Calculation of the cross sections of the formation of nuclei in isomeric states in reactions with neutrons

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Abstract

An analysis of reliability of existing experimental (EXFOR database) and evaluated (TENDL-2021 and IRDFF-II libraries) cross section data for $(n, 2n)$, $(n, n'\gamma)$ and (n, p) reactions initiated by neutrons with energies up to 20 MeV with the formation of ^{114,115}In and ^{91}Y isotopes in isomeric metastable states is performed. This examination is motivated by the results of recently carried out measurements at the National Research Centre "Kurchatov Institute" with neutrons with energies close to 14 MeV: these data are important for designing facilities suitable for controlled thermonuclear fusion. An independent method based on TALYS-1.9 software package calculations using parameters provided in RIPL-3 library for evaluating both the cross sections of mentioned reactions and the errors for such evaluations is proposed. Implemented error of the cross section evaluation allows for realistic conclusions about the reliability of data obtained in various experiments to be drawn.

Motivation

When designing facilities suitable for controlled thermonuclear deuterium-tritium fusion reaction with the formation of neutrons with an energy of 14.1 MeV it is important to take into account reactions leading to the formation of nuclei in metastable (isomeric) states. They decay with the emission of high-energy γ rays. Recent NRC "Kurchatov Institute" measurements [1] include such reactions as $^{115}\mathrm{In}(n, 2n)^{114m}\mathrm{In}$, $^{115}\mathrm{In}(n, n'\gamma)^{115m}\mathrm{In}$, $^{91}\mathrm{Zr}(n, p)^{91m}\mathrm{Y}$, and some more. Latest libraries (IRDFF-II, JEFF-3.3, JENDL-5.0, ENDF/B-VIII.0, FENDL-3.0) provide sparse information regarding the cross sections of nucleus formation in isomeric states for incident neutrons with energies near 14 MeV.

Significant progress has been made in the field of numerical simulation of nuclear reactions. RIPL-3 [2] provides a standard collection of input parameters for nuclear models utilised in software packages. Among the programs utilising them is TALYS-1.9, an open-source software package [3]. Evidently, there is a need to analyse the reliability of data related to the formation of isomeric nuclei in neutron reactions. We consider the potential of utilising TALYS-1.9 for this analysis. Using only recommended RIPL-3 parameters we compare experimentally obtained data [4], NRC "Kurchatov Institute" measurements, reliable estimated data (IRDFF-II [5] and TENDL-2021 [6] libraries) to our own TALYS-1.9 calculations.

Analysis Method

TALYS-1.9 calculations are highly sensitive to the chosen model of density of excited levels: Composite Gilbert-Cameron Model [7] — "Model 1"; The Back-shifted Fermi gas Model [8] — "Model 2"; Generalised Superfluid Model [9, 10] — "Model 3". None of the three models has advantages over the others.

However, if we consider the arithmetic mean

$$\sigma_{avg}(E) = \frac{\sigma_1(E) + \sigma_2(E) + \sigma_3(E)}{3} \qquad (1)$$

with the suggested error of

$$\Delta\sigma_{avg}(E) = \max\{\epsilon_{12}(E), \epsilon_{23}(E), \epsilon_{31}(E)\}, \qquad (2)$$

where $\epsilon_{ij}(E) = \left|\sigma_i(E) - \sigma_j(E)\right|$, then the corridor between $\sigma_{min} = \sigma_{avg} - \Delta\sigma_{avg}$ and $\sigma_{max} = \sigma_{avg} + \Delta\sigma_{avg}$ determines the region in which the true cross section is located with high probability. For the three presented reactions ~65% of experimental data on average is contained within the proposed cross section region in the energy range of 14-15 MeV.

Results and Discussion

Fig. 1 depicts experimental data and evaluations for the $^{115}\mathrm{In}(n, 2n)^{114m}\mathrm{In}$ reaction. Near the energy of 14 MeV the cross section $\sigma_{\text{IRDFF-II}}(E)$ lies above the majority of experimental data points. On the other hand, most of the experimental data points are distributed uniformly within the corridor between $\sigma_{min}(E)$ and $\sigma_{max}(E)$. The calculated average cross section is located at the centre of the corridor. Therefore, as an estimate for the cross section of isomer formation, $\sigma_{avg}(E)$ is superior to $\sigma_{\text{IRDFF-II}}(E)$.

