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JENDL-4.0: A New Library for Innovative Nuclear Energy Systems

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The fourth version of Japanese Evaluated Nuclear Data Library (JENDL-4.0) has been produced in cooperation with the Japanese Nuclear Data Committee. In the new library, much emphasis is placed on the improvements of fission product and minor actinide data. Achieving this, nuclear model codes were developed. Coupled-channel optical model parameters, which can be applied to a wide mass range, were obtained for evaluations. Thermal cross sections of many actinides were revised on the basis of experimental data or systematics. Simultaneous evaluation was performed for the fission cross sections of important uranium and plutonium isotopes above 10 keV. The new library JENDL-4.0 is made available on the Web site of the JAEA Nuclear Data Center.

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I. INTRODUCTION

The JAEA Nuclear Data Center has produced a series of Japanese Evaluated Nuclear Data Libraries (JENDLs) in cooperation with the Japanese Nuclear Data Committee since early 1970s. We continue to update the library in order to improve its reliability and meet users' requirements. The general-purpose library JENDL-3.3 [1] was released in 2002. It revealed good performances for reactor and shielding applications. The JENDL-4 project officially started in 2005 after the foundation of the Japan Atomic Energy Agency. The new library aims at applications to the R&D of innovative reactors, the high burn-up and use of MOX fuels for the current LWRs, the burn-up credit, and so on. Therefore, minor actinide and fission product data become more important than before. Nuclear model codes were developed to raise the reliability of evaluated cross sections, since experimental data are scarce for those nuclides. Using the codes, we evaluated the cross sections in the energy region above resolved resonances. The parameters for the resolved resonances were re-adjusted or updated so as to reproduce available experimental data. Fission cross sections of important uranium and plutonium isotopes were evaluated by using absolute and ratio measurements simultaneously. Evaluation and compilation of the new library are finished and it is made available as JENDL-4.0.

This paper presents how the evaluation was performed. Section II. deals with the evaluation methodology. In Sect. III. , the evaluated results are described. Section IV. summarizes the conclusion.

II. EVALUATION METHODOLOGY

1. Development of Nuclear Model Codes

As mentioned above, it is necessary to raise the reliability of fission product and minor actinide data for JENDL-4. Nuclear model calculations play a significant role in the evaluation of those nuclei. Two statistical model codes POD [2] and CCONE [3] were developed to reflect recent advances in nuclear theories on evaluation. The POD code is mainly used for medium and medium-heavy nuclei. It consists of the spherical optical model, the one-component exciton model, the distorted-wave Born approximation (DWBA), and the Hauser-Feshbach statistical model with width fluctuation corrections. Moreover, for deformed nuclei, the code is capable of reading the transmission coefficients and direct reaction cross sections calculated by other coupled-channel optical model codes. As an example, Fig. 1 shows the differential cross sections for the elastic scattering on ^{89}Y. The angular distributions, which are calculated from the spherical optical model parameters of Koning and Delaroche [4], are in good agreement with experimental data, while the JENDL-3.3 evaluation deviates from the measurements at backward angles.

The other code CCONE was developed to evaluate actinide nuclei. It is written in C++ programming language. Nuclear properties, decay channels, spectra, *etc.*, are treated as objects. These objects are created dynamically at an execution time, which enables one to

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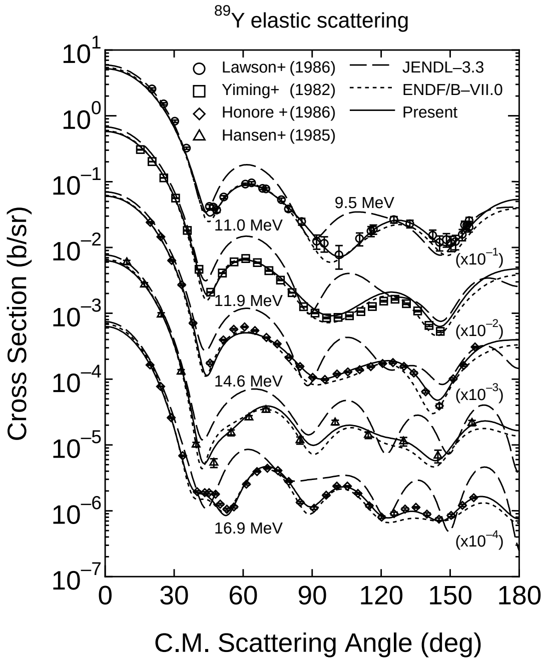

Fig. 1. Angular distributions of neutrons elastically scattered from ^{89}Y.

