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Effective temperatures and scattering cross sections in water mixtures determined by Deep Inelastic Neutron Scattering

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ABSTRACT

The present work shows a series of results of Deep Inelastic Neutron Scattering (DINS) experiments on light and heavy water mixtures performed at the spectrometer VESUVIO (Rutherford Appleton Laboratory, UK) employing an analysis method based on the information provided by individual detectors in forward and backward scattering positions. We investigated the effective temperatures of the different atoms composing the samples, a magnitude of considerable interest for Nuclear Engineering. The peak intensities and their relation with the bound-atom cross sections is analyzed, showing a good agreement with tabulated values which supports the use of this technique as non-destructive mass spectrometry. Previous results in the determination of scattering cross sections by this technique (known in the literature) that were at variance with the present findings are commented.

1. Introduction

Neutron cross sections of the different species of water constitute a topic of permanent interest in pure and applied Physics, and of particular importance in Nuclear Engineering since it is at the core of nuclear reactors calculations. In this regard an adequate description of the mechanisms of neutron thermalization is a permanent requirement of this discipline. The problem of neutron thermalization is usually treated with different approaches according to energy regimes. Thermal neutron interactions are described in cross section libraries while the epithermal regime is treated as a free gas model. A precise description of the latter case must take into account an effective temperature of the atoms that differs substantially from the thermodynamic temperature because it takes into account the molecular internal degrees of freedom. This is often overlooked in Nuclear Engineering calculations, thus causing inaccuracies in the results.

Deep Inelastic Neutron Scattering provides a direct measurement of effective temperatures, which makes this technique a potential source of data with direct applications to Engineering. In addition to its well-known application in the study of momentum distributions, the new prospects that offers the DINS technique to applied research were the focus of interest of a recent International Workshop (Seel et al., 2014). The present paper is in line with the idea of promoting the use of the technique in Applied Physics and discusses a method to determine effective temperatures in DINS experiments. Also with this premise, we recently published on the possibility of performing transmission and DINS measurements simultaneously at VESUVIO (Rodríguez Palomino et al., 2014).

In this work we determine effective temperatures by a direct analysis of the time-of-flight spectra on individual detectors, without going through the intermediate step of transformation into the West scaling variable *y* (described in detail in Mayers, 1990). The model employed in the analysis corresponds to that of an ideal gas with an effective temperature that accounts for the internal molecular vibration modes, corresponding to the usual Nuclear Engineering calculations. Since one of the main points of interest of this work is focused on these Engineering calculations, we briefly present its use and the data sources employed. We also present the relationship of the present findings with the most updated model employed in Engineering calculations developed in our laboratory.

The data analysis procedures required to go from the raw data in time-of-flight scale, to the effective temperatures are described in detail. The *modus operandi* includes residual background subtraction, multiple scattering corrections and data fitting.

At the end of this paper we revisit an old topic of the DINS technique about the peak intensities observed in water samples, and its relation with the scattering cross sections of the atoms. We show a full agreement with tabulated cross sections, thus adding support

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to the idea of mass-selective neutron spectroscopy (Krzystyniak et al., 2014) in current development.

2. Experimental details

Measurements were performed on three different light water/heavy water mixtures at room temperature. The Deuterium molar concentrations of the mixtures were $x_D = 0$ (light water), 0.25, and 0.5. An additional measurement was performed with a sample of $x_D = 0.62$ with lower statistics, so only some of its results will be shown. The mixtures were prepared from known volumes of pure light water and heavy water, which were verified by weight. All the samples were contained in a coin-shaped aluminum can 1.4 mm thick and 5.01 cm diameter. The sample covered the entire penumbra of the beam at the sample position, a necessary condition to perform both transmission and the standard Deep Inelastic Neutron Scattering (DINS) experiments at VESUVIO.

The setup of VESUVIO spectrometer is thoroughly described in Mayers and Reiter (2012), from where we take the nomenclature of the detectors used in this work. Forward scattering detectors are yttrium aluminum perovskite (YAP) γ-ray detectors (S135 to S198), and backscattering detectors (S3 to S134) are ^{6}Li-doped glass scintillators. Detector S1, located 8.6 m from the moderator was used as incident beam monitor, and its number of counts was employed to normalize all the measured spectra. Detector S2, placed at 13.43 m from the neutron moderator is the transmission monitor. The sample is located inside an evacuated bell, at 11 m from the moderator. In addition to the measurements on water samples mentioned above, we performed ancillary measurements on a 2 mm-width lead sample (for standard calibrations), on the empty-cell and on the empty instrument. Fig. 1 (based on Mayers and Reiter, 2012) describes schematically the experimental setup.

