7 Interdisciplinary Research

7.1

7.1.1 Comparison of Experimental Data and Theoretical Predictions for the n-d Cross-Section at Low Energies

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The neutron-deuteron (n-d) cross-section at low energies plays an important role in the design and operation of heavy-water moderated nuclear fission reactors. Therefore, we calculated the n-d differential cross-section in the incident neutron energy range from 1 to 3.3 MeV and compared the theoretical results to the available experimental data. The Pair Correlated Hyperspherical Harmonic method developed by the Pisa group was used [Kie93]. The Argonne AV18 nucleon-nucleon interaction [Wir95] was employed and the three-nucleon interaction (TNI) of Urbana (UR) was added. The combination of AV18+TNI [Pud95] correctly describes the $^3$H binding energy. It has been shown [Kie96] that the rigorous proton-deuteron (p-d) calculations of the Pisa group below the deuteron breakup threshold ($E_p=3.33$ MeV), again using AV18+TNI, are in excellent agreement (≈1% deviation) with experimental p-d cross-section data in this energy range. Therefore, we expect the present n-d calculation to have the same accuracy as well.

Figure 7.1.1 shows our calculations in comparison to the experimental data. Except for the forward angle data at 1.0 MeV (Figure 7.1.1 a), the data of Adair et al. [Ada53] (Figure 7.1.1 c, e and j) and Seagrave and Cranberg [Sea57] (Figure 7.1.1 h and n) are in very good agreement with the theoretical predictions. This is very satisfying, considering the fact that these data are some 40 years old. However, the 30 year old data of Vedrenne [Ved66] (Figure 7.1.1 b, d, g, and m) have both the wrong shape and magnitude. The data of Weber [Web81] (Figure 7.1.1 f) and Chatelain et al. [Cha79] (Figure 7.1.1 i and o) are too high at backward angles. Finally, (Figure 7.1.1 k and l) the data of Schwarz et al. [Sch83] are compared to the theoretical results at $E_n=2.5$ and 3.0 MeV. These are the most recent data for the n-d differential cross-section in the energy range of interest and the associated experimental uncertainties are rather small. The agreement between data and theoretical predictions is very good.

We conclude that the n-d differential cross-section can now be predicted reliably in the energy range of interest. In fact, the theoretical calculations are probably more accurate than the accuracy of the best experimental data. Therefore, for heavy-water moderated

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Figure 7.1-1: Comparison of experimental n-d differential cross-section data with theoretical predictions.
fission reactor design studies, n-d cross-sections calculated using AV18+TNI can be used in the energy range of interest without any reservation.


7.1.2 Sonoluminescence and High-Pressure Gas Scintillators

W. Tornow

Sonoluminescence (SL) is a nonequilibrium phenomenon which occurs when acoustic energy is focused on a bubble of air trapped in water such that the bubble emits light [Bar91]. The light emission is visible to the unaided eye and appears blue. The acoustic energy (10^{-11} eV/atom) enters in a continuum at the macroscopic level and spontaneously focuses down to the molecular, atomic, and electron degrees of freedom, concentrating the ambient energy by more than twelve orders of magnitude.

The experimental arrangement for achieving stable single-bubble SL consists of piezoelectric transducers that excite breathing resonances in a water-filled spherical glass flask to which they are attached [Put95]. Above a certain threshold acoustic amplitude a bubble can be trapped. The water acts like a piston that compresses and decompresses the air periodically and the collapse of a bubble formed by cavitation occurs such that the energy of collapse is delivered to a small number of molecules, which are thus excited or dissociated. Light is emitted in the deexcitation or recombination process. The light emission occurs only during an interval of less than 100 ps or 150 ps within each cycle in the sound field, which has a period of a few tens of microseconds (depending on the diameter of the glass flask). The temperature of 10^5 K required to explain the ultraviolet light emitted by the
bubble suggests that an inward-moving shock wave remains intact to a radius of $2.5 \times 10^{-4}$ cm from the center of the bubble. If the shock front survives down to 20 nm, the temperature would reach $10^6$ K. However, the associated photons (soft X-rays) do not propagate through water and therefore it is not clear what the highest temperature associated with the sonoluminescence really is.

According to Refs. [Put95, Hil94], pure N$_2$ bubbles produced hardly any light. The same observation was made for O$_2$, a 80%-20% mixture of N$_2$ and O$_2$, and gas from a liquid-air container. It is the 1% presence of Ar in natural air that is responsible for the vast majority of the light emission. Subsequently, it was found that Ar can be replaced by other noble gases like He and Xe. The admixture of Xe (He) produces more (less) light than the admixture of Ar. The observed light emission depends strongly on the nature of the gas inside the bubble. For example, Xe yields a spectral peak at about 300 nm, whereas in the case of other noble gases the peak is located further in the ultraviolet region, which is obscured by the cutoff of water.

The importance of noble gases for observing SL raised our suspicion of a possible relationship between the light emission processes in SL and high-pressure gas scintillators. In the following we will review some of the information necessary to support our conjecture.