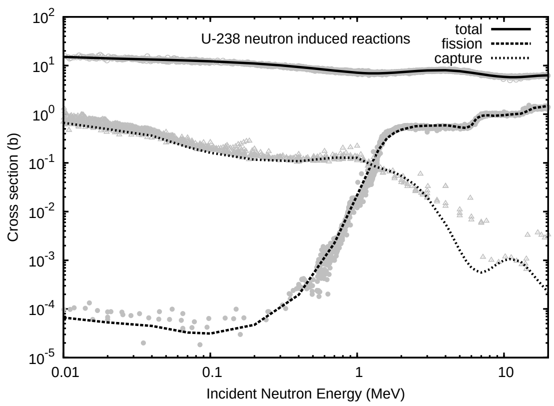

Fig. 2. ^{238}U cross sections calculated with CCONE.

handle a large number of reaction chains. The CCONE code is based on the coupled-channel optical model, the two-component exciton model, and the Hauser-Feshbach theory. The DWBA method is applied to calculate the direct reaction cross section for the excitation of vibrational states. For fission, a double-humped parabolic barrier is assumed and all transition states are approximated by a level-density formula. The cross sections of ^{238}U are illustrated in Fig. 2. The calculated cross sections reproduce experimental data very well.

2. Coupled-Channel Optical Model Parameters

Optical model parameters are the most important parameters for nuclear model calculations. Koning and Delaroche [4] derived the spherical optical model parameters which can be applied to a wide mass range. However, the use of the spherical parameters is not preferable for heavy fission products and actinides which are highly deformed. Kunieda *et al.* [5] obtained the local and global optical model parameters for mass numbers $50 \lesssim A \lesssim 240$ in the incident neutron or proton energy region from 1 keV to 200 MeV. They used the coupled-channel method based on the rigid-rotator model [6] and adopted the functional forms proposed by Soukhovitski *et al.* [7] for the analyses of neutron total cross sections and angular distributions of elastically and inelastically scattered neutrons and protons. The calculated s-wave neutron strength functions are illustrated in Fig. 3, together with the experimental values taken from RIPL-2 [8]. The present coupled-channel calculations agree with experimental data, whereas a remarkable overestimate is seen in the spherical model calculations for the mass range $150 \lesssim A \lesssim 180$, where the nuclei are deformed. This exhibits the reliability of the parameters presently obtained even in the low energy region below 1 MeV.

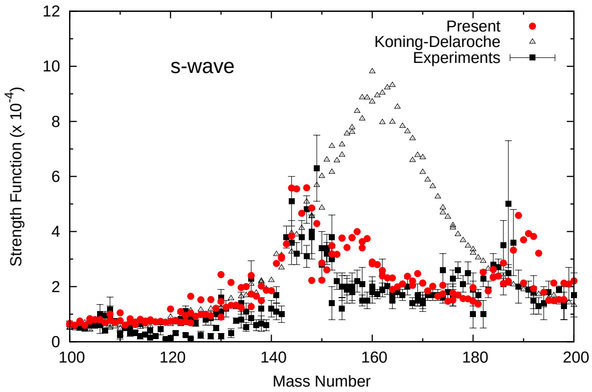

Fig. 3. (Color online) s-wave neutron strength function.

