Application of Energy Window Concept in Doppler Broadening of ^{238}U Cross Section

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1. Introduction

The huge amount of data required has been a big issue in the generation of resonance cross sections. In order to perform thermo-hydraulic feedback, cross section data at temperatures with intervals of 10-50 K is required. However, for each temperature there is around 1 GB of cross section data that needs to be generated. On the fly Doppler broadening is one of the techniques used to reduce the amount of storage, and one of the key elements is application of the energy window concept. Currently, the NJOY code is used for construction and Doppler broadening of microscopic cross sections. [1] There exist several methods or formalisms to produce microscopic cross sections and there are also different methods of Doppler broadening.

In this paper, Multi-Level Breit-Wigner (MLBW) formalism and the $\psi-\chi$ method are used for generation and Doppler broadening of the resonance cross section. Accuracy of the energy window concept applied MLBW (EW MLBW) Doppler broadened cross section was compared with that of the cross section generated by conventional MLBW (Con MLBW) formalism for ^{238}U isotope using MATLAB. The conventional method requires Doppler broadening of all resonances, including resonances far from the target energy point, which do not change much with respect to the temperature change. The energy window concept makes Doppler broadening possible with a smaller number of resonances neighboring to the energy point we are interested in, and just adds up 0 K temperature cross sections of other resonances.

2. Methods and Results

In this section, the following microscopic cross section generation techniques are described: Multi-level Breit-Wigner formalism, $\psi-\chi$ Doppler broadening method, and energy window concept.

2.1 Multi-Level Breit-Wigner Formalism

Resonance parameters from the ENDF/B-VII.0 file are converted into cross sections using R-matrix theory, and then approximated into the MLWB formalism.

Eqs. (2), (3), (4) and (5) show the potential, elastic scattering, radiative capture, and fission cross sections, respectively, in terms of the resonance parameters.

$$\sigma_{mr} = \frac{4\pi}{k^2} g_J \frac{\Gamma_{nr}}{\Gamma_r} \ , \tag{1}$$

$$\sigma_p = \sum_l 4\pi / k^2 (2l+1) \sin^2 \phi_l \ , \tag{2}$$

$$\sigma_n = \sigma_p + \sum_l \sum_{rc} \sigma_{mr} \{A\psi(\theta, x) + B\chi(\theta, x)\} \ , \tag{3}$$

$$\sigma_\gamma = \sum_l \sum_r \sigma_{mr} \frac{\Gamma_{\gamma r}}{\Gamma_r} \psi(\theta, x) \ , \tag{4}$$

$$\sigma_f = \sum_l \sum_r \sigma_{mr} \frac{\Gamma_{fr}}{\Gamma_r} \psi(\theta, x) \ , \tag{5}$$

$$\mathrm{A} = \cos 2\phi_l - (1 - \frac{\Gamma_{nr}}{\Gamma_r}) + \frac{\mathrm{G}_{rl}}{\Gamma_{nr}} \ , \tag{6}$$

$$B = \cos 2\phi_l - (1 - \frac{\Gamma_{nr}}{\Gamma_r}) + \frac{\mathrm{G}_{rl}}{\Gamma_{nr}} \ , \tag{7}$$

where r is the resolved resonance index, l is the angular momentum, Γ_r, $\Gamma_{\gamma r}$, Γ_{fr} and Γ_{nr} are the total, capture, fission, and neutron widths, respectively, g_J is the spin statistical factor, ϕ_l is the phase shift, and k is the neutron wave number. The parameters x and θ are defined as:

$$x = \frac{2(E - E_r)}{\Gamma_r} \ , \tag{8}$$

$$\theta = \frac{\Gamma_r}{\sqrt{\frac{4k_b TE}{A}}} \ , \tag{9}$$

where E and E_r are energy point and resonance peak energy point, respectively; k_b is the Boltzmann constant; T is absolute temperature; A is atomic weight ratio to the neutron for the given isotope.

