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Impact of the Doppler Broadened Double Differential Cross Section on Observed Resonance Profiles

R. Dagan,[1,*] B. Becker,[2] Y. Danon,[3] F. Gunsing,[4] S. Kopecky,[2]
C. Lampoudis,[4] O. Litaize,[5] M. Moxon,[6] and P. Schillebeeckx[2]

[1] *Karlsruhe Institute of Technology, INR, 76344 Eggenstein-Leopoldshafen, Germany*
[2] *EC-JRC-IRMM, Retiesweg 111, 2440 Geel, Belgium*
[3] *Rensselaer Polytechnic Institue, Gaerttner LINAC Center, Troy, New York 12180, USA*
[4] *CEA Saclay, DSM/DAPNIA/SPhN, 91911 Gif-sur-Yvette, France*
[5] *CEA, DEN, Cadarache, F-13108 Saint Paul Lez Durance, France*
[6] *Hyde Copse 3, Marcham, United Kingdom*

This paper is sequential to studies discussing with the impact of the Doppler broadening of the Double Differential Cross Section (DDXS) on nuclear reactor core calculations. In this study, the influence of the resonance dependent DDXS on the observed resonance line shape in time of flight capture experiments is investigated. The importance of the correct formalism is illustrated by comparing Monte Carlo simulations with and without a resonance dependent DDXS model to measured data of a saturated ^{238}U resonance. The resonance dependent DDXS is taken into account via its stochastic implementation known as Doppler Broadening Rejection Correction (DBRC). In addition, the increased impact of the resonance dependent DDXS model for higher temperatures is shown via a simulation of capture yields for ^{238}U and ^{183}W at different sample temperatures.

I. INTRODUCTION

The improvement of theoretical models for the Doppler broadened Double Differential Cross Section (in following referred to as DDXS) has been going on since 1944. At first, the simple two body collision (asymptotic approach) was developed, then the impact of the temperature [1] was introduced, followed by energy dependent cross sections [2] and solid state effects [3]. In parallel, considerable effort was invested in a new accurate formalism and in appropriate computational methods to determine the complete effect of DDXS on reactor calculation. A full practical formalism based on the free gas model was developed [4] and implemented [5] in the data processing code NJOY [6]. $S(\alpha,\beta)$ tables of the scattering angle and neutron energy after a collision were extracted [7], in a way that they could be read by varieties of Monte Carlo codes. The computational process was further improved by the development of the so called DBRC (Doppler Broadening Rejection Correction) method [8] which allowed for relatively easy implementation of the resonance and the temperature effects on the calculated DDXS. As far as reactor simulations are concerned the introduction of the new resonance dependent DDXS brought a well noticeable shift in the criticality of a variety of core simulations ranging from 200 to 600 pcm.

A series of angle dependent experiments were performed at the Rensselear Polytechnic Institute [9, 10] to confirm the validity of the resonance dependent DDXS theory and its computational approach. In several cases the correct DDXS is also required for the description of capture measurements, in relative thick samples, as the yield has a substantial contribution from multiple scattering events. In particular, the DDXS is needed for heavy nuclei with low energy resonances for which the neutron width is larger than the radiation width. Examples of the impact of the DDXS on the profile are given in Refs. [11] for the 69.2 eV resonance of ^{232}Th. However, in Ref. [12] it is shown that for the sample at room temperature the observed resonance profile can also be described by an approximation for the DDXS where only the temperature (first differential part) is introduced as it is implemented in REFIT [13].

This contribution aims at a more elaborated study of the influence of the DDXS on line shapes observed in capture experiments using experimental data for ^{238}U obtained at the GELINA TOF-facility. The experiments were performed within the EFNUDAT project.

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[*] Corresponding author: Ron.Dagan@kit.edu

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II. DDXS IN VIEW OF NUCLEAR DATA EVALUATION

The correct formula of the resonance dependent DDXS that was developed in Ref. [4] was manipulated (Eq. (1)) in such a way that it became feasible to introduce it within the data processing code NJOY [6] to generate the resonance dependent scattering $S(\alpha,\beta)$-tables [7]. For isotropic scattering the DDXS is given by

$$\begin{aligned}\sigma_s(E \to E', \vec{\Omega} \to \vec{\Omega}') = &\\ &\frac{1}{4\pi E}\sqrt{\frac{A+1}{A\pi}} \int\limits_{\epsilon_{max}}^{\infty} d\xi \int\limits_{\tau_0(\xi)}^{\tau_1(\xi)} d\tau \left(\frac{\xi+\tau}{2}\right)\\ \times \quad & \sigma_s\left(\frac{A+1}{A^2}\frac{(\xi+\tau)^2}{4}k_BT, 0\right)\\ \times \quad & \exp\left(v^2 - \left[\frac{(\xi+\tau)^2}{4A} + \frac{(\xi-\tau)^2}{4}\right]\right)\\ \times \quad & \left(\frac{\epsilon_{max}\epsilon_{min}(\xi-\tau)^2}{B_0 \sin(\hat{\varphi})}\right). \qquad (1)\end{aligned}$$