3. Fission Cross Sections above Resonance Region

The fission cross sections above the resolved resonance region were evaluated on the basis of experimental data if available. For the important nuclides ^{233,235,238}U and ^{239,240,241}Pu, the simultaneous evaluation was employed by considering absolute and ratio measurements. The procedure is the same as that used for the JENDL-3.3 evaluation, although experimental data were carefully selected in the present analysis. The energy regions, where the simultaneous evaluation was performed, are 400 keV – 20 MeV for ^{238}U, 100 keV – 20 MeV for ^{240}Pu, and 10 keV – 20 MeV for ^{233,235}U and ^{239,241}Pu. As examples, Figs. 4 and 5 show the fission cross sections of ^{235}U and ^{239}Pu, respectively. The fission cross sections of ^{235}U presently evaluated are a few percent smaller than the JENDL-3.3 values in the energy region where k_{eff} of small fast critical assemblies is sensitive. On the other hand, in the case of ^{239}Pu, the present evaluation is almost consistent with JENDL-3.3.

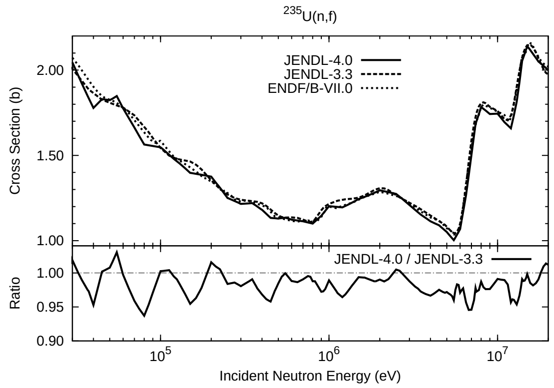

Fig. 4. Fission cross section of ^{235}U.

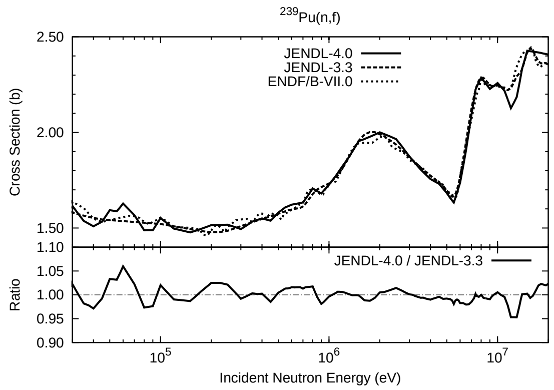

Fig. 5. Fission cross section of ^{239}Pu.

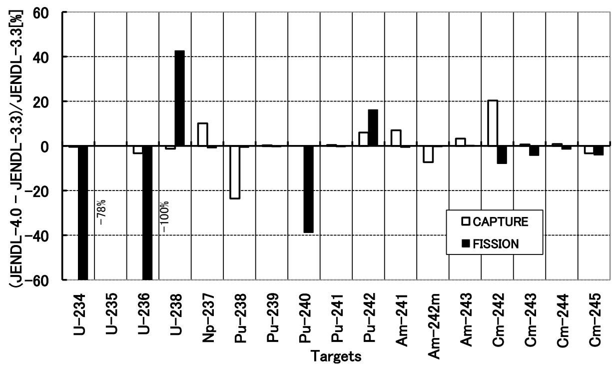

Fig. 6. Differences in thermal cross sections.

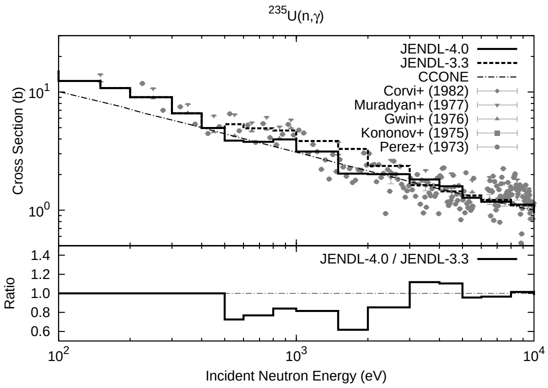

Fig. 7. Capture cross section of ^{235}U.

