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EVALUATION AND VALIDATION OF ^{28,29,30}SI CROSS SECTIONS IN THE RESOLVED RESONANCE REGION

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ACRONYMS

BFS	Big Physical Stand
ENDF	Evaluated Nuclear Data File
IAEA	International Atomic Energy Agency
ICSBEP	International Criticality Safety Benchmark Evaluation Project
NSNFP	National Spent Nuclear Fuel Program
ORNL	Oak Ridge National Laboratory
RRR	resolved resonance region

ABSTRACT

Resonance parameter evaluations of the three stable silicon isotopes $^{28,29,30}Si$, were performed at Oak Ridge National Laboratory in 2002 and the results of those evaluations were restored from the archives in 2018. The evaluations also accounted for the contribution of the direct component of the capture cross sections computed over the neutron resonance range. For the most abundant isotope, ^{28}Si, the value of the thermal capture cross sections was increased by 10% on the basis of analyses devoted to reevaluating the thermal radiative neutron capture cross sections. The contribution of the direct capture cross sections was recomputed for each isotope, and its energy-dependent behavior improved. Results of benchmark calculations performed at the International Atomic Energy Agency showed an excellent agreement with integral measurements.

1. BACKGROUND

In the newly released Evaluated Nuclear Data File (ENDF)/B-VIII.0 library (2018), the ^{28,29,30}Si capture and elastic cross sections for incident neutron energies up to 150 MeV were adopted from the ENDF/B-VII.1 nuclear data library (2011), which, in turn, adopted the evaluated data from previous releases of the ENDF/B library. In the neutron energy range up to 20 MeV, the set of evaluations was performed by Hetrick [1]. The corresponding resonance parameter evaluations ranged from thermal up to 1.5–2 MeV but did not account for the description of the direct neutron component contribution of the capture cross sections.

In 2001 Oak Ridge National Laboratory (ORNL) performed neutron capture cross-section experiments on light nuclei [2] in response to a request from the Nuclear Criticality Safety Program. For light nuclei the direct capture component represents a nonnegligible part of the neutron capture cross section. Thus, in the subsequent resonance analysis of the data, for the first time, the direct capture component was included using the R-Matrix code SAMMY [3]. In 2002, before the release of the ENDF/B-VII.0 (2006) nuclear data library, ORNL released and submitted to the ENDF repository a set of silicon evaluations [4] in the resolved resonance region (RRR). This evaluation accounted for the description of the direct capture component calculated by the TEDCA code [5] and included in the fitting procedure the capture cross sections of natural silicon measured at Oak Ridge Electron Linear Accelerator [2] in the energy range 1 to 700 keV. The SAMMY recipe was followed to guarantee the unitary condition on the calculated cross sections. The total capture cross sections, obtained as the sum of the direct component and the compound component, were obtained by determining the difference of the total cross sections and reaction cross sections.

We believe that the resonance parameter evaluations were never included in the ENDF/B-VII.0 release because of the difficulty, at that time, to process ENDF files containing direct neutron capture contributions.

2. DISCUSSION OF THE UPDATES

In the present work, the updates to the set of ORNL silicon evaluations released in 2002 were focused on the ^{28,29,30}Si capture cross sections in the thermal energy range and the related direct capture contributions. Particularly for ^{28}Si(n_{th},γ) evaluation, the capture cross section has always been controversial due to the discrepant values found in the experimental database. As shown in Table 1, measurements performed in the early nineties by Kennett [6] and Raman [7] are discrepant by almost 40 mb with respect to a previous measurement performed by Islam [8]. Raman and Kennett briefly explained this discrepancy due to stoichiometry problems in Islam's measurement. Further analyses devoted to reevaluating the thermal radiative neutron capture cross sections [9] for a large set of nuclides adopted a value of 186 mb for the ^{28}Si(n_{th},γ) cross section.

The present work produced two sets of silicon evaluations, namely ORNL (2018[1]) and ORNL (2018[2]). The first set of evaluations modified the existent direct component of the ^{28}Si capture cross sections by decreasing it 20% up to 1.5 MeV (as shown in Fig. 1), and, at the same time, the capture width parameters Γ_γ of the bound levels were fitted to obtain a value of ^{28}Si(n_{th},γ) cross section of 184.5 mb. Since, at thermal energies, the elastic scattering cross section of ^{28}Si (about 1.89 b) is considerably bigger than the capture cross section, the capture resonance widths could be varied with no impact on the elastic channel. The reconstructed capture cross sections in the neutron energy range up to 1.75 MeV plotted in Fig. 4 show

Table 1. Measured and evaluated ^{28}Si(n_{th},γ) cross sections (in mb). The direct and resonance component to the total capture cross section is shown when possible.

