(From Minutes of SG39 Meeting in Nov. 2013)

C9. Methodology issues

- *Prepare a list of priority missing covariance data types (see also points C4 and C5) and list of "suspect" low values (file dependent) (Action on M. Ishikawa). This list will be discussed with CIELO evaluators.*

Comments on Covariance Data of JENDL-4.0 and ENDF/B-VII.1

April 22, 2014

M. Ishikawa, JAEA

Summary

- Number of nuclides surveyed : 5

  --> Pu-239, U-235, U-238, Fe-56 and Na-23

- Number of nuclides, reactions and energy regions focused on: totally 14

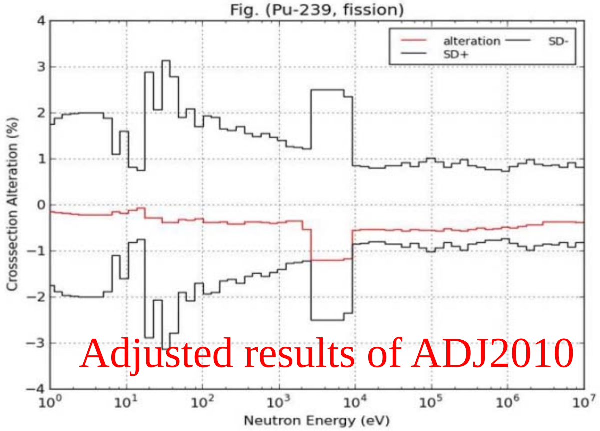
  ✓Pu-239: 1) fission (2.5~10keV) and 2) capture (2.5~10keV).
  ✓U-235: 3) fission (500eV~10keV) and 4) capture (500eV~30keV).
  ✓U-238: 5) fission (1~10MeV), 6,7) capture (below 20keV, 20~150keV), 8) inelastic (above 100keV) and 9) elastic (above 20keV).
  ✓Fe-56: 10) elastic (below 850keV) and 11) mu-bar (above 10keV).
  ✓Na-23: 12) capture (600eV~600keV), 13) inelastic (above 1MeV) and 14) elastic (around 2keV).

- References used to get information

J-1) K.Shibata, et al.: JENDL-4.0 evaluation report, JNST, 48, 1, pp.1-30 (2011).
J-2) O.Iwamoto, et al.: JENDL-4.0 covariance evaluation report, JKPS(ND2010), 59, 2, pp.1224-1229 (2011).
J-3) JNDC: JENDL-4.0 comment file, http://wwwndc.jaea.go.jp/jendl/j40/j40.html (2014).
J-4) K.Shibata, et al.: JENDL-3.2 covariance evaluation report, JAERI-Research 97-074 (1997) (in English).
J-5) K.Shibata: private communication (2014).
J-6) O.Iwamoto: private communication (2014).

E-1) M.Chadwick, et al.: ENDF/B-VII.1 evaluation report, Nuclear Data Sheets, 112, pp.2887-2996 (2011).
E-2) M.Herman, et al.: COMMARA-2.0 covariance evaluation report, BNL-94830-2011 (2011).
E-3) NNDC: ENDF/B-VII.1 comment file, http://www.nndc.bnl.gov/endf/b7.1/index.html (2014).
E-4) P.Oblozinsky, et al.: AFCI-1.2 covariance evaluation report, BNL-90897-2009 (2009).
E-5) M.Chadwick: private communication (2013).

Pu-239 Fission (1/3)



<Energy Range>

2.5~10keV (lower part of unresolved resonance region)

<Observed Facts>

In **JENDL-4.0**, the standard deviation (**STD) of 2.5~10keV** is **significantly large** in the unresolved resonance region of 2.5~30keV. No such discontinuity is seen in ENDF-7.1.