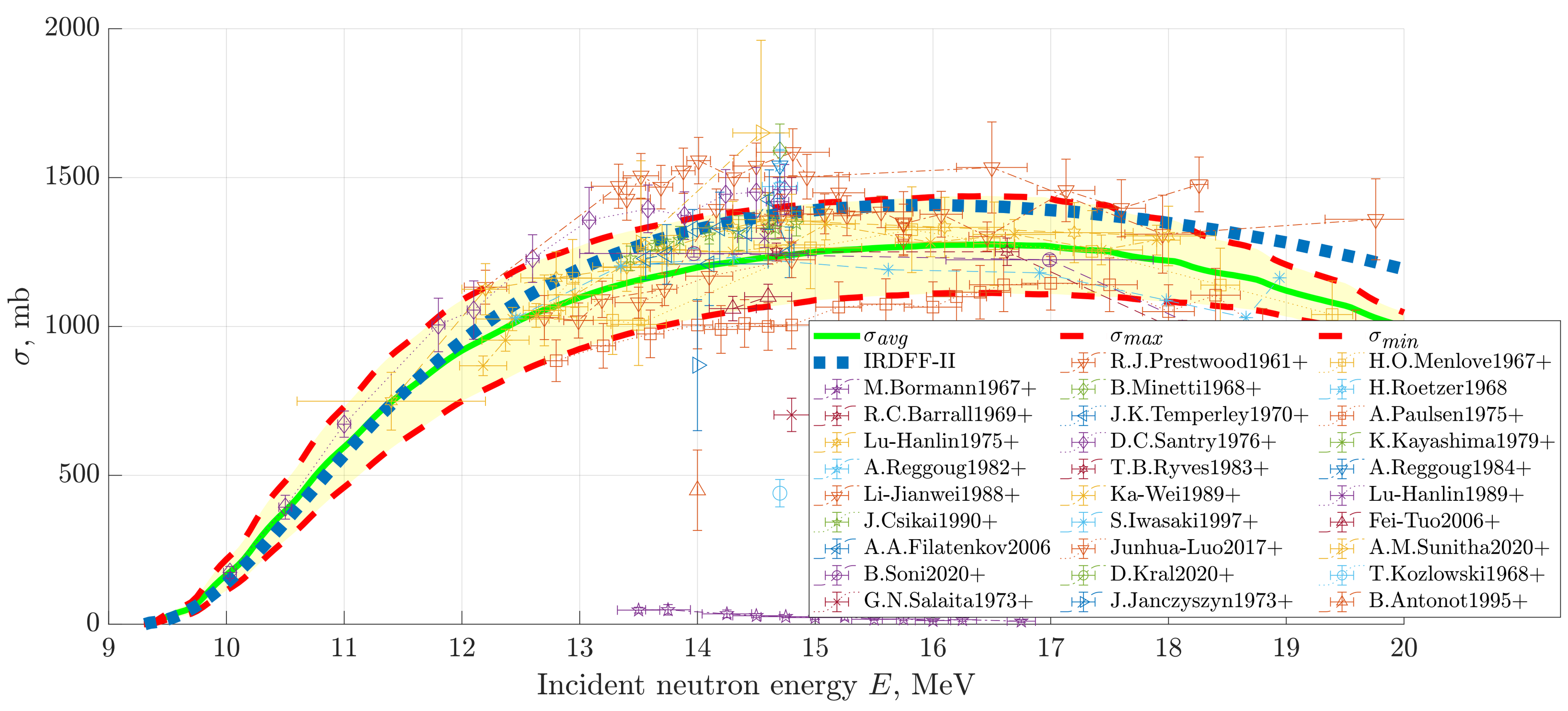

Figure 1. Cross section of isomeric (m) state in the $^{115}\mathrm{In}(n, 2n)^{114m}\mathrm{In}$ reaction as a function of incident neutron energy. TENDL-2021 graph is absent as it coincides with the corresponding IRDFF-II graph.

