RESONANCE EVALUATION OF TITANIUM-48 INCLUDING COVARIANCE FOR CRITICALITY SAFETY APPLICATIONS*

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ABSTRACT

In this work we report the methodology and the results of an evaluation carried out for ^{48}Ti in the resolved resonance region for applications in criticality safety calculations. The evaluation was performed using the computer code SAMMY with the reduced R-matrix Reich-Moore formalism. The Bayes' scheme was utilized for fitting the experimental data. New transmission and capture data were essential in the evaluation process. A complete set of resonance parameters was obtained in the energy region from thermal to 400 keV. In addition to the resonance parameters, a resonance parameter covariance matrix was also obtained. The impact of the new resonance parameter evaluation in benchmark calculations, as well as the uncertainty, was verified.

Key Words: Neutron Cross-Section, Nuclear Data Evaluation, Covariance Generation

1 INTRODUCTION

Titanium is an effective neutron absorber that serves as baseline material for chemical separation in high-activity waste solutions. Titanium has not been considered for use in nuclear applications such as reactor design and analysis. Rather, it normally appears as a structural material that may be present in fuel cycle facilities or canisters for transport and disposition of nuclear waste. Criticality safety evaluations of systems in which titanium is present require an understanding of the nuclear data and its uncertainty. To improve the cross-section data and uncertainty for titanium in the thermal and epithermal energy regions, a resonance parameter (RP) and resonance parameter covariance matrix (RPCM) evaluation for ^{48}Ti was done with the computer code SAMMY [1]. New capture and transmission measurements for enriched ^{48}Ti and natural titanium were made at the Oak Ridge Electron Linear Accelerator (ORELA) of the Oak Ridge National Laboratory (ORNL) [2]. The neutron transmission and capture cross section were measured in the energy range 10 eV to 500 keV. The transmission data were measured at the 80 m flight station of ORELA using flight path 1. The neutron detector was an 11.1-cm-diameter, 1.25-cm-thick ^{6}Li-glass scintillator positioned in the beam at 79.815 m from the neutron source. The scintillator was viewed on edge by two 12.7-cm-diameter photomultipliers that were placed outside the neutron beam to decrease backgrounds. The neutron capture experiments were performed at the 40 m flight station using flight path 7.

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Since no previous capture cross-section measurements were available in the resonance region, the ORELA data were essential for determining the shape and the uncertainty in the capture cross section. The resonance evaluation for ^{48}Ti was done in the energy range 10^{-5} eV to 400 keV. Thermal cross-section data available in the EXFOR data system [3] were also used in the evaluation.

2 EXPERIMENTAL DATA BASE

The new transmission and capture data measurements performed at ORELA were used in the evaluation to improve the accuracy of the titanium resonance parameters primarily below 100 keV, where no data were available in the literature. Indeed, the availability of new experimental data below 100 keV permitted a comprehensive evaluation of the total and capture cross section and the resonance parameters covariance from thermal to 100 keV. The measurements were done at room temperature (293.6 K). The measurements consisted of four transmission measurements, specifically, two measurements for natural titanium and two measurements for enriched ^{48}Ti with 99.32% enrichment. In addition to the transmission data, two capture measurements were also carried out at ORELA—one set of measurements for natural titanium and another for a 99.32% enriched ^{48}Ti. The data used in the evaluation are described in Table I. For the evaluation in the thermal energy region, the values indicated in the Atlas of Neutron Resonances (ANR) [4] were used.

Table I. Experimental description for titanium measurements

Data Set	Energy range (keV)	Flight path (m)	Density (at/b)
Natural titanium			
Transmission	0.01–500.0	79.827	0.052966 (thick)
Transmission	0.01–500.0	79.827	0.008785 (thin)
Capture	0.01–500.0	40.116	0.035158
Enriched ^{48}Ti (99.32%)			
Transmission	0.01–500.0	79.827	0.028185 (thick)
Transmission	0.01–500.0	79.827	0.0011821 (thin)
Capture	0.01–500.0	40.116	0.0091386

3 DATA EVALUATION PROCEDURE

The Reich-Moore formalism of the code SAMMY and the Bayes' method for data fitting were used to evaluate the resonance parameters for ^{48}Ti in the resolved energy region from 10^{-5} eV to 400 keV. The resonance parameters listed in the existing cross-section libraries, as for instance the ENDF/B version VII release 0, were done in the energy region up to 300 keV. In this work the upper energy limit of the ^{48}Ti resonance evaluation was extended to 400 keV by taking advantage of the high-quality resolution data listed in Table I.