As can be noted, Eq. (1) depends on the temperature as well as on the scattering cross section σ_s at zero Kelvin temperature as indicated by the second argument. A detailed explication of Eq. (1) can be found in Ref. [5]. The explicit appearance of the energy dependent cross section and the correct temperature in the second argument of Eq. (1) are the essence of the resonance dependent Doppler broadened differential cross section.

The implementation of the analytical formula of resonance dependent DDXS in existing Monte Carlo transport codes or those for resonance shape analysis in a deterministic approach might be cumbersome. An additional way to handle the resonance and temperature dependent scattering kernel in Monte Carlo codes was introduced in Ref. [14]. It is based on a modification of the commonly used target velocity and directional probability distribution $P(V,\mu)$. The modified probability distribution is given by

$$\begin{aligned}P(V,\mu) = C' \left\{\frac{\sigma_s(v_r,0)}{\sigma_s^{max}(v_\xi,0)}\right\} \times \left\{\frac{v_r}{v+V}\right\}&\\ \times \left\{\frac{2\beta^4V^3e^{-\beta^2V^2} + (\frac{\beta v\sqrt{\pi}}{2})(\frac{4\beta^3}{\sqrt{\pi}})V^2e^{-\beta^2V^2}}{1+\beta v\sqrt{\pi}/2}\right\}, & \qquad (2)\end{aligned}$$

where C' is a normalization constant depending on the neutron speed v, but not on the speed V of the target or the neutron speed v_r relative to the target at rest. For details see Ref. [14]. The approach in Eq. (2) is known as the Doppler Broadened Rejection Correction (DBRC) [8]. It extends the common approach in Monte Carlo simulation [15] by adding another rejection for the ratio of the 0 K scattering cross section, corresponding to the velocity term v_r, and an arbitrary maximal scattering cross section σ_s^{max}. In comparison to Eq. (1) the first term in the parentheses is the additional rejection which replaces the integration over the energy dependent cross section, the second term is the rejection of the chosen velocities (based on the third term) in an adequate sampling procedure commonly used in MC codes. The third term includes the temperature through the Maxwell Boltzmann target velocity distribution. From physical point of view Eqs. (1) and (2) are similar, however the introduction and use of the second equation is by far more simple and allows for an accurate implementation in Monte Carlo codes used for the calculations of line shapes of capture yield near pronounced resonances.

The determination of resonance parameters is performed in general by dedicated codes [13, 16, 17] which compare experimental measurements to numerical model calculations. In case of capture yield experiments, the quantity of interest is the reaction yield, which is the fraction of the neutron beam being captured in the sample. The theoretical yield Y can be expressed as sum of primary yield Y_0 and multiple interaction correction Y_m

$$Y = Y_0 + Y_m. \qquad (3)$$

The latter is due to a capture reaction after at least one neutron scattering in the sample. The primary capture yield is given by

$$Y_0 = \left(1 - e^{-n\sigma_t}\right)\frac{\sigma_c}{\sigma_t}, \qquad (4)$$

where n is the areal density and σ_c and σ_t are the Doppler broadened capture and total cross section, respectively.

Using the DDXS, the single scattering correction Y_1 (absorption after 1 scattering collision), given for the 0 K temperature limit in Ref. [17], can be generalized to

$$\begin{aligned}Y_1(E) \;=\; & \frac{1}{S}\int\limits_S dxdy \int\limits_{z=0}^{D} dz \frac{n}{D}\exp\left(-\frac{n}{D}\sigma_t z\right)\\ & \int\limits_{\vec{\Omega}'} d\vec{\Omega}' \int\limits_{E'} dE' \sigma_s(E \to E', \vec{\Omega} \to \vec{\Omega}')\sigma_c' \frac{n}{D}\\ & \int\limits_q dq \exp\left(-\frac{n}{D}\sigma_t' q\right), \qquad (5)\end{aligned}$$

where S and D are surface area and thickness of the sample, respectively. q is the distance of a collision point (x,y,z) to the surface of the sample. σ_c' and σ_t' are evaluated at the energy E' of the scattered neutron. For a thick sample and a strong scattering resonance Y_1 can significantly increase the capture yield. The expression for Y_2 (absorption after 2 scattering collisions) is more complicated and several approximations are usually employed [13, 17].

