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New evaluations of n + Cu and n + Zr cross-section data for neutron energies up to 200 MeV

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Abstract. This work presents evaluated general purpose nuclear data files for the n+^{63,65}Cu and n+^{90,91,92,94,96}Zr reactions for neutron energies up to 200 MeV. The TALYS-1.8 code was used for the nuclear model simulations in the energy range from 1 keV to 200 MeV. To improve the pre-equilibrium particle emission the Geometry-Dependent Hybrid model (GDH) was used as option implemented in an extended version of the code as option. Resonance data based on recent measurements and their covariances were included in the files. A set of covariance data for all nuclear reactions was also prepared and included in the evaluations. The adjustments of the nuclear model parameters were performed to fit both available differential and integral measured data. The evaluated data were carefully checked against the latest fusion relevant integral measurements.

1. Introduction

In the framework of the European fusion programme nuclear data evaluations are performed to enable qualified particle transport calculations of fusion devices such as ITER and DEMO. The improvement of the nuclear data base is an important element of quality assured analyses for the design and optimisation of these facilities and related neutron sources like IFMIF (International Fusion Materials Irradiation Facility) or DONES (DEmo Oriented NEutron Source).

The available nuclear data evaluations for the stable Cu isotopes included in the JEFF-3.2 library show some deficiencies as revealed in the analyses of a 14-MeV neutron benchmark experiment conducted at the Frascati Neutron Generator (FNG) on copper [1]. The available nuclear data evaluations for stable ^{90,91,92,94,96}Zr isotopes are not as consistent as required for accurate activation and particle transport calculations. Therefore n+Zr data were newly evaluated. Consistent evaluated data sets are of high priority for applications to ITER, DEMO and IFMIF/DONES with quality assured design, optimisation and performance analyses. As a common requirement to the new evaluated data files they must include all information required for a variety of nuclear analyses including high energy particle transport simulations of neutrons and photons as well as the assessment of the nuclear radiation damage and gas production.

2. Nuclear models and computer codes

The nuclear model simulations of the n+^{63,65}Cu and n+^{90,91,92,94,96}Zr interactions were performed with the TALYS-1.8 code [2] for the neutron energies from 1 keV up to 200 MeV. The performed pre-analyses for the n+Cu and n+Zr reactions demonstrate the necessity of an accurate adjustment of the TALYS nuclear model parameters to fit available experimental data. In spite of TALYS' high predictive power, additional specific improvements can be reached by using in the TALYS calculations an extra model for the pre-equilibrium reactions description, Geometry Dependent Hybrid model (GDH) [3]. This model was implemented in the extended version of TALYS. With the GDH model included, TALYS-1.8 gives more precise results for n+Cu reactions compared to the original version. The GDH model is called in the calculations by using the keyword *preeqmode* 5. The nuclear level density was described with a back-shifted Fermi gas model [4] (*ldmodel* 2).

All optical model calculations for neutrons and protons were performed using TALYS built-in Optical Model Potentials (OMPs). In case of other charged particles the external global OMPs of Ref. [5,6] were used for deuterons and alphas, respectively. For tritons and helions, new OMPs were elaborated using a large experimental data base and available OMPs for some target nuclides [7]. The parameters of the global OMPs for charged particles except proton were separately prepared and used in the TALYS calculations invoking *optmod* option. For all OMPs the same incident energy range from keVs up to 200 MeV was used to keep continuity and consistency of the evaluated data. All uncertainties arising in the evaluations due to the adjustment procedure of the reaction cross sections are accounted for in the elastic scattering cross section, thus keeping the total cross section unchanged.

3. Nuclear data evaluations

3.1. Resonance data

The resonance data evaluated at Oak Ridge National Laboratory for n+^{63,65}Cu reactions [8] were adopted. New low energy measurements for the total cross sections and for the neutron transmission (energy range 0.01 eV–0.1eV) were used for the resonance parameter

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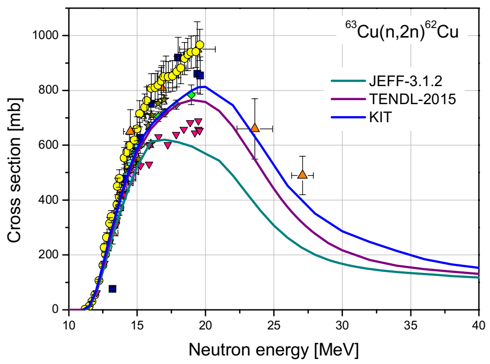

Figure 1. Evaluated ^{63}Cu(n,2n)^{62}Cu cross section.