Author (Year)	Value (mb)	σ_γ(res)	σ_γ(dir)
Islam (1990)	207±4		
Kennett (1992)	171±3		
Raman (1992)	169±4	34.9$^{(a)}$	134.1$^{(b)}$
Mughabghab (2006) [10]	177±4	45$^{(a)}$	132
ORNL (2002)	168.9	103.1	65.8
IAEA (2007)	186±3	N/A	N/A
ENDF/B-VIII.0 (2018)	169.1	169.1	0.00
ORNL (2018[1])	184.5	131.9	52.6
ORNL (2018[2])	186.0	76.0	110.0

$^{(a)}$Computed by subtraction.
$^{(b)}$Computed from the values reported in the 'G+V' column for ^{28}Si in Table V of Ref. [7].

the differences between the ORNL (2002) evaluation and the current evaluation featuring a higher thermal capture cross section but a decreased direct component of the ^{28}Si capture cross sections. The thermal values and direct capture component for ^{29,30}Si were kept unchanged, as shown in Figs. 2 and 3.

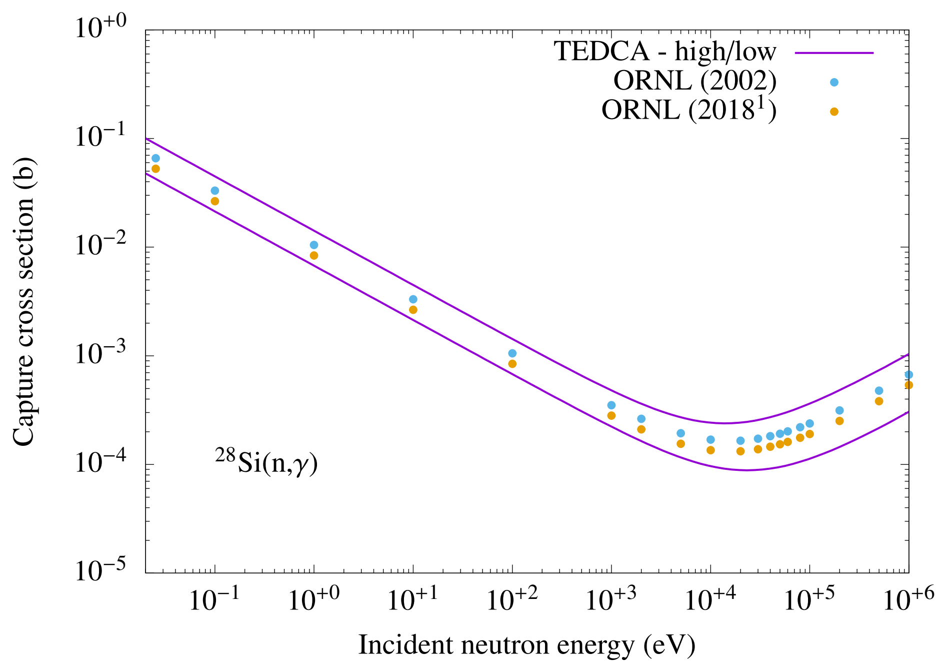

Figure 1. High and low direct capture components of n+^{28}Si cross sections (in purple) calculated from analytic equations as reported in [4]. The evaluated data are shown with light blue and yellow dots.

A second set of silicon evaluations was also generated. The motivation was to improve the unfavorable behavior of the component of the direct capture cross section. As shown in Figs. 1, 2, and 3, the capture cross sections included in the ORNL (2002) evaluations predicted an increasing direct capture for neutron energy in the keV region. The nonphysical behavior predicted by the TEDCA code might be due to the use