Elastic scattering interference parameters can be found in the following way:

$$G_{rl} = \frac{1}{2} \sum_{r \neq r'} \frac{\Gamma_{nr} \Gamma_{nr'} (\Gamma_r + \Gamma_{r'})}{(\mathrm{E}_r - \mathrm{E}_{r'})^2 + \frac{1}{4} (\Gamma_r + \Gamma_{r'})^2} \ , \tag{10}$$

$$H_{rl} = \frac{1}{2}\sum_{r\neq r'} \frac{\Gamma_{nr}\Gamma_{nr'}(\mathrm{E}_r - \mathrm{E}_{r'})}{(\mathrm{E}_r - \mathrm{E}_{r'})^2 + \frac{1}{4}(\Gamma_r + \Gamma_{r'})^2} \ . \qquad (11)$$

Eqs. (1) to (9) are given in the NJOY2012 manual book [1], but the fission cross section Eq. (5) should be improved in order to consider the interference effect in ^{238}U. This modification was done by Hideki Takano (September 1977) [2]:

$$\sigma_f = \sum_l \sum_r \sigma_{mr}\{(\frac{\Gamma_{fr}}{\Gamma_r} + \frac{u_{fr}}{\Gamma_{nr}})\psi(\theta,x) + \frac{v_{fr}}{\Gamma_{nr}}\chi(\theta,x)\} \ , (12)$$

with fission interference parameters:

$$u_{fr} = \frac{1}{2}\sum_{r\neq r'} \frac{\sqrt{\Gamma_{nr}\Gamma_{nr'}}\,\mathrm{G}^f_{rr'}(\Gamma_r - \Gamma_{r'})}{(\mathrm{E}_r - \mathrm{E}_{r'})^2 + \frac{1}{4}(\Gamma_r - \Gamma_{r'})^2} \ , \qquad (13)$$

$$v_{fr} = \sum_{r\neq r'} \frac{\sqrt{\Gamma_{nr}\Gamma_{nr'}}\,\mathrm{G}^f_{rr'}(\mathrm{E}_r - \mathrm{E}_{r'})}{(\mathrm{E}_r - \mathrm{E}_{r'})^2 + \frac{1}{4}(\Gamma_r - \Gamma_{r'})^2} \ , \qquad (14)$$

where $G^f_{rr'} = \sqrt{\Gamma_{f1r}\Gamma_{f1r'}} + \sqrt{\Gamma_{f2r}\Gamma_{f2r'}}$

The $\psi - \chi$ terms used for the Doppler Broadening of the resonance cross section will be described in the next subsection.

It can be easily understood that the resonance method requires large computational time, because there is a double sum over resonances at every energy point.

2.2 $\psi - \chi$ Doppler Broadening Method

This method makes it possible to directly generate the broadened cross section from resonance parameters given in the ENDF/B-VII.0 data file of ^{238}U. However, in the NJOY2012 code, the resonance cross section of the given material is produced by Reich-Moore formalism which does not support the $\psi - \chi$ broadening method. Therefore, a 0 K cross section should be produced at first, and only then Doppler broadening can be performed. $\psi(\theta,x)$ and $\chi(\theta,x)$ are the actual line shape functions, which are defined in Eq. (15) and (16):

$$\psi(\theta,x) = \frac{\sqrt{\pi}}{2}\,\mathrm{Re}(\mathrm{W}(\frac{\theta x}{2}, \frac{\theta}{2})) \ , \qquad (15)$$

$$\chi(\theta,x) = \frac{\sqrt{\pi}}{2}\,\mathrm{Im}(\mathrm{W}(\frac{\theta x}{2}, \frac{\theta}{2})) \ , \qquad (16)$$

$$\mathrm{W}(\frac{\theta x}{2}, \frac{\theta}{2}) = e^{-z^2} erfc(-iz) = \frac{i}{\pi}\int_{-\infty}^{\infty} \frac{e^{-t^2}}{z-t}\,dt \ , (17)$$

$$z = x + iy \ . \qquad (18)$$

Eq. (17) illustrates the Complex Probability Function, which plays a key role in broadening of the resonance cross section. From Eqs. (15) and (16) it is clear that ψ and χ are just real and imaginary parts of the Complex Probability Function, respectively.