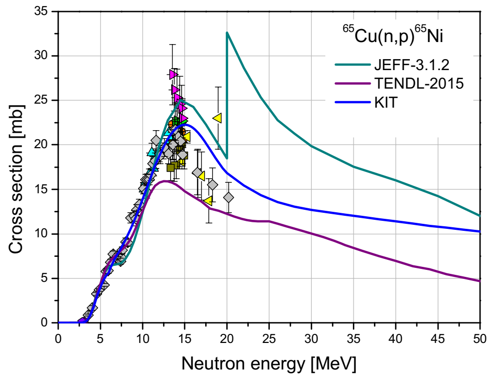

Figure 2. Evaluated ^{65}Cu(n,p)^{65}Ni cross section.

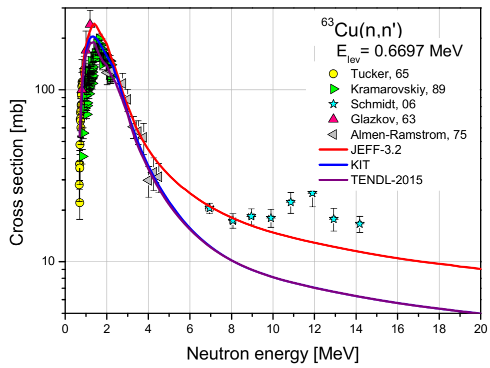

Figure 3. Evaluated ^{63}Cu(n,n′) cross section.

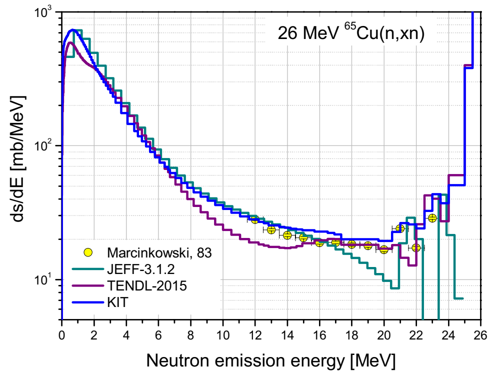

Figure 4. Evaluated neutron emission spectra for n+$^{nat.}$Cu at 26 MeV.

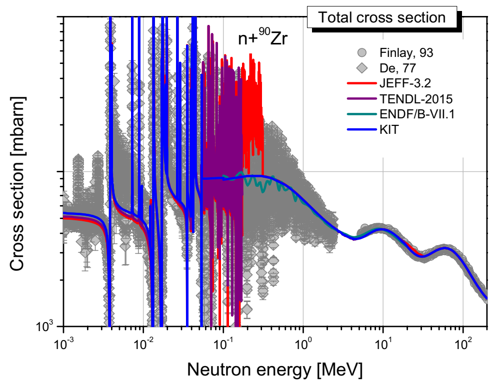

Figure 5. Evaluated total cross section for the n+^{90}Zr.

evaluation. Also the available experimental data for higher energies were accounted for the calculations of the new resonance parameters and their co-variances. For both Cu nuclei the resonance region was set from 10^{-5} eV to 300 keV. For n+^{90,91,92,94,96}Zr reactions the resonance data for resolved and unresolved regions were taken from the available ENDF/B-VII.1 evaluations.

3.2. 3.2 n+Cu nuclear data evaluation

The procedure applied for the nuclear data evaluation is based on a consistent approach to an optimal fit of the experimental data. The nuclear model parameters were adjusted stepwise resulting in an optimal set [9].

Shown in Figs. 1 and 2 are the newly evaluated ^{63}Cu(n,2n) and ^{65}Cu(n,p) cross sections compared to the measured and other evaluated data. The present results are the re-evaluations of the n+Cu data included in the JEFF-3.2 library due to some deficiencies found. Great attention was paid to the evaluation of the inelastic scattering cross sections for all excitation states of the ^{63,65}Cu. The previous n+Cu evaluation for (n,n’) reactions from JEFF-3.2 was based on latest measured data [10] that cannot be reproduced by any nuclear model simulations, Fig. 3.

The equilibrium part of the particle emission spectra is calculated in TALYS in the framework of the multiple Hauser-Feshbach statistical model [2]. With the new GDH option the calculated pre-equilibrium particle emission spectra fit much better the experimental data compared to the original TALYS-1.80 results included in TENDL-2015, Fig. 4.

3.3. n+Zr nuclear data evaluation

For the evaluation of the n+Zr nuclear data a special care was given to the evaluation of the exclusive reaction cross sections where sufficient experimental data exist. In Fig. 5 the evaluated total cross section for the n+^{90}Zr based on the optical model calculations is presented and compared to the available low and high energy experimental data. The newly produced data fit very well high energy experimental results. The representations of the resonance region are different in all libraries. Shown in the Fig. 6 are results of the evaluation for the neutron inelastic scattering (n,n’) for the 2nd excited state of the ^{91}Zr. The present results are close to the TENDL-2015 ones but they are quite different from the ENDF/B-VII.1 data.