3.1 Fitting Procedure

Natural titanium consists of five isotopes, namely ^{46}Ti, ^{47}Ti, ^{48}Ti, ^{49}Ti, and ^{50}Ti, with thermal capture cross sections ranging from about 0.18 to 8.3 barns. The percentage isotopic abundances for natural titanium are, respectively, 8.25, 7.44, 73.72, 5.41, and 5.18. Besides being the most

abundant isotope, ^{48}Ti also has the largest thermal capture cross section. Furthermore, criticality safety benchmark experiments, for which natural titanium is present, are predominantly sensitive to ^{48}Ti cross sections. The work described in this paper was carried out in response to criticality safety needs for improved nuclear data for systems in which titanium is present. Therefore, ORNL was targeted to produce a resonance evaluation for ^{48}Ti.

The six experimental measurements listed in Table I were used in the evaluation of the ^{48}Ti isotope. In addition, the thermal cross section and resonance integral listed in the ANR were also used. For a complete SAMMY analysis of the natural and enriched ^{48}Ti, one must include the resonance parameters for the remaining titanium isotopes. For that purpose, the ENDF/B-VII.0 resonance parameters for ^{46}Ti, ^{47}Ti, ^{49}Ti, and ^{50}Ti were used. In SAMMY, the experimental data can be fitted simultaneously or sequentially. The latter was used in the present evaluation. In the sequential Bayes' analysis the RP and the RPCM obtained from fitting one data set are used in the analysis of the next data set. This procedure should yield a unique set of resonance parameters with the corresponding RPCM at the end of the evaluation for all data analyzed. In practice this is usually not possible in view of the fact that the experimental data carry systematic uncertainties as a result of, for instance, normalization process, background correction, neutron energy calibration, and others. Because of these systematic uncertainties, the experimental data basis used in the evaluation is seldom consistent. Consistency in the experimental data basis can be achieved by varying the experimental parameters in a sequential fitting using the SAMAMR modules of SAMMY.

3.2 ^{48}Ti Resonance Evaluation

A set of resonance parameters describing the experimental data up to 400 keV was obtained in the SAMMY analysis. The initial set of resonance parameters used in the evaluation up to 300 keV was retrieved from ENDF/B-VII.0 [5]. Above 300 keV up to 400 keV new resonance parameters were generated using the peak-search option of the RSAP code [6]. The resonance spin assignment was done using the methodology described in the code SUGGEL [7]. The final set of resonance parameters for ^{48}Ti contains a total of 120 resonances—118 in the energy region up to 400 keV and two external energy levels, one negative level and another level above 400 keV. Of the 118 resonances 17 are s-wave resonances, 67 are p-wave, and 36 are d-wave. The results of the total and capture cross sections calculated with the resonance parameters and compared with the experimental data for ^{48}Ti are displayed in Fig. 1 in the energy range 10 eV to 100 keV. The total cross section was derived from the two transmission measurements indicated in Table 1. Comparisons of the total and capture cross section in the energy region from 100 keV to 400 keV are shown in Fig. 2.

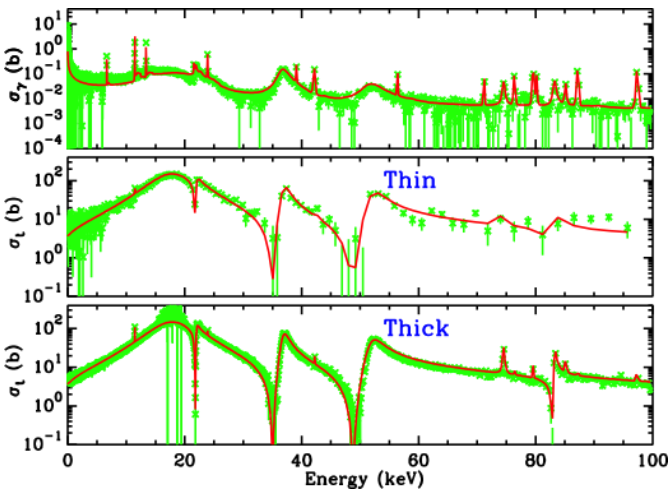

Figure 1. Comparison of the total (two transmission data) and capture cross section calculated in the energy range 10 eV to 100 keV with the resonance parameters and the experimental data for ^{48}Ti.

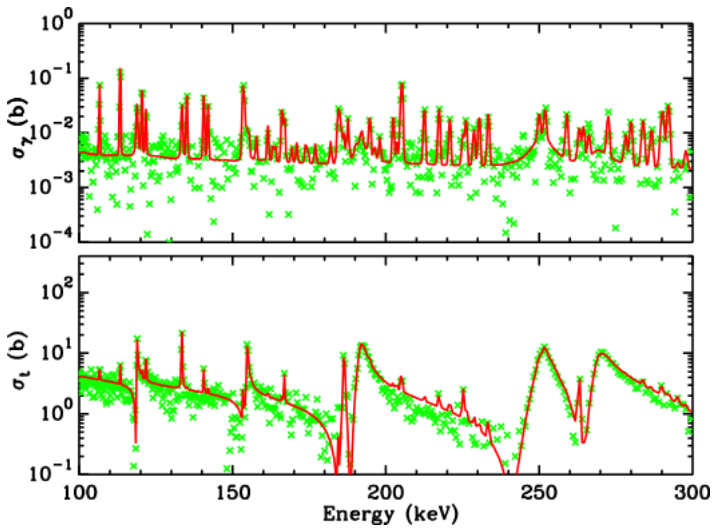

Figure 2. Comparisons of the total and capture cross section in the energy region 100–400 keV calculated with the resonance parameters and the experimental data for ^{48}Ti.