Table. 1. 0 K cross section and 1200 K cross section generation computational time using conventional MLBW formalism

Temperature (K)	Computational time (sec)
0	41.05
1200	42.45

From Table 1 it can be seen that the Doppler broadening computational time is very small (around 1.40 sec) in contrast to cross section generation computational time. However, it is still a large amount of time just for broadening of one energy point.

2.3 Energy Window Concept

The total number of resolved resonances for the given isotope is 3343, where there are 926 s-wave and 2417 p-wave resonances.

According to the conventional Doppler broadening used in the MLBW formalism, at every single energy point all existing s- and p-wave resonances of ^{238}U should be broadened.

On the other hand, the energy window concept is based on the fact that every separate resonance (no matter s- or p-wave) is a smooth function far from its peak. In Figs. 1 and 2, which separately show the generated s- and p-wave capture resonance cross sections in the energy range of the 1st resonance, it can be easily observed that resonances are smooth and have relatively low cross section values in contrast to the dominating resonance. Through Figs. 1 to 4 point-line functions represent the remaining resonances.

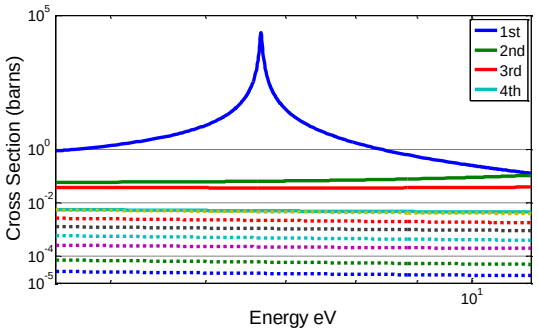

Fig.1. First 11 s-wave resonances in capture reaction.

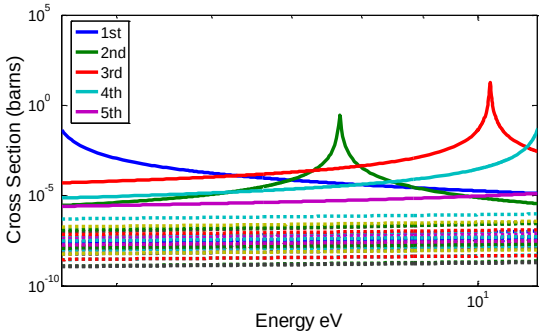

Fig.2. First 40 p-wave resonances in capture reaction.

Another important step is to check the relative difference with respect to temperature change for every resonance that has a big impact on the final capture cross section. The results of relative difference calculations can be well observed from Figs. 3 and 4:

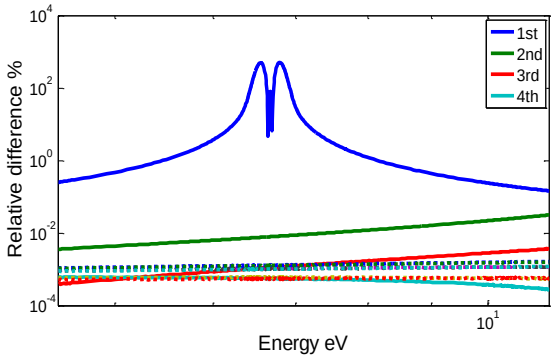

Fig.3. Relative error between 7 s-wave resonance cross sections at 0 K and 1200 K.