Examples of the evaluated exclusive (n,2n), (n,p) and (n,α) cross sections are given in Figs. 7–10. The new evaluated results account for the latest measured data and

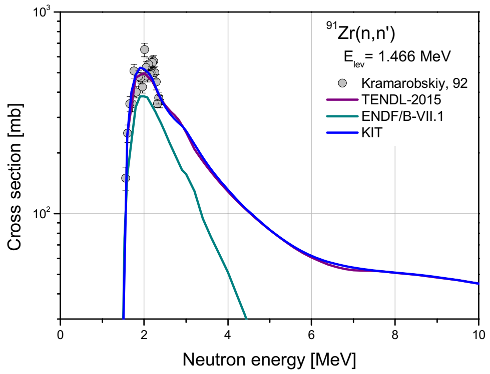

Figure 6. The evaluated (n,n′) cross section for the 2nd excited level of the ^{91}Zr.

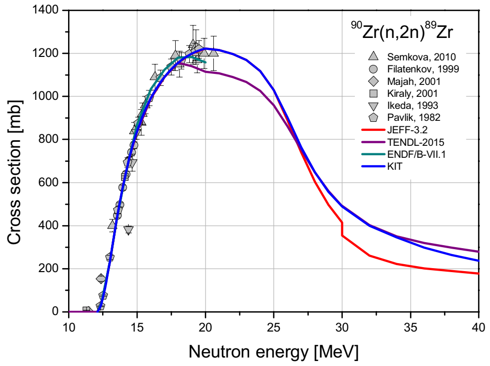

Figure 7. Evaluated ^{90}Zr(n,2n) cross section.

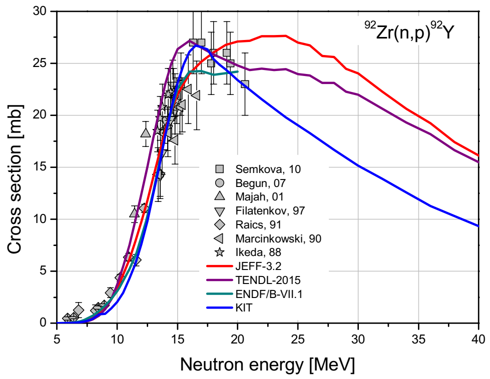

Figure 8. Evaluated ^{92}Zr(n,p) cross section.

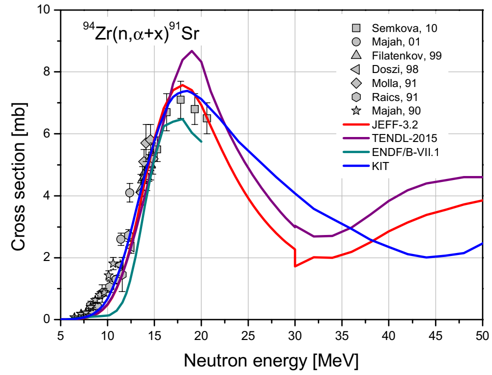

Figure 9. Evaluated ^{94}Zr(n,α+x) cross section.

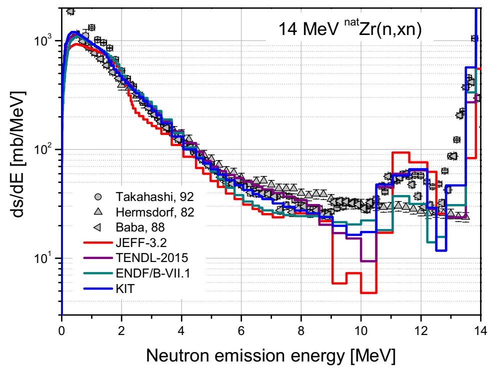

Figure 10. Neutron emission spectrum for Zr with incident neutrons of 14 MeV.

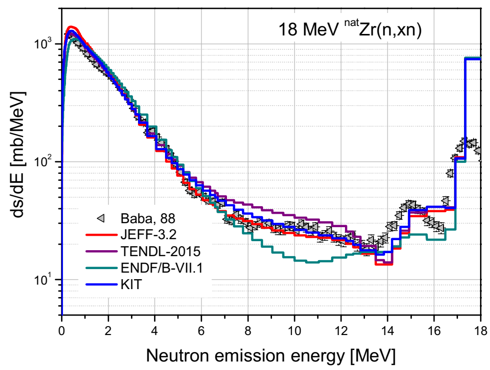

Figure 11. Neutron emission spectrum for Zr with incident neutrons of 18 MeV.

show a good agreement with the available experimental data below 20 MeV compared to other evaluations. The inclusion of the GDH model in the TALYS simulations improves the description of the pre-equilibrium neutron emission spectra, as shown in Figs. 10, 11. The peaks in the spectra due to collective excitations are reproduced also well.