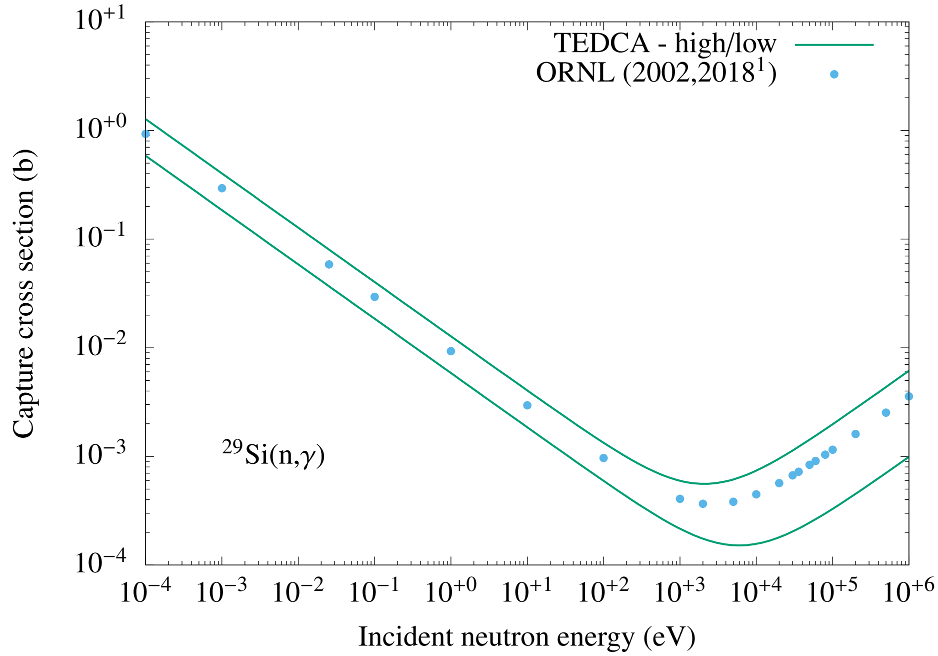

Figure 2. High and low direct capture components of n+^{29}Si cross sections (in green) calculated from analytic equations as reported in [4]. The evaluated data are shown with light blue.

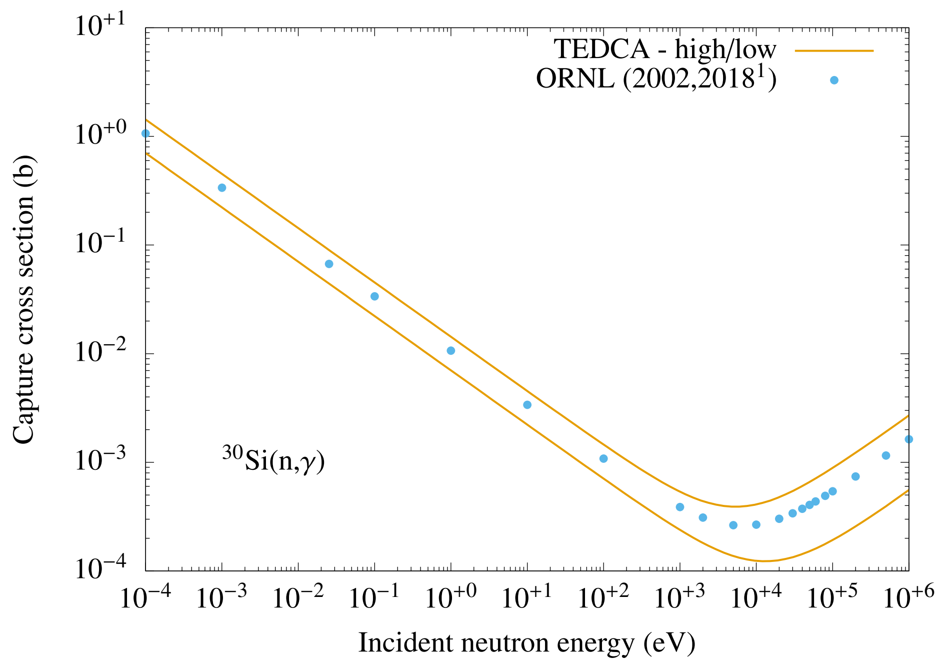

Figure 3. High and low direct capture components of n+^{30}Si cross sections (in yellow) calculated from analytic equations as reported in [4]. The evaluated data are shown with light blue.

of an optical model potential that accounts only for the real part component. New calculations with the

CUPIDO code [11][12] were performed by using a complex optical potential, consistently accounting for the absorption cross sections, as shown in Figs. 4–6. For the ^{30}Si evaluation, the capture cross-section values calculated by CUPIDO were decreased by 5% in order to fit the capture thermal value of 107 mb by the bound levels of the resonance parameters.