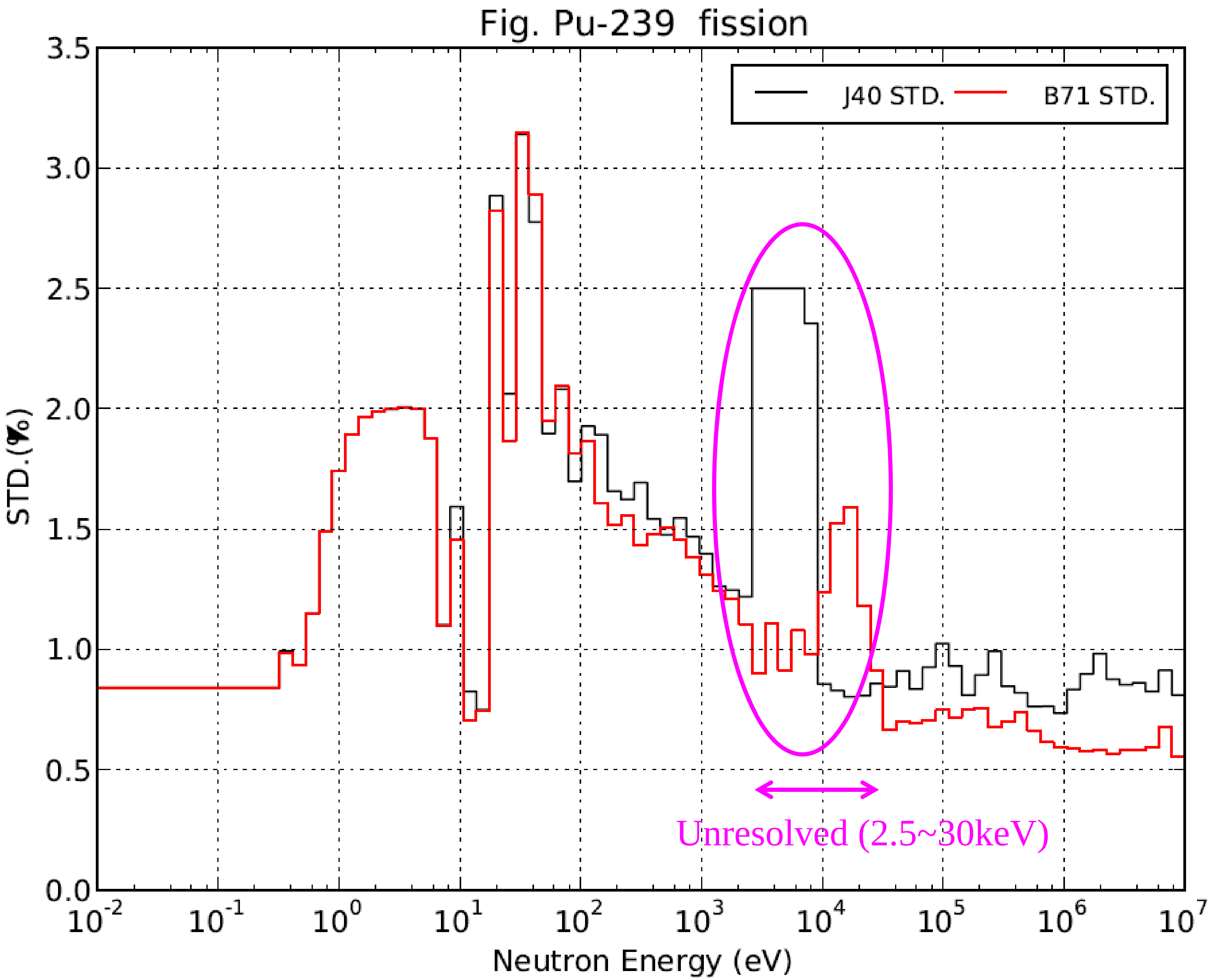
<Obtained Information and/or Comments>

In the former JENDL-3.3, the covariance of the whole unresolved resonance region was evaluated from the uncertainty of resonance parameters, therefore, the STD was generally large. Above 10keV, JENDL-4.0 changed to adopt the simultaneous evaluation for major fission isotopes for the center values of fission cross-section, and the resonance parameters were only used to calculate the shielding factors. Since the simultaneous evaluation was found to evaluate the STD too small, the variance of JENDL-4.0 was multiplied by