Fig. 2 depicts corresponding graphs for the $^{115}\mathrm{In}(n, n'\gamma)^{114m}\mathrm{In}$ reaction. Notably, both TALYS-1.9 and IRDFF-II (or TENDL-2021) estimates in the 14–15 MeV range align well with the EXFOR library's experimental data.

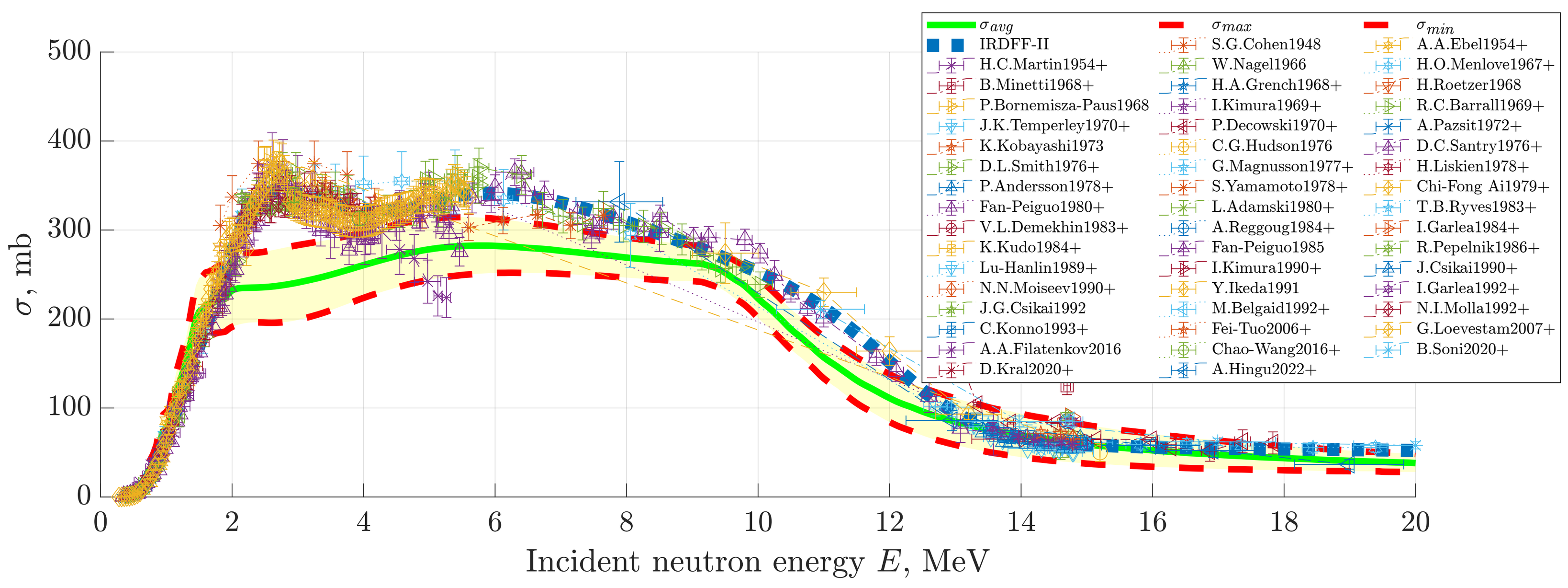

Figure 2. Cross section of isomeric (m) state in the $^{115}\mathrm{In}(n, n'\gamma)^{115m}\mathrm{In}$ reaction as a function of incident neutron energy. TENDL-2021 graph is absent for the same reason as in Fig. 1.

Finally, Fig. 3 depicts corresponding graphs for the $^{91}\mathrm{Zr}(n, p)^{91m}\mathrm{Y}$ reaction. In the energy range of 14–15 MeV, which is of our interest, we find that the calculated average cross section $\sigma_{avg}(E)$ correlates with experimentally available data better than the corresponding $\sigma_{\text{TENDL-2021}}(E)$.