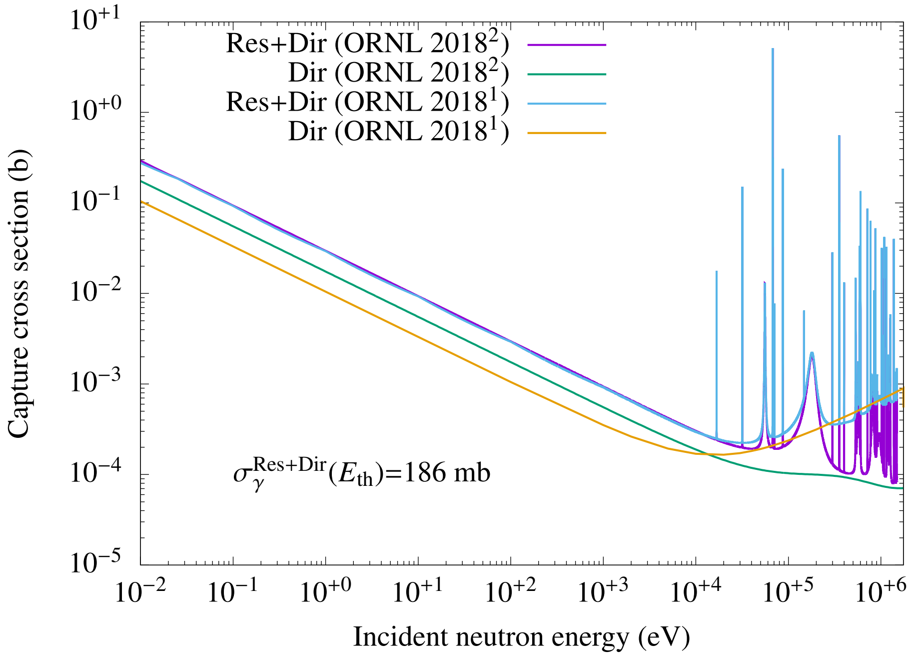

Figure 4. ^{28}Si(n,γ) cross sections reconstructed from the ORNL (2002) evaluation and the ORNL (2018^{1,2}) evaluation in the neutron energy range up to 1.75 MeV.

3. VALIDATION

Only very few benchmark cases containing significant amount of silicon are available in the International Criticality Safety Benchmark Evaluation Project (ICSBEP) collection. Sponsored between 1999 and 2000 by the US National Spent Nuclear Fuel Program (NSNFP) at the Idaho National Engineering and Environmental Laboratory, the ICSBEP identified a list of benchmarks that consists of a series of critical heterogeneous configurations of silicon dioxide with uranium and polyethylene with plutonium fuels performed at the Institute of Physics and Power Engineering, Obninsk, Russia, at the Big Physical Stand (BFS) facility. The purpose of those experiments was to obtain data that are applicable to a wide range of criticality safety operations involving fissile contaminated waste streams. In particular, the data were intended for NSNFP validations of criticality safety calculations performed in support of storage of highly enriched spent nuclear fuels in the US geologic repository at Yucca Mountain, Nevada. In that regard, the experiments covered a very broad range of spectra and provide an excellent case study for the validation of the silicon nuclear data evaluations.

After the recent release of the ENDF/B-VIII.0 library, numerical calculations were performed to test the BFS-79 group of benchmarks (HEU-MET-MIXED-005) that were designed to validate the predictions of reactivity for criticality safety in systems containing silicon. With the ENDF/B-VIII.0 library, the