a factor of 2 **[J-2, p.1226]**, but still small compared with the STD of JENDL-3.3, which was carried over to JENDL4.0 in 2.5~10keV **[J-6]**. Since the evaluation method of the covariance is consistent with that of the central value of cross-section, the discontinuity at 2.5~10keV is physically acceptable. However, the cross-section change by adjustment followed this covariance discontinuity as the figure above.

<Recommendations>

It is **desirable** for **JENDL-4.0** to **improve** the evaluation of **2.5~10keV region** soon.

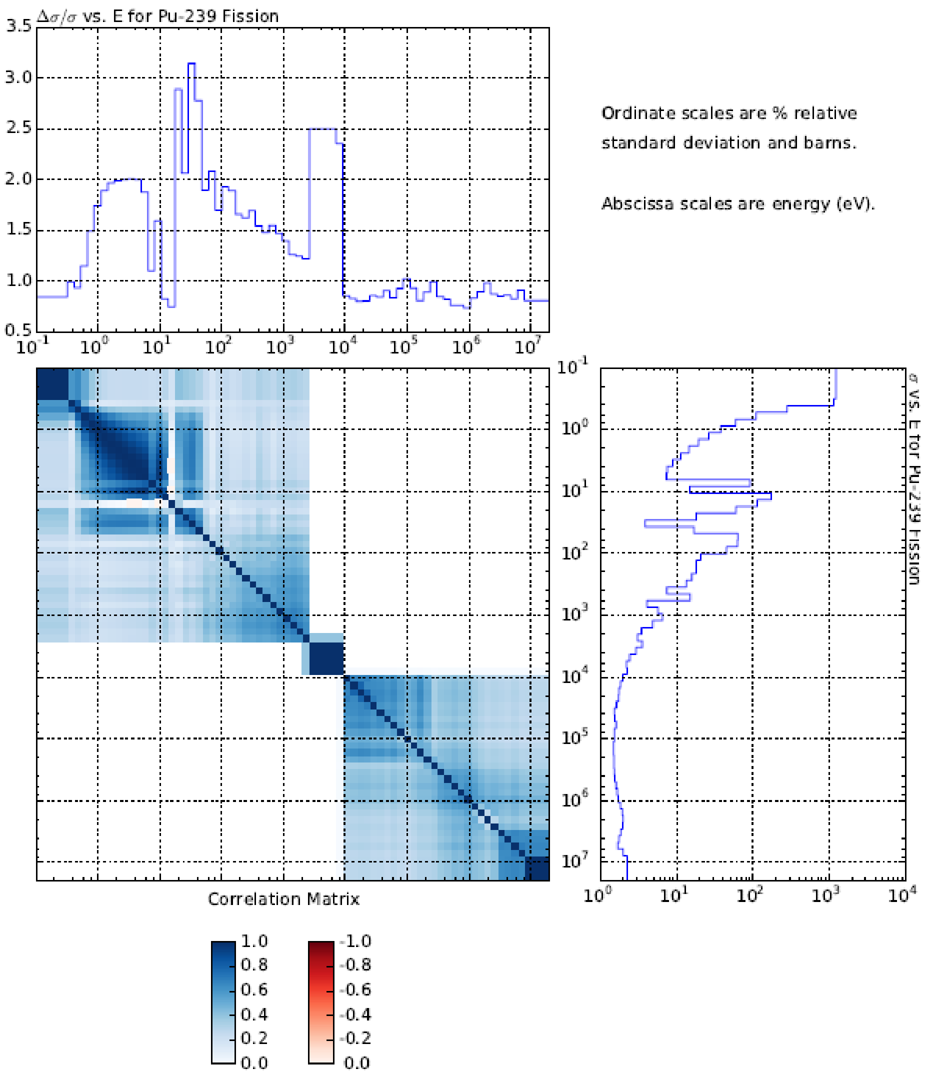
Pu-239 Fission (2/3)