4. Thermal Cross Sections of Actinides

The thermal cross sections are the most important data to be reproduced by resolved resonance parameters. The measured thermal cross sections were taken mainly from EXFOR and averaged to estimate the fission and capture cross sections at 0.0253 eV. Weights for averaging were determined from the reported uncertainties, year of publication, and so on. The parameters of negative and low-lying positive resonances were adjusted so as to reproduce the average cross sections. For the nuclides whose measured cross sections do not exist, we obtained the systematics of thermal fission and capture cross sections as a function of neutron binding energy. Figure 6 shows the difference in the thermal cross sections between JENDL-3.3 and JENDL-4.0. It is found from the figure that large differences are seen for sub-threshold fission reactions. As for ^{235}U, the cross sections remain unchanged from JENDL-3.3.

5. Prompt Fission Neutron Spectra

The fission neutron spectra were essentially calculated with the modified Los Alamos model [9]. In the energy region below 5 MeV, the data on ^{233,235,238}U and ^{239}Pu were taken from JENDL-3.3. The fission neutron spectra for $^{241-243}$Am and $^{242-246,248}$Cm were obtained from the multi-modal analyses in the energy region below 6 MeV. For other nuclides, Iwamoto [10] developed a simplified formula with the systematics of its parameters. In the energy region above 5 or 6 MeV, where multi-chance fission occurs, the same systematics were used, although pre-fission neutrons were calculated with CCONE.

III. EVALUATED RESULTS

1. Actinides

The cross sections were evaluated for 79 nuclides in the range of Z = 89 − 100, where JENDL-3.3 contained the data for 62 nuclides.

As for resolved resonance parameters (RRPs), we adopted the new sets evaluated by the ORNL group for ^{232}Th, ^{233,238}U, ^{239,241}Pu. The parameters of ^{236,238}Np were evaluated at JAEA. Those of other nuclides were revised by comparing with measured cross sections. The present evaluation and JENDL-3.3 adopted the same RRPs evaluated by Leal *et al.* [11] for ^{235}U. However, in the present work, the upper boundary of the resolved resonance region was changed to 500 eV from 2.25 keV. This change is due to the fact that the capture cross sections calculated from their RRPs seem too large as a result of the benchmark analyses of fast-neutron cores with uranium fuels. The capture cross sections were de-

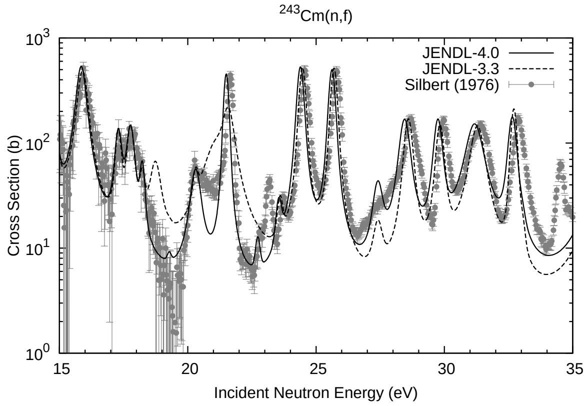

Fig. 8. Fission cross section of ^{243}Cm.

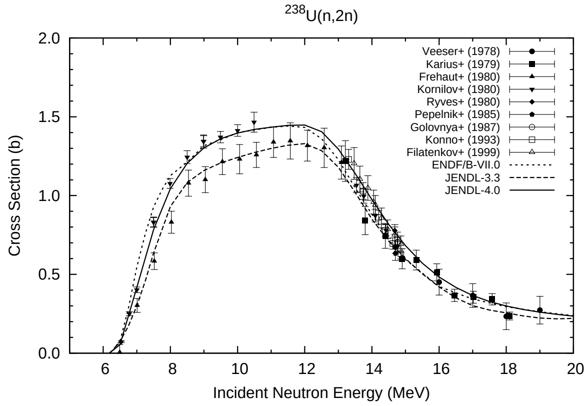

Fig. 10. ^{238}U$(n,2n)$ cross section.