As can be noted from Eq. (5), Y_1 is directly dependent on the DDXS. Consequently an accurate formalism and numerical implementation in the relevant fitting code is mandatory to estimate the effect of the resonance dependent DDXS on the line shape and eventually on the resonance parameters themselves.

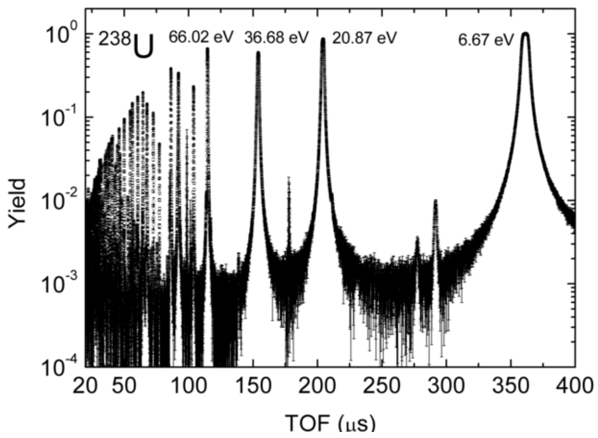

FIG. 1. Experimental capture yield of a 0.46 mm (1.920×10^{-3} at/b) thick ^{238}U sample in the 20 μs (2.1 keV) to 400 μs (5.4 eV) TOF frame measured at 300 K [18].

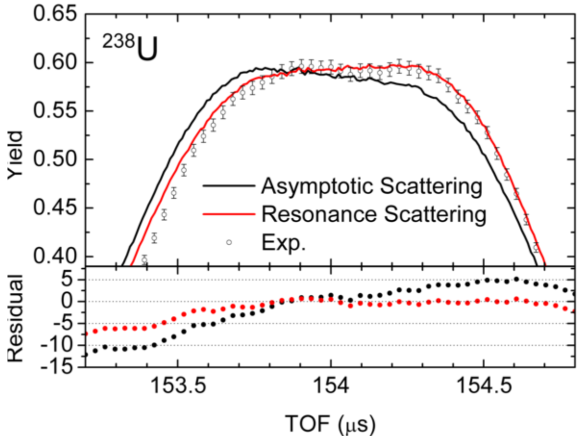

FIG. 2. Experimental and simulated capture yield as function of TOF of a 0.46 mm (1.920×10^{-3} at/b) thick ^{238}U sample the vicinity of the 36.68 eV resonance measured at 300 K.

III. IMPACT OF THE RESONANCE DEPENDENT DDXS ON THE CAPTURE YIELD LINE SHAPE OF ^{238}U

A capture measurement on a ^{238}U sample [18] was carried out at the multi-user TOF facility GELINA [19]. The GELINA facility provides a pulsed white neutron source with an energy range from 10 meV to 20 MeV. The sample consisted out of two back-to-back ^{238}U (^{235}U: 11 ppm) foils with a combined thickness of 0.46 mm (1.920×10^{-3} at/b), an eqivalent diameter of 4.52 cm and a total mass of 12.2 g. The sample was placed at a flight path length of 12.908 m. The capture rate was then measured based on the total energy detection principle [20] in combination with the pulse height weighting technique using two C_6D_6 gamma-ray detectors [20]. The detectors were placed at a 125° angle with respect to the incident neutron beam. The energy dependence of the neutron flux was continuously monitored with a ^{10}B Frisch-gridded ionization chamber placed at about 80 cm before the sample. The measured spectra were used to deduce the experimental capture yield using the AGS code [21]. The normalization of the capture yield was based on the saturated resonance of ^{238}U at 6.67 eV. Fig. 1 shows the deduced capture yield in the TOF frame from 20 μs (2.1 keV) to 400 μs (5.4 eV).

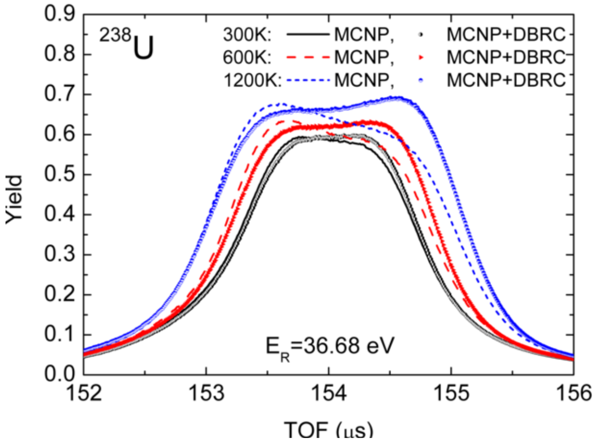

FIG. 3. Simulated capture yield as function of time of flight (TOF) of a 0.46 mm (1.920×10^{-3} at/b) thick ^{238}U sample in the vicinity of the 36.68 eV at 300 K, 600 K and 1200 K.