3. Data analysis formulation

3.1. Basic expressions

In this paper we work with the experimental data represented in the time-of-flight scale, such as they result from the experiment. We will explicitly avoid passing through the y-scale as is traditional for this technique, to show an alternative route in the data analysis. By choosing this procedure we obviate the use of the convolution approximation on which we formulated some objections in the past, particularly in relation to the analysis of the Compton profiles of light atoms (Blostein et al., 2005). The analysis that we will perform is only on individual-detector spectra, so we will not add up the signals of different detectors, to preserve the best possible angular resolution.

The basic expression for the difference filter-out minus filter-in spectra in the time-of-flight scale, is based in the equation stated by Powles (1976). The basic setup consists in incident neutrons traveling an incoming path of length L_0 with energy E_0 (wave vector $\mathbf{k}_0$), that are scattered in the sample at an angle θ, and travel along a distance L_1 up to the detector position with a final energy E (wave vector $\mathbf{k}$)

$$C(t,\theta)\Delta t = \int_{\substack{E_{0,\inf}\\ t=\text{const}}}^{\infty} dE_0\,\Phi(E_0)\sigma(E_0,E,\theta)\,\varepsilon(E)\left[1-e^{-nT_F\sigma_F(E)}\right]\left|\frac{\partial E}{\partial t}\right|\Delta\Omega\Delta t \tag{1}$$

where $\Phi(E_0)$ is the incident neutron flux, $\sigma(E_0,E,\theta)$ the double-differential scattering cross section of the sample (defined below in Eq. (2)), $\varepsilon(E)$ the detector efficiency, $\Delta\Omega$ is the solid angle subtended by the detector, $(1-e^{-nT_F\sigma_F(E)})$ the absorption probability of the resonant filter, characterized by a number density n, a thickness T_F, and a total (scattering plus absorption) cross section $\sigma_F(E)$. The lower limit of integration $E_{0,\inf} = m/2(L_0/t)^2$ is determined by kinematic condition that in the second flight path the neutron spends a time tending to zero. The spectrum $C(t,\theta)$, known as neutron Compton profile, is a microscopic magnitude. Its link with the measured spectrum that comprises multiple scattering events, and container contributions is shown in Rodríguez Palomino et al. (2013). At the end of the multiple-scattering and beam attenuation corrections we will be able to access $C(t,\theta)$.

The systems we consider are light/heavy water mixtures, with different Deuterium molar concentrations x_D. The double differential cross section of such mixtures is described by

$$\sigma(E_0,E,\theta) = \sqrt{\frac{E}{E_0}}\left[2(1-x_D)\,\sigma_{b,H}\,s_H(E_0,E,\theta) + 2x_D\,\sigma_{b,D}\,s_D(E_0,E,\theta) + \sigma_{b,O}\,s_O(E_0,E,\theta)\right], \tag{2}$$

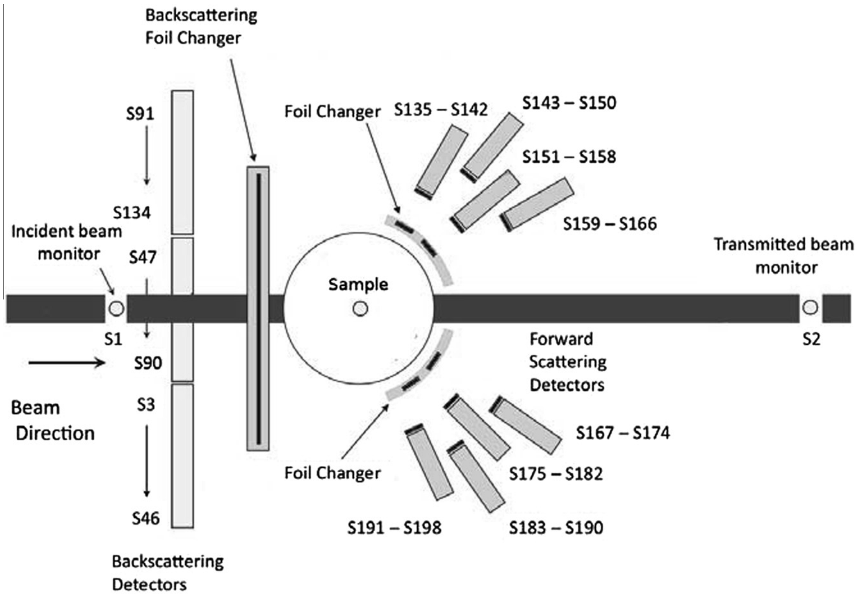

Fig. 1. VESUVIO experimental setup, showing the detector positions.