In addition to the resonance evaluation, an RPCM was generated for ^{48}Ti as a result of the evaluation. In the SAMMY fit of the experimental data, systematic uncertainties such as data normalization, background, etc. were propagated into the final RPCM. The RPCMs were converted in the ENDF format using the LCOMP=1 option and processed with PUFF-IV module of AMPX-6 [8]. Although no resonance evaluations were done for ^{46}Ti, ^{47}Ti, ^{49}Ti, and ^{50}Ti, RPCMs for these isotopes were generated based on the retroactive approach of the SAMMY code. The RPCM for ^{48}Ti processed with the PUFF-IV code using the SCALE [9] 44-group neutron group structure for the capture cross section is shown in Fig. 3. The relative uncertainty in the capture cross section of ^{48}Ti in the resolved resonance region varies between 2% and 10%.

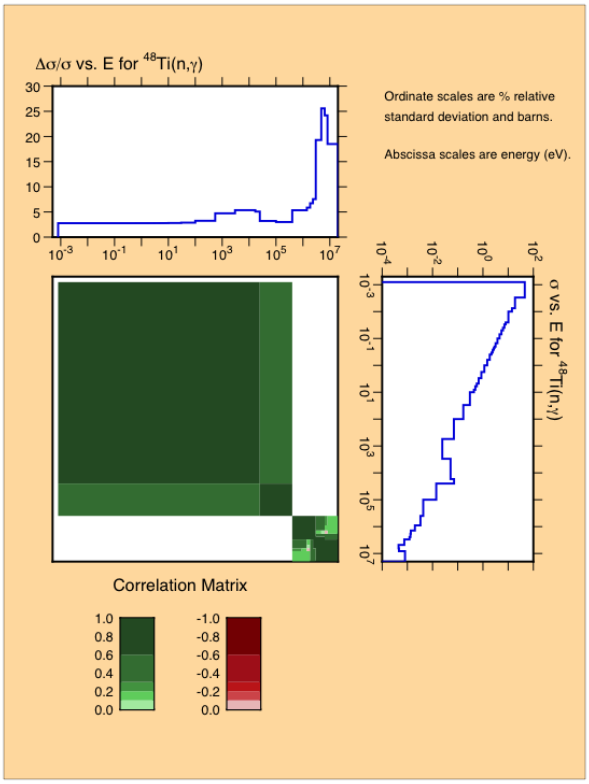

Figure 3. Covariance for the ^{48}Ti capture cross section.

The covariance results shown in Fig. 3 above 400 keV correspond to an evaluation done at Los Alamos National Laboratory (LANL) for ^{48}Ti [10]. Both the ORNL resonance evaluation and the LANL high-energy evaluation were combined to produce a new evaluation. The new evaluation was submitted for inclusion in the most recent ENDF library, i.e., the ENDF/B-VII.1.

Thermal cross-section results for the new ^{48}Ti evaluation were computed and compared with existing results. The thermal cross sections and their uncertainties for the total, capture, and scattering cross sections for ^{48}Ti are displayed in Table II. Also listed in Table II are the ANR results and those of ENDF/B-VII.0. The capture resonance integral and uncertainty calculated with the RPCM is 3.78 ± 0.17 barns and for the ANR is 3.90 ± 0.25 barns, whereas for ENDF/B-VII.0 the value is 3.68 barns. It should be noted that the RPCM leads to an uncertainty in the thermal cross section of about 2.7%.

Table II. Thermal cross section and uncertainties for ^{48}Ti

Cross section	ENDF/B-VII.0 (barns)	ANR (barns)	This work (barns)
Capture	7.84	8.32 ± 0.16	8.32 ± 0.23
Total	12.16	12.42 ± 0.25	12.35 ± 0.30
Scattering	4.32	4.10 ± 0.20	4.03 ± 0.20

