures between 0 and 100 °C.
- The cross section model has been generalized to the one of liquid D_2O. Coherent neutron scattering is treated in view of a microscopic static structure and molecular motions through the Vineyard's convolution approximation [5]: a set of partial static structure factors for pairs of DD, DO and OO, determined experimentally [6], is utilized to express interference scattering from distinct molecules.
- A full set of double-differential and total cross sections for neutron incident energies from 0.1 μeV (ultra-cold) to 10 eV (epi-thermal) has become numerically calculable. Satisfactory agreement with the neutron scattering experiments and computer simulations [7–19] has been shown at several different temperatures. For reference, such a typical example is given in Fig. 1 for scattering laws for liquid H_2O and D_2O. Inclusion of water molecule dynamics well reproduces the experimentally observed behavior [14–16,20] especially at small momentum and energy transfer, which is in contrast to the molecular gas models for H_2O [21] and D_2O [22].

In the present paper, eight sets of multigroup constants (energy-averaged cross sections) for liquid H_2O and D_2O at

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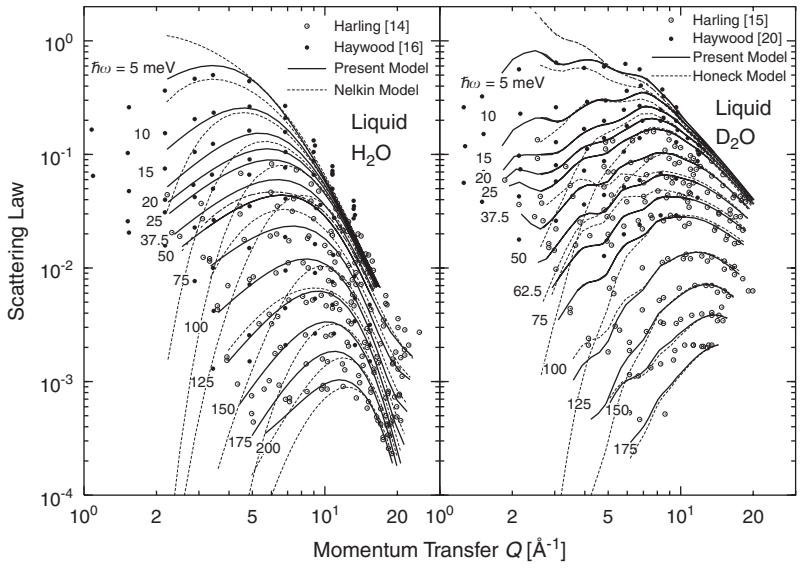

Fig. 1. Calculated scattering laws as a function of energy transfer $\hbar\omega$ and momentum transfer Q for liquid H_2O and D_2O at 20 °C, compared with the experimental results [14–16,20] and the Nelkin and Honeck models [21,22].

5, 27, 52 and 77 °C are newly generated using the cross section model mentioned above. A wide range of neutron energies from 0.1 μeV to 10 MeV is covered and forward scattering inherent to H by epi-thermal and fast neutrons is adequately represented by the Legendre polynomial expansion up to order 3. By the combined use of the already-developed multigroup constants for liquid H_2 and D_2 [23], liquid and solid CH_4 [24], and liquid ^{4}He [25], it becomes possible to treat quantitatively neutron slowing down and thermalization over the extremely wide energy range, say, from fission/spallation to ultra-cold-neutron energies. All the sets of multigroup constants are expected to serve for research and development of an advanced neutron source.

The purpose of the present paper is to report that the newly generated multigroup constants exhibit not only all of the essential characteristics of liquid water dynamics, but also yield proper energy spectra of fast and thermal neutron fluxes inherent to liquid H_2O and D_2O. The former is assured by calculating group-transfer scattering cross sections, angular distributions of scattered neutrons and total scattering cross sections especially at low energies below 10 eV. Good agreement with many experimental results [14,15,17,19,26–29] is found, for instance, with respect to the temperature dependence of total scattering cross sections at very-cold neutron energies around 0.01 meV. The latter spectral analysis is performed by a multigroup neutron transport calculation for pure liquid H_2O and D_2O and their mixtures at each temperature. The thermal neutron spectra are compared with the experimental ones in water and aqueous boric acid solutions [29] and characterized in terms of effective neutron temperature and thermal neutron gain with a change in liquid temperature and H_2O/D_2O content. Furthermore, non-Maxwellian deviations of the calculated spectra are found and clarified in view of water molecular dynamics such as quasi-elastic scattering and hindered rotation, which is essentially in contrast to the molecular gas models [21,22].

Section 2 describes briefly the procedures of multigroup constant generation. Section 3 illustrates physical characteristics of the multigroup constants. Section 4 is devoted to the concluding remarks.

2. Generation of multigroup constants

Since the method and procedure of multigroup constant generation have been described [30], only the main points concerned hereupon are touched. The energy range of incident and scattered neutrons from 0.1 μeV to 10 MeV is divided at equal logarithmic intervals into 140 groups: total number of groups is $G = 140$ with 10 groups per one energy decade. The angular distribution of scattering cross section is represented by the Legendre polynomial expansion up to a maximum order $L = 3$, i.e. in the P_3 approximation, which is almost adequate for reproducing forward scattering in free H, D and O by epi-thermal and fast neutrons. Hence the multigroup constants are defined using the double-differential scattering cross section $d^2\sigma_s^X(E \to E', \theta)/d\Omega\, dE'$ for liquid H_2O and D_2O ($X = H_2O$ or D_2O) at scattering angle θ with the change of neutron energy from E toE':

$$\sigma_{s,g\to g'}^{l,X} = 2\pi \int_{-1}^{1} d\mu \int_{E_g}^{E_{g-1}} dE \int_{E_{g'}}^{E_{g'-1}} dE' \times w(E) \frac{d^2\sigma_s^X(E \to E', \theta)}{d\Omega\, dE'} P_l(\mu) \quad (1)$$

where $\mu = \cos\theta$, $P_l(\mu)$ is the Legendre polynomial function of order l (= 0, 1, 2, 3), E_g and E_{g-1} are the lower and upper boundaries of the energy group g ($g = 1, 2, 3, \ldots, G$), and $w(E)$ is the weighting spectrum of neutron flux consisting of