High-pressure N$_2$-Ar and N$_2$-Xe mixtures were investigated by Engelke [Eng60] and Tornow et al. [Tor76]. It was found that the light output is independent of pressure at pressures above a few atmospheres. In Ref. [Tor76], it was reported that a high-pressure N$_2$-Xe gas scintillator produces about a factor of 7 more light than a N$_2$-Ar gas scintillator at the same pressure. This observation is in qualitative agreement with the gas doping results of SL bubbles by Hiller et al. [Hil94].

The relative scintillation efficiencies of noble gases and their mixtures were investigated by Northrop and Gursky [Nor58]. Of all the noble gases, Xe produces the largest light output. In striking similarity to the work of Ref. [Nor58], Xe produced the largest light intensity in the SL studies of Ref. [Hil94].

Most of the light arising in a noble gas following the passage of a charged particle lies in the ultraviolet. Strickler and Arakawa [Str64] showed that pure Ar bombarded by α-particles emits a continuum which extends from about 110 nm to 280 nm. The decay of the scintillation light has been reported to be as fast as $10^{-9}$ s with a decay period inversely proportional to pressure. The first excited state of non-ionized and ionized noble gas atoms lies very high (i.e., at about two-thirds the energy required for ionization). Therefore, transitions from excited states to the ground state produce ultraviolet light. The energies of resonance levels of noble gas atoms from which the atoms are able to return directly to the ground state without passing through intermediate excited states are given in Table 7.1–1. According to this table, the statement made in Ref. [Hil92] that the spectral peak of SL appears to be located at photon energies above 6 eV is not surprising. In fact, Table 7.1–1 explains why a spectral peak was observed in Ref. [Hil94] for Xe and not for Ar and He. According to Table 7.1–1, in the latter two cases the spectral peaks are expected to lie at
Table 7.1-1: Energies (in eV) and associated wavelengths $\lambda$ (in nm)

<table>
<thead>
<tr>
<th>Level Type</th>
<th>para He</th>
<th>ortho He</th>
<th>Ne</th>
<th>Ar</th>
<th>Kr</th>
<th>Xe</th>
</tr>
</thead>
<tbody>
<tr>
<td>1st metastable level</td>
<td>20.7</td>
<td>19.7</td>
<td>16.50</td>
<td>11.5</td>
<td>9.9</td>
<td>8.2</td>
</tr>
<tr>
<td>1st resonance level</td>
<td>21.1</td>
<td>16.55</td>
<td>11.59</td>
<td>10.0</td>
<td>8.4</td>
<td></td>
</tr>
<tr>
<td>2nd metastable level</td>
<td></td>
<td>16.60</td>
<td>11.61</td>
<td>10.5</td>
<td>9.41</td>
<td></td>
</tr>
<tr>
<td>1st ionization level</td>
<td>24.46</td>
<td>21.5</td>
<td>15.7</td>
<td>13.9</td>
<td>12.1</td>
<td></td>
</tr>
<tr>
<td>$\lambda$ of resonance radiation</td>
<td>50.2</td>
<td>58.4</td>
<td>74.5</td>
<td>106.3</td>
<td>117.5</td>
<td>146.0</td>
</tr>
</tbody>
</table>

...a much shorter wavelength.

The speed of the scintillation light depends on the speed of its radiative transition and on the probability for reabsorption and subsequent reemittance (resonance radiation trapping). The lifetime of resonance levels of noble gas atoms or ions is $<10^{-9}$ s. It is well known that the effect of pressure broadening reduces the trapping time of resonance radiation at high pressures. In addition, considering the pressure and temperature associated with SL, the lifetime of the metastable levels given in Table 7.1–1 may be reduced by collisions with neutral or excited atoms or ions to the level of that expected for resonance radiation. Therefore, the sub-nanosecond time scale of SL is not too surprising. However, presently unknown mechanisms, most likely related to the high pressure in the bubble, must be responsible for the pico-second SL light pulses.

In Ref. [Hil92], it was found that by lowering the temperature from 20°C to below 10°C the total light emission from a single bubble can be enhanced by over a factor of ten. In a subsequent paper, Barber et al. [Bar94] reported that as the water temperature decreased from 40°C to 1°C the intensity of the light emission increased by a factor of over 200.

To establish the connection to gas scintillators we notice that they are very susceptible to poisoning of the light by contaminants, especially to organic substances like hydrocarbons. Therefore, we speculate that the strong increase of light emission observed in SL with decreasing temperature is (similarly to gas scintillators) a direct consequence of the purification process accompanied with the temperature decrease. Not only is the partial vapor pressure of light absorbing contaminants in the bubble and the surrounding driving fluid reduced, but the contaminants are also preferentially absorbed at the inner wall of the glass container where the temperature is lowest.

In summary, the existing experimental information suggests that the light emission processes associated with SL are closely related, if not identical, to the ones known to occur in high-pressure gas scintillators. In fact, we think that the small SL-bubble trapped in water acts like a high-pressure micro gas scintillator.