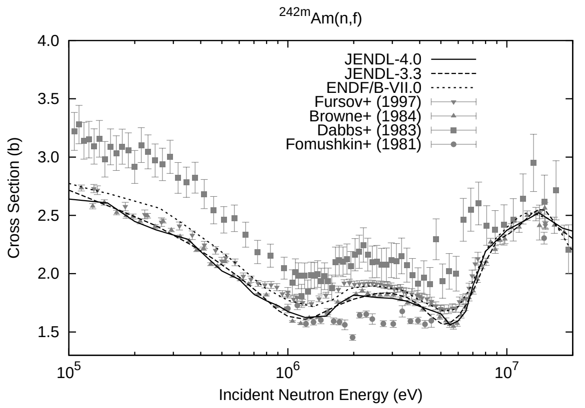

Fig. 9. Fission cross section of $^{242\text{m}}$Am.

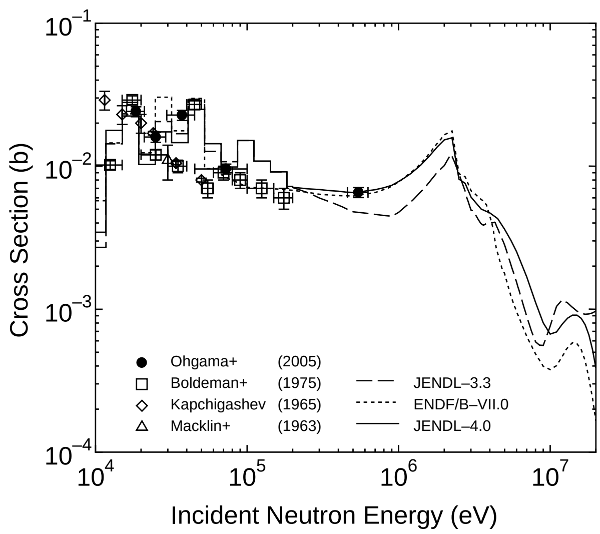

Fig. 11. Capture cross section of ^{90}Zr.

creased in the energy region from 500 eV to 3 keV, as seen in Fig. 7. The present evaluation is also consistent with the statistical model calculations obtained by CCONE. As another example, the fission cross section of ^{243}Cm is illustrated in Fig. 8. It is found from the figure that the revised cross sections reproduce the measured data better than JENDL-3.3.

The fission cross sections above the resolved resonance region were evaluated by the least-squares fitting to experimental data if many measurements were available. The fission cross sections of ^{233,235,238}U and ^{239,240,241}Pu were obtained from the simultaneous evaluation as mentioned in Section II. 3. Figure 9 shows the fission cross section of $^{242\text{m}}$Am.

The nuclear model code CCONE was extensively used for the evaluations of cross sections and spectra. The $(n,2n)$ cross section of ^{238}U was evaluated by using CCONE. As seen in Fig. 10, the present evaluation is systematically larger than the JENDL-3.3 evaluation that is based on the experimental data of Frehaut *et al.* [12].

2. Fission Products

The RRPs of JENDL-3.3 FP nuclides were examined for JENDL-4.0 by taking account of recent measurements. As a result, the parameters of 109 nuclides were updated. Moreover, the parameters of additional 15 nuclides were newly evaluated. The calculated thermal cross sections and resonance integrals were compared with the compilation of Mughabghab. [13] One of the issues on the RRPs is related to ^{157}Gd. The thermal capture cross section of ^{157}Gd, which is calculated from the resonance parameters obtained recently by Leinweber *et al.* [14], is about 10% smaller than the value adopted in JENDL-3.3. Using their parameters as they are, the calculations almost reproduce the power distribution for the core with Gd_2O_3-UO_2 fuel, but considerably overestimate the criticalities for the cores having Gd in water. According to the sensitivities analyses of the two systems, the former one is sensitive to the capture cross section of ^{157}Gd in the energy region above 0.1 eV, whereas the latter one is sensitive to it below 0.1 eV. We tried to adjust the parameters so as to reproduce both integral measurements, but in vain. Finally, the background cross sections were added to the capture cross sections calculated from the parameters of Leinweber *et*