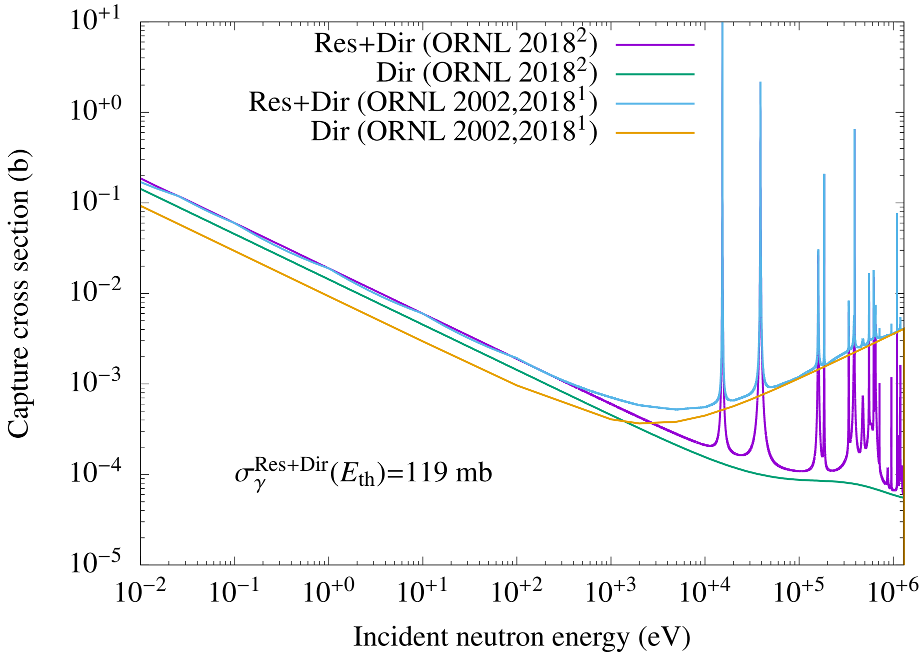

Figure 5. ^{29}**Si(n,γ) cross sections reconstructed from the ORNL (2002) evaluation and the ORNL (2018[1,2]) evaluation in the neutron energy range up to 1.75 MeV.**

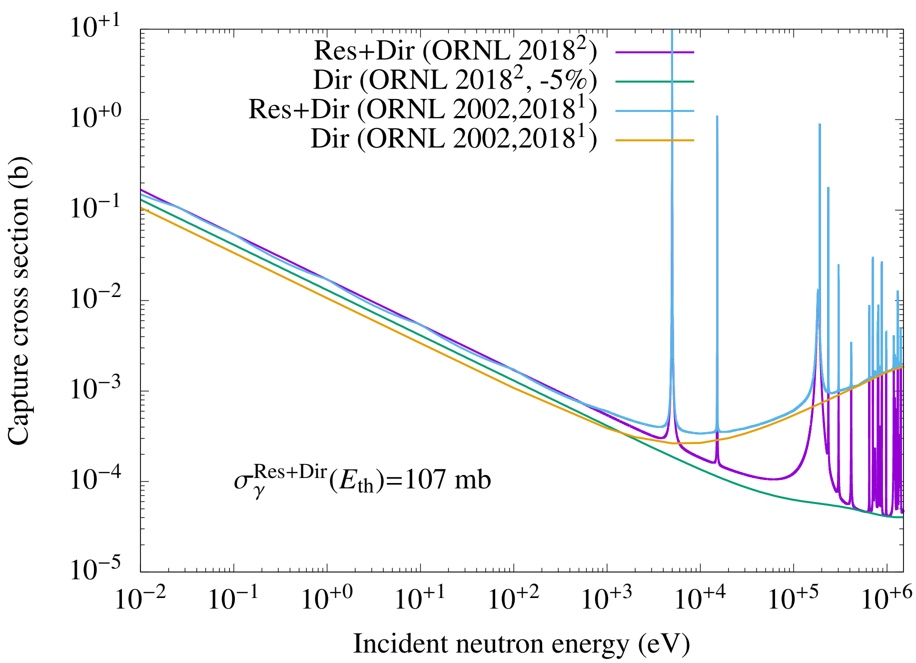

Figure 6. ^{30}**Si(n,γ) cross sections reconstructed from the ORNL (2002) evaluation and the ORNL (2018[1,2]) evaluation in the neutron energy range up to 1.75 MeV.**

prediction very much improved. The two remaining outliers had a pronounced thermal spectrum, suggesting the possibility that the Si thermal capture cross section was underestimated, as clearly shown in Figure 7, where the results of Δk_{eff} between calculated and measured values as a function of the epithermal fission fraction (FEPIT) for the HEU-MET-MIXED-005 experiments are reported for the ENDF/B-VIII.0 (in red) together with calculations from ENDF/B-VII.1 (in black) and JEFF-3.3 libraries (in green). The calculations using the ORNL evaluations (in blue and pink) are also shown.

The increased value of the $^{28}Si(n_{th},\gamma)$ cross sections induces a reduction of about 800 pcm in the thermal assemblies (e.g. HEU-MET-MIXED-005.3 or BSF-79/3 in yellow), showing that the criticality is independent of the epithermal fraction spectra. The significantly improved performance in predicting the reaction rates is shown in Fig. 7, where the calculations were based on the two sets of evaluations, namely ORNL (2018[1]) and ORNL (2018[2]).