4 BENCHMARK CALCULATIONS AND UNCERTAINTY

The impact of the ^{48}Ti cross sections and uncertainties in benchmark calculations was studied. The benchmark system for which the uncertainty in the multiplication factor (k_{eff}) was investigated consists of a thermal critical heterogeneous cylinder of highly enriched uranium polyethylene, and titanium with a polyethylene reflector. The experiment was performed at the Russian Federal Nuclear Center – Institute of Technical Physics (VNIITF) [11]. The benchmark is referred to in the International Criticality Safety Benchmark Evaluation Project (ICSBEP) [12] as the HEU-MET-MIXED-001 benchmark. The calculations were done with the TSUNAMI-3D sequence of the SCALE code, which uses the KENO V.a Monte Carlo neutron transport code to produce the sensitivity of k_{eff} to the cross-section data on an energy-dependent, nuclide-reaction-specific basis. In this calculation, the sensitivities to k_{eff} for the problem-dependent multigroup cross-section data are produced with adjoint-based perturbation theory. The sensitivities of the multiplication factor to the ^{48}Ti capture cross section are shown in Fig. 4. Also shown for comparison is the sensitivity of k_{eff} to the ^{235}U capture cross sections. Calculations with TSUNAMI using the ENDF/B-VII.0 238-group cross-section library result in a k_{eff} = 1.0083 ± 0.0001. The quoted uncertainty is due to the stochastic aspect of the Monte Carlo calculation. Calculations with the ENDF/B-VII.1 cross sections, including the ORNL (resonance region) and LANL (high-energy region) ^{48}Ti evaluation, produced a value for k_{eff} of 1.0053 ± 0.0001. The ^{48}Ti covariance was used in the TSUNAMI code to assess the uncertainty in the k_{eff} due to the uncertainty in the nuclear data. The TSUNAMI-calculated percentage uncertainty in k_{eff} due to the ^{48}Ti data is 0.1139 ± 0.0001. The total percentage contribution to the uncertainty in k_{eff} due to the various isotopes is 1.1880 ± 0.0004. Hence, the uncertainty in k_{eff} due to ^{48}Ti is ~11% of the total uncertainty for the HEU-MET-MIXED-001 benchmark.

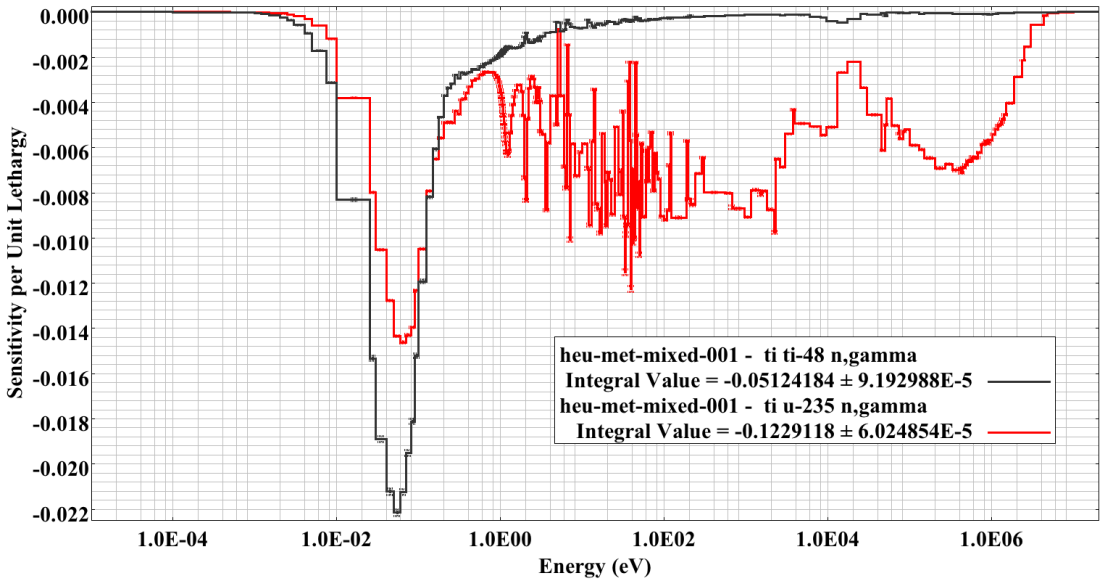

Figure 4. Sensitivity of the multiplication factor to the capture cross sections of ^{48}Ti and ^{235}U for the HEU-MET-MIXED-001 benchmark system.

5 CONCLUSIONS

A new resolved resonance evaluation for ^{48}Ti has been described in this paper. The results of the evaluation are a set of resonance parameters and RPCMs in the energy range 10^{-5} eV to 400 keV. The evaluation was performed with the computer code SAMMY using the Reich-Moore resonance formalism. New transmission and capture measurements done at ORELA were used in the evaluation, which allowed the evaluation to be extended up to 400 keV. The evaluation is part of the new ENDF/B-VII.1 cross section. An example of the application of the new data and uncertainty data was presented for the HEU-MET-MIXED-001 benchmark system.

6 ACKNOWLEDGMENTS

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