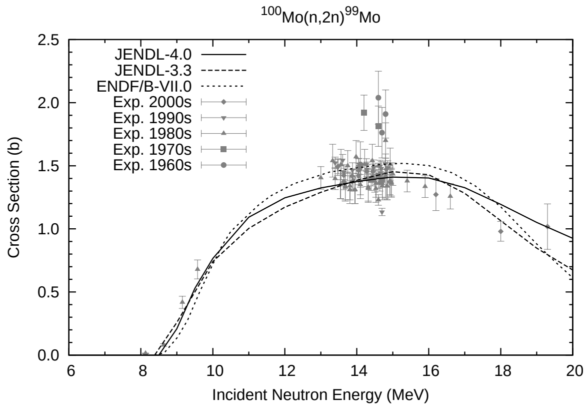

Fig. 12. ^{100}Mo$(n,2n)$ cross section.

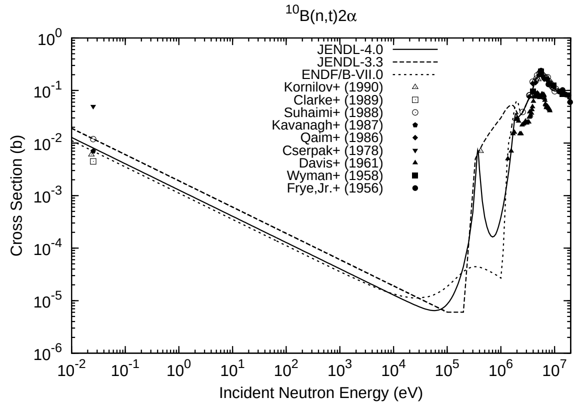

Fig. 14. ^{10}B$(n,t)2\alpha$ cross section.

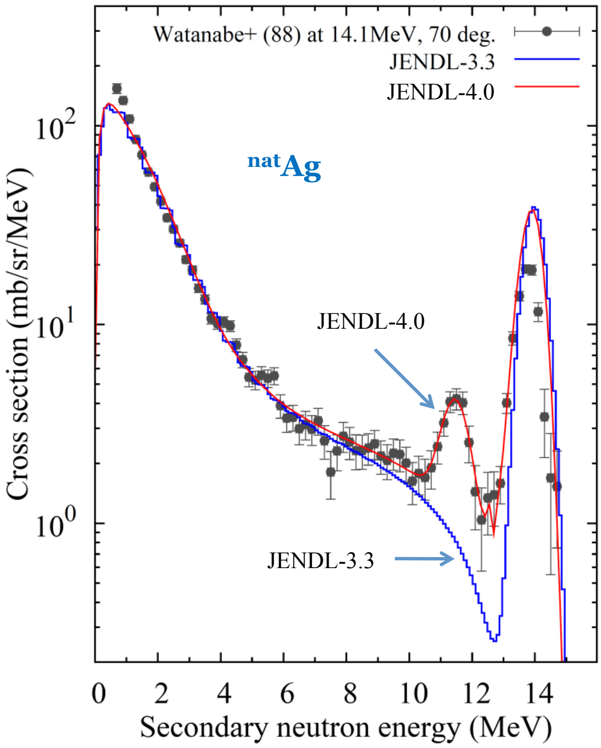

Fig. 13. (Color online) $^{\rm nat}$Ag(n,xn) spectrum at 14.1 MeV.

al. below 0.1 eV.

In the energy region above resolved resonances, nuclear model calculations were performed by using POD and CCONE. The cross sections were revised for 140 FP nuclides. Moreover, the data for another 30 FP nuclides were newly calculated. After combined with the RRPs mentioned above, we obtained a total of 215 FP nuclides in the range of Z = 30 − 68, where 185 nuclides are included in JENDL-3.3. The capture cross section of ^{90}Zr is shown in Fig. 11. The gamma-ray strength function was normalized so as to reproduce the data measured by Ohgama *et al.* [15]. Figure 12 shows the ^{100}Mo$(n,2n)^{99}$Mo cross section. This $(n,2n)$ reaction draws attention recently, since it is one of the feasible ways to produce ^{99}Mo, which is requisite for nuclear medicine applications. The neutron emission spectra from elemental Ag are shown in Fig. 13 at an incident neutron energy of 14.1 MeV. In this case, we assumed a pseudo resonance at an excitation energy of 2.5 MeV. Such pseudo resonances are often needed to reproduce measured neutron emission spectra in the FP mass region. The JENDL-3.3 evaluation obviously underestimates the measured data in the region of 10 – 12 MeV, since no direct reaction process is taken into account.