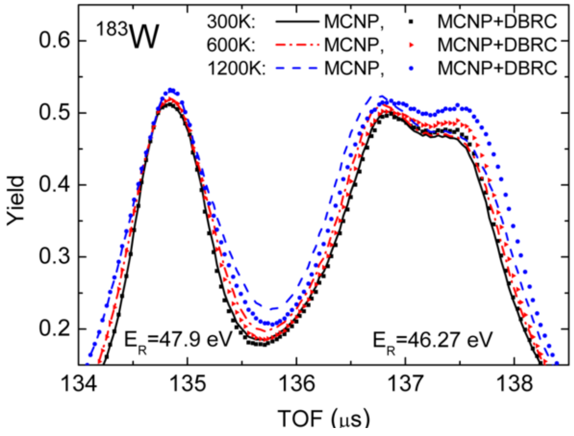

FIG. 4. Simulated capture yield as function of TOF of a 0.065 mm (3.07×10^{-4} at/b) thick ^{183}W sample in the vicinity of the 46.27 eV and 47.9 eV resonances at 300 K, 600 K and 1200 K using the EC-JRC-IRMM evaluation of the ^{183}W cross section [23].

The measurement was simulated with the Monte Carlo code MCNP5 [15] (ver. 1.40) using the ENDF/B-VII.1 nuclear data library [22]. A standard version of the code applying the asymptotic DDXS above 10 eV at 300 K and a modified version including DBRC were used. The experimental resolution of the TOF measurement was taken into account by using a probability distribution of the equivalent flight path distance [20]. The effect of the resonance dependent DDXS is strongly pronounced in cases where the scattering cross section is of the same order of magnitude as the absorption cross section. The well pronounced resonance at 36.68 eV has the most "convenient" ratio Γ_γ/Γ_n as far as the importance of the DDXS is concerned. Fig. 2 presents the measured and simulated capture yields as well as the relative deviation between the simulations and the experimental results close to the 36.68 eV resonance of ^{238}U at 300 K. It is evident that the introduction of the resonance dependent DDXS model is mandatory. Nevertheless, the slight differences on the lower time (higher energy) wing might be due additional experimental effects such as γ-ray attenuation or the used resolution function. The experiment resolution could be improved by using a 60 m flight path of the GELINA facility. Since the strongest deviation between the two simulations can be noticed at the wings of the resonance, a selfindication measurement (or the simple application of numerical filter on the present data set) which decreases the peak count rate would stronger illustrate the obtained differences.

IV. TEMPERATURE DEPENDENCE OF THE IMPACT

Since the resonance dependent DDXS is directly dependent on the sample temperature, it's impact on the capture yield was studied by simulating the capture yield of ^{238}U and ^{183}W at different temperatures (300 K, 600 K, 1200 K). Figs. 3 and 4 show the yield in the vicinity of the 36.68 eV resonance of ^{238}U and the 46.27 eV and 47.9 eV resonances of ^{183}W, respectively. A flight path of 12.908 m was assumed, however neglecting any resolution effect. Both figures show that while at 300 K the impact of the introduction of the DBRC within the MCNP code is low, it enhances considerably with a temperature increase.

An experimental evidence similar to the one shown in Fig. 2 would be necessary to confirm the validity of the differential Doppler broadening part embedded in the DBRC formalism at higher temperatures. Moreover it would confirm the use of the current resonance parameters and the free gas based Doppler broadening concept.

V. CONCLUSIONS

A full (temperature and resonance dependent) formalism of the DDXS was introduced to study its impact on the line shape of pronounced resonances in capture yield experiments. It was shown that for the saturated resonance of ^{238}U at 36.68 eV the capture yield is better reproduced using the resonance dependent DDXS in form of DBRC. The growing impact of the DBRC on the capture yield with increased temperatures, as was calculated for ^{238}U and ^{183}W, emphasizes the need of experiments at higher temperatures. Such measurements are foreseen to be done at the GELINA facility. With them, the validity of the complete Doppler Broadening formalism (including its differential part) can be rigorously analyzed which in return will increase the confidence in the use of the current applied resonance parameters.

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