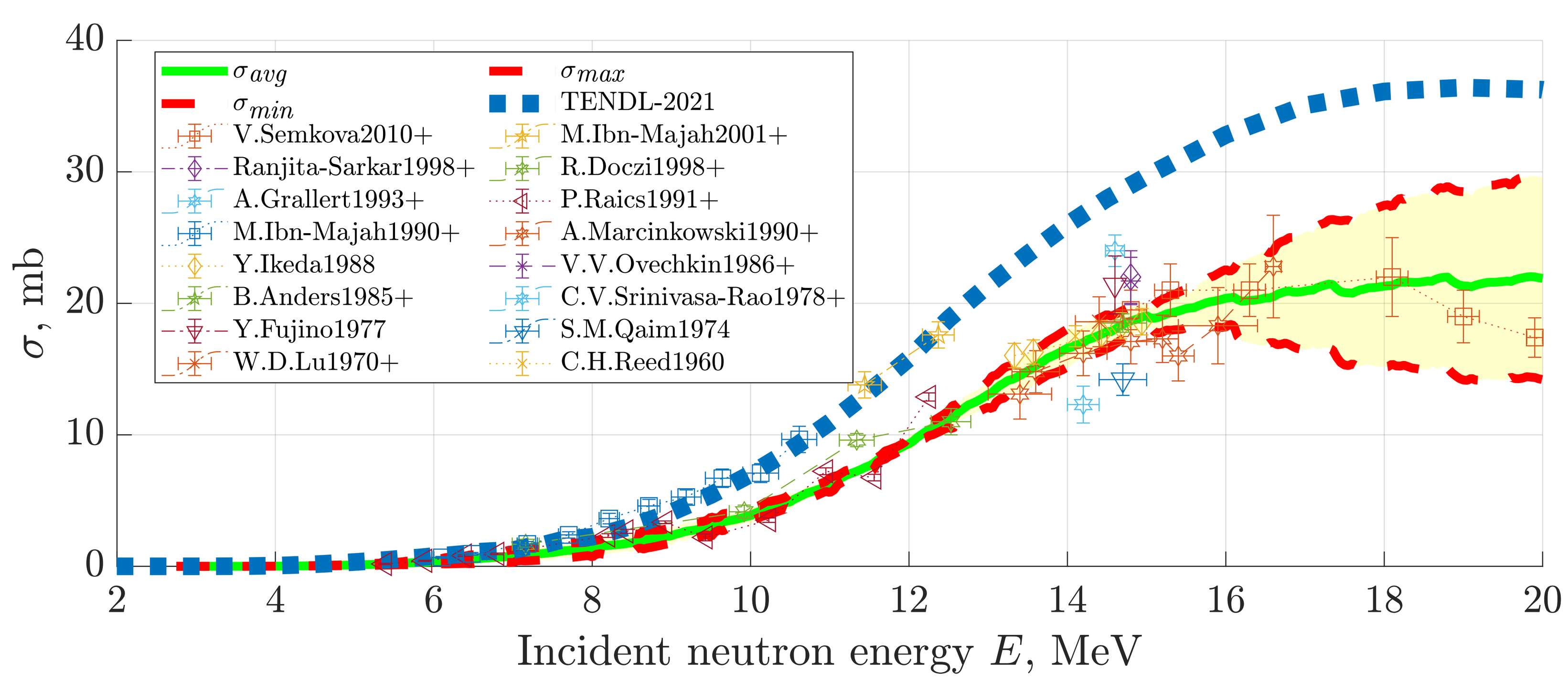

Figure 3. Cross section of isomeric (m) state in the $^{91}\mathrm{Zr}(n, p)^{91m}\mathrm{Y}$ reaction as a function of incident neutron energy. No IRDFF-II data are available for this reaction.

Conclusion

We analysed three particular neutron reactions that result in the creation of metastable nuclei in isomeric states. Our aim was to determine the reliability of estimates for the associated cross sections. We demonstrated that available experimental data, as well as IRDFF-II (and/or TENDL-2021) estimates are reproduced within "reasonable accuracy" by means of TALYS-1.9 software package calculations relying solely on recommended RIPL-3 parameters. The implemented error (which is interpreted as a theoretical uncertainty) $\Delta\sigma_{avg}(E)$ can serve as a quantitative assessment of said "reasonable accuracy" of cross sections obtained as a result of calculations with TALYS-1.9.

Therefore, we conclude that in certain cases TALYS-1.9 package could be utilised as a cross section predictive tool, using only suggested level density models and default parameters with no fitting parameters needed.

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