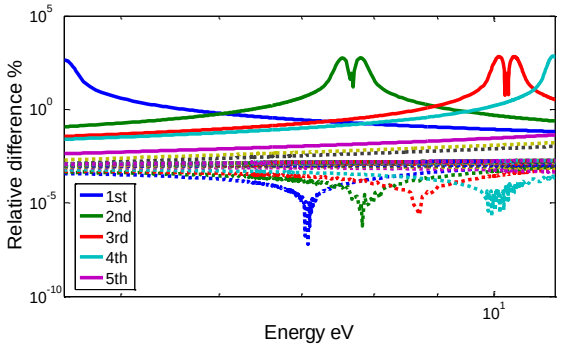

Fig.4. Relative error between 40 p-wave resonance cross sections at 0 K and 1200 K.

From the relative differences for every s- and p-wave resonance between 4.5 and 11.2 eV, it was observed that only a few resonances, which are close to the target energy range, vary with regard to temperature variations.

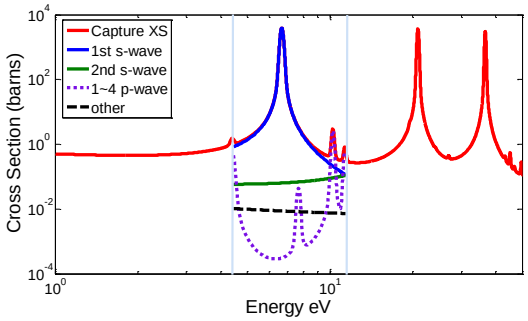

Fig.5. Energy window for capture cross section.

In Fig. 5. the sum of all other resonances far from the given energy range has very little change with respect to temperature or has a relatively small cross section value. The cross sections of other resonances at 1200 K can be replaced by 0 K generated cross sections, for the reasons mentioned above. Conventional MLBW Doppler broadening is not efficient because of broadening of resonances which are located at relatively higher energies and have no crucial impact at lower energies with respect to temperature change. Therefore, the energy window concept is suggested as an alternative to the conventional Doppler broadening method.

A case was tested in such a way that 7 s-wave and 40 p-wave consecutive resonances were broadened in the energy region of the 1st resonance at 1200 K.

Figs. 6 to 9 illustrate the 1st resonance energy interval (4.5~11.2 eV) where the total, capture, elastic scattering, and fission cross sections were broadened by the energy window applied Multi-level Breit-Wigner approach, and compared with the corresponding cross sections generated by the conventional MLBW.

The relative difference between reference and EW MLBW according to every reaction type is shown in Fig. 10. The maximum relative error among fission, capture, elastic scattering, and total cross sections is less than 0.0016 %.

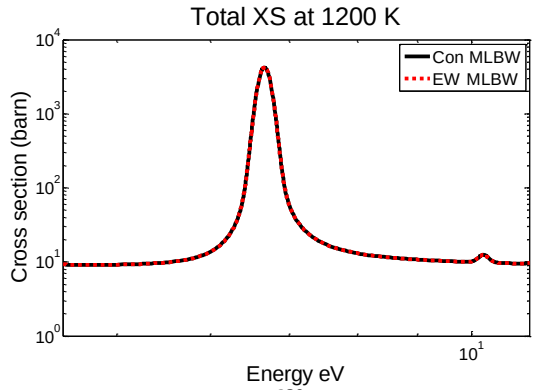

Fig. 6. Total cross section of ^{238}U at 1200 K generated by EW MLBW.

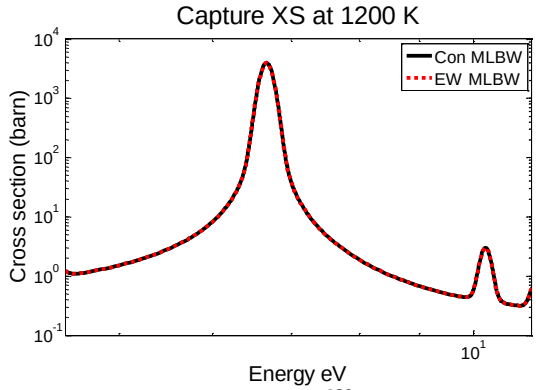

Fig. 7. Capture cross section of ^{238}U at 1200 K generated by EW MLBW.