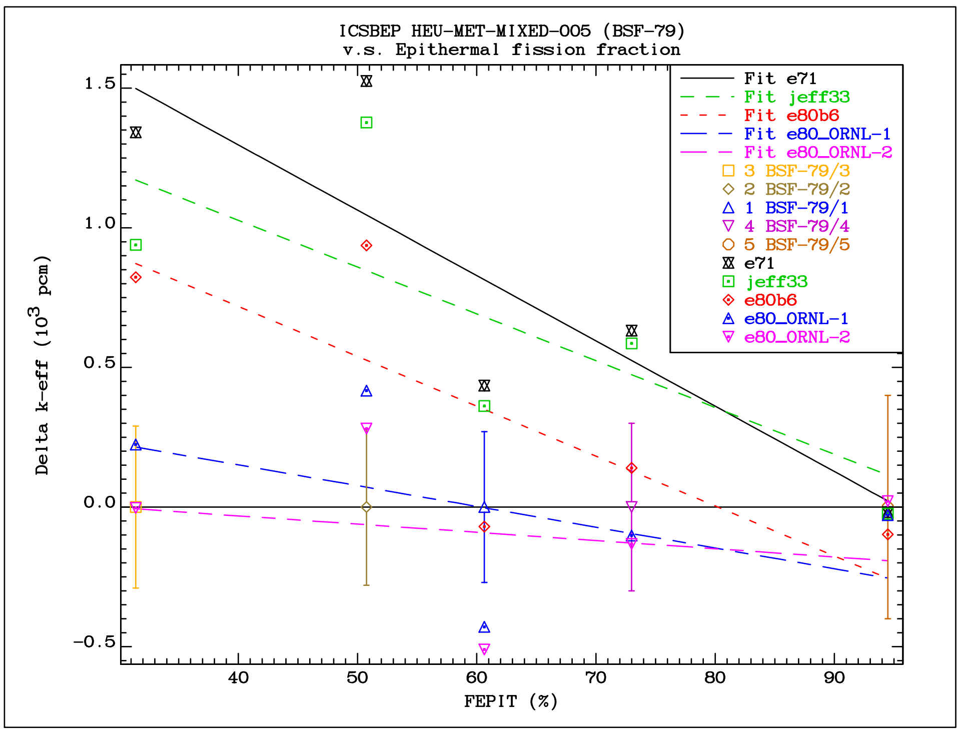

Figure 7. Results for the HEU-MET-MIXED-05 experiments from the ICSBEP compilation. Comparison between ORNL (2018[1]) and ORNL (2018[2]) are shown in blue and pink, respectively.

4. CONCLUSIONS

Since 1997 Hetrick evaluation [1] till the recent release of the ENDF/B-VIII.0 library (2018), the silicon cross section evaluations were not updated in the releases of the ENDF library although a new set of silicon evaluations in the RRR was performed at ORNL in 2002. The 2002 ORNL evaluations were submitted for inclusion into the ENDF/B-VII.0 library, however, they were not included in the ENDF/B-VII.1 release.

One of the reasons may be the difficulty, at that time, to include in the processing procedure of the ENDF files the neutron direct component of the capture cross sections.

After the recent release of the ENDF/B-VIII.0 library and the testing of a group of benchmarks designed to validate the predictions of reactivity for criticality safety in systems containing silicon, it was found that the predictions of those benchmarks were remarkably improved and that the remaining outliers had a pronounced thermal spectrum, suggesting the possibility that the silicon thermal capture was underestimated.

In the present work, two sets of silicon evaluations were generated, ORNL (2018^1) and ORNL (2018^2). ORNL (2018^1) accounted for an updated value of the $^{28}\mathrm{Si}(\mathrm{n_{th}},\gamma)$ cross section and a direct capture contribution decreased by 20% from the ORNL (2002) evaluation in order to match the thermal capture cross section suggested by a study performed at IAEA [9]. For ORNL (2018^1), the $^{29,30}\mathrm{Si}$ evaluations were kept unchanged. Due to both changes in the thermal cross-section value and the direct capture cross section, an improved agreement with benchmarks in the thermal spectrum was achieved for ORNL (2018^1).

The ORNL (2018^2) set of evaluations accounted for updating the direct capture contributions for all three isotopes and the $^{28}\mathrm{Si}(\mathrm{n_{th}},\gamma)$ value as done for ORNL (2018^1). This was motivated by the unfavorable behavior of the component of the direct capture cross sections reported in ORNL (2018^1). With the second set of evaluations, an excellent agreement with benchmarks was achieved. The ORNL (2018^2) set of evaluations was submitted to the ENDF repository to be included in the next ENDF/B release.

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