3. Other Nuclides

For light elements, data were revised for ^{1,2}H, ^{9}Be, ^{10}B, C, ^{14}N, and ^{16}O. The data on ^{1}H were taken from ENDF/B-VII.0 by considering the results of thermal reactor benchmarks. The ^{10}B$(n,t)2\alpha$ cross section was re-evaluated, since accurate estimate of tritium production from boron is required for PWRs as a result of high burn-up. It is found from Fig. 14 that the present evaluation is 33% smaller than JENDL-3.3 at thermal energy. The thermal (n,p) cross section of ^{14}N was increased to 1.93 b from 1.83 b.

Concerning structural materials, the data on Si, Ca, Ti, ^{55}Mn, Cr, ^{56,57}Fe, and Cu were revised. Elemental V data were replaced with the new isotopic evaluations of ^{50,51}V; the data on ^{59}Fe and ^{59}Ni were newly evaluated. The ^{59}Ni(n,α) cross section is important to estimate the radiation damage of reactor vessels.

In the heavy mass region, we revised the data on $^{174,176-180}$Hf, $^{182-184,186}$W, Pb, and ^{209}Bi. The data on ^{169}Tm, Yb, ^{181,182}Hf, ^{180}W, Os, and ^{197}Au were newly evaluated. The nuclide ^{182}Hf has a half life of 8.9 million years, and its production cross section is needed to estimate the activation of control rods for BWRs. The reliability of the revised Pb data was confirmed by the results of fast-reactor and fusion benchmark calculations. The $(n,2n)$ cross section of elemental Pb is illustrated in Fig. 15. The present evaluation is smaller than the JENDL-3.3 evaluation at 14 MeV, while the data measured by Frehaut *et al.* [12] are systematically smaller

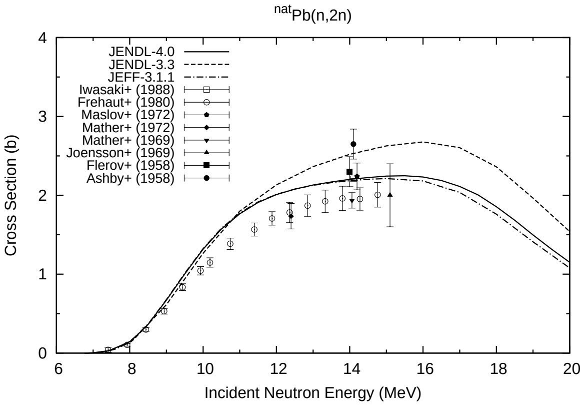

Fig. 15. $^{\text{nat}}$Pb$(n, 2n)$ cross section.

than the present work and the JEFF-3.1.1 evaluation, as in the case of ^{238}U (Fig. 10).

4. Fission Product Yield

Most of the fission yield data in JENDL-3.3 were taken from those of JNDC library version 2 [16], which were compiled in 1990. However, the data for only 12 fissioning nuclides are available. For JENDL-4.0, we decided to adopt the ENDF/B-VII.0 fission yield data which were based on the compilation of England and Rider. [17] Modifications were made to the ENDF/B-VII.0 data, namely the nuclides and decay chains being consistent with those contained in JENDL FP Decay Data File 2000 [18]. Moreover, ternary fission was taken into account.

IV. CONCLUSIONS

The evaluation and compilation of JENDL-4.0 were performed for applications to innovative nuclear energy systems. The new library consists of the sub libraries, *i.e.*, the neutron cross section data for 406 nuclides, the fission product yield data for the neutron-induced fission of 31 nuclides and the spontaneous fission of 9 nuclides, the thermal scattering law data for 15 materials selected from ENDF/B-VI.8 and -VII.0, and the photo-atomic and electro-atomic data taken from ENDL. The new library is made available on the Web site of the JAEA Nuclear Data Center.

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