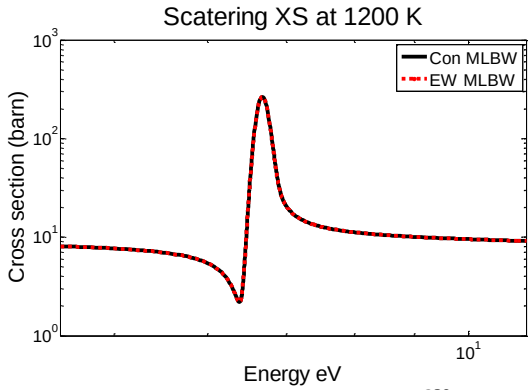

Fig. 8. Elastic Scattering cross section of ^{238}U at 1200 K generated by EW MLBW.

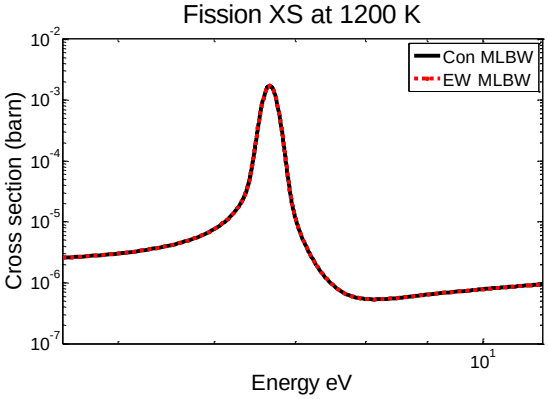

Fig. 9. Fission cross section of ^{238}U at 1200 K generated by EW MLBW.

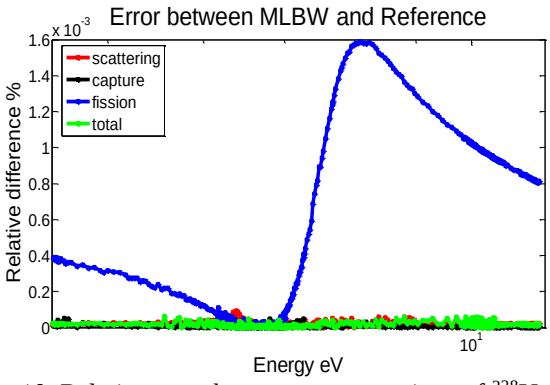

Fig. 10. Relative error between cross sections of ^{238}U at 1200 K generated by EW MLBW and conventional MLBW.

The computational time comparison between conventional MLBW and energy window applied MLBW Doppler broadenings for the given case was done and the result is shown below:

Table. 2. Computation time for Doppler broadening at single energy point by using conventional MLBW and EW MLBW at 1200 K.

Method	**Computation Time (sec)**	**Improvement (%)**
Con MLBW	1.40	-
EW MLBW	0.79	43.57

Doppler broadening using $\psi - \chi$ does not take much time in contrast to generation of cross sections as shown in the previous subsection; however, there is a good improvement in case of just 7 s-wave and 40 p-wave resonances broadening, which is slightly bigger than 43 %.

3. Conclusions

Multi-level Breit-Wigner formalism and the $\psi - \chi$ Doppler broadening method were used to construct microscopic cross sections of ^{238}U at different temperatures. The energy window concept was applied only for the 1st resonance energy region (4.5~11.2 eV). The cross sections generated by both methods in this energy range were compared with each other.

The energy window concept demonstrates high competitiveness because the relative differences were less than 0.0016% for all types of cross sections.

The advantage of the energy window concept is that the number of resonances broadened for every energy point is significantly reduced, which allows a reduction of computation time by almost 45 % of Doppler broadening time of the cross section generation at temperatures higher than 0 K.

ACKNOWLEDGEMENTS

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