4. Benchmark calculations

The nuclear data evaluation procedure utilizes multi-faceted tests of the results using both formal checkers for the correctness of the data and benchmark analyses of integral experiments to check the data quality in application calculations. The newly evaluated Cu data was tested against the integral benchmark experiment performed at FNG on a copper assembly including measurements of specific reaction rates, neutron and photon flux spectra. Neutron induced reaction rates, neutron and photon spectra were measured at several positions inside the massive copper block. Shown in the Figs. 12 and 13 are the C/E ratios for ^{27}Al(n,α) rate and a neutron spectrum at ∼17 cm in the Cu block.

The results obtained with the revised ^{63,65}Cu evaluation demonstrate better agreement with the measured data as compared with the previous evaluation included in the JEFF-3.2 release. The main differences come from the re-evaluated inelastic scattering data for all excitation levels of ^{63,65}Cu, Fig. 3.

5. Calculations of the data covariances

The inclusion of covariance data in the general purpose evaluated data files is a general requirement to the candidates to be included in the international nuclear

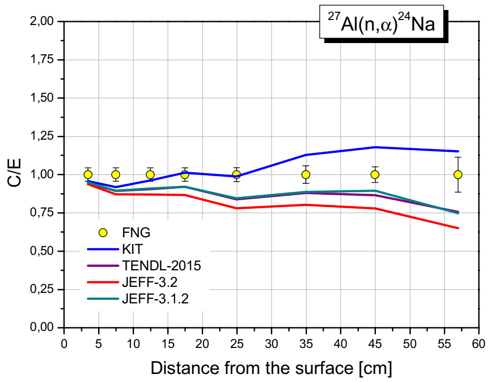

Figure 12. C/E for ^{27}Al(n,α) reaction rate.

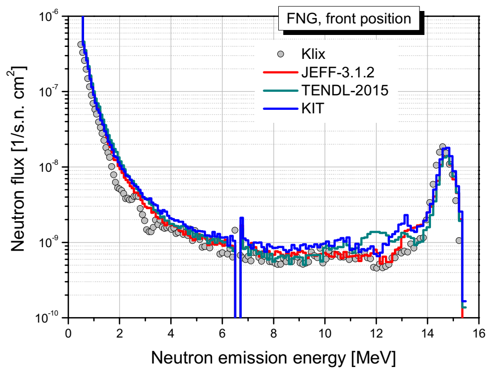

Figure 13. Neutron emission spectra.

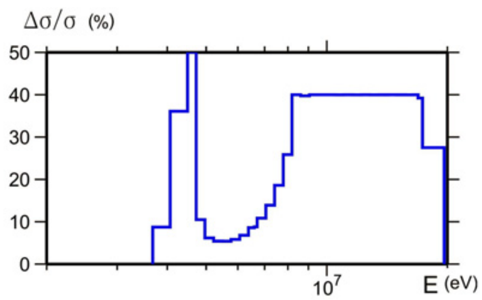

Figure 14. The evaluated variances for the ^{92}Zr(n,p) cross section.

data libraries. In the present work, the co-variances were prepared by making use of the BEKED system [11] and the modified TALYS-1.8 codes. A Monte Carlo approach for calculations of the covariance matrices for the cross-sections is applied in the BEKED code for the random sampling of the nuclear model parameters. Typically the optical model parameters, deformation parameters for coupled channels calculations and nuclear level density parameters are sampled to get the nuclear models responses. With this method experimental uncertainties are also taken into account in the calculations of the final evaluated nuclear data covariances. The Monte Carlo samplings are performed until the deviation of the final results for two sequential runs becomes negligible. The example of the evaluated variances for the ^{92}Zr(n,p) cross section (Fig. 8) is shown in the Fig. 14.

6. Evaluated data files

For the present evaluation, we adopted the following structure of the data files: below 20 MeV of the neutron incident energy the full detailed information for all open reaction channels is given and above 20 MeV we present total and elastic scattering cross sections as well as particle emission spectra, total cross sections for the residuals production and their recoil spectra.

7. Conclusions

Within the European fusion program new data evaluations were performed for the n+Cu and n+Zr nuclear reactions in the energy range from 10^{-5} eV to 200 MeV. The data for n+Cu were revised taking into account the results of the benchmark analyses on an integral 14 MeV neutron experiment. The nuclear model calculations were performed with a suitably modified version of the TALYS-1.8 code. The new data files enable full particle transport and nuclear damage calculations in the whole energy range. Co-variance data are also included in the evaluated data files to enable uncertainty analyses in fusion neutronics calculations.

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