Pu-239 Fission (3/3)

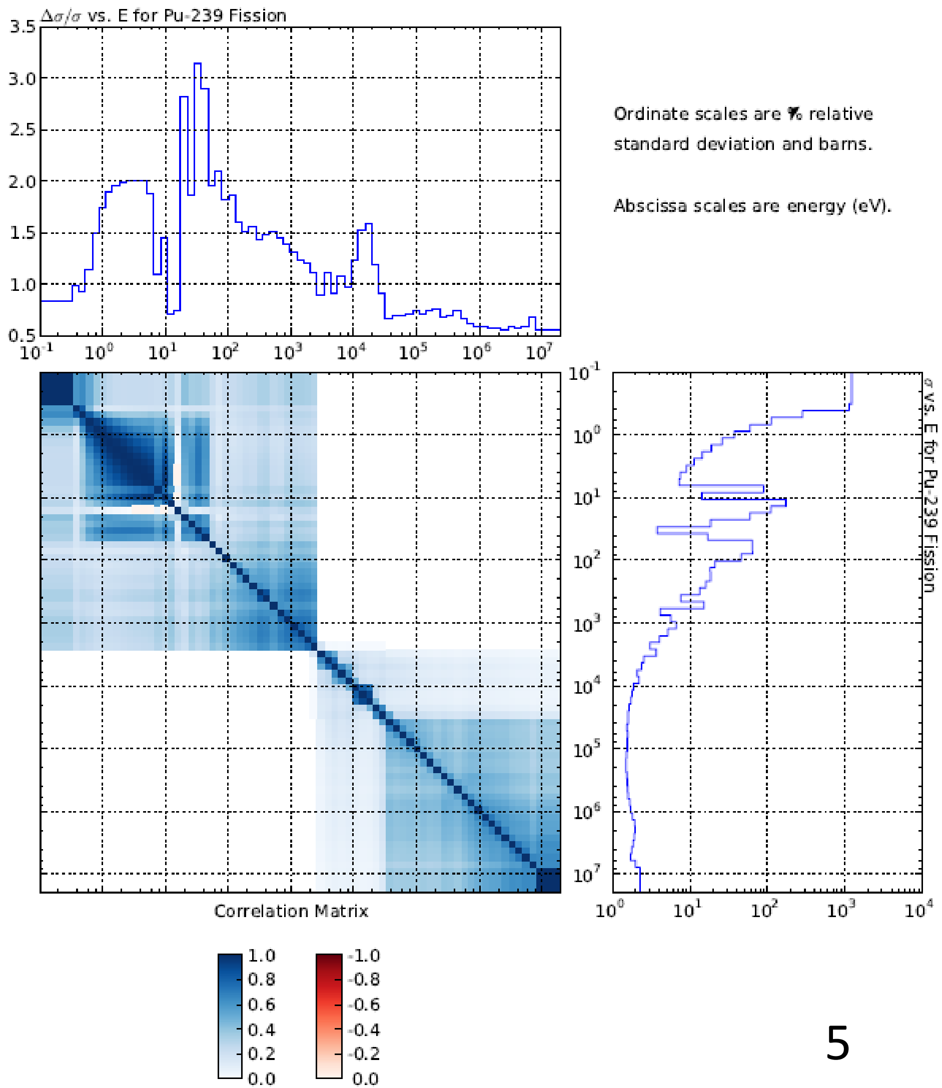
JENDL-4.0

Fig. Pu-239 Fission (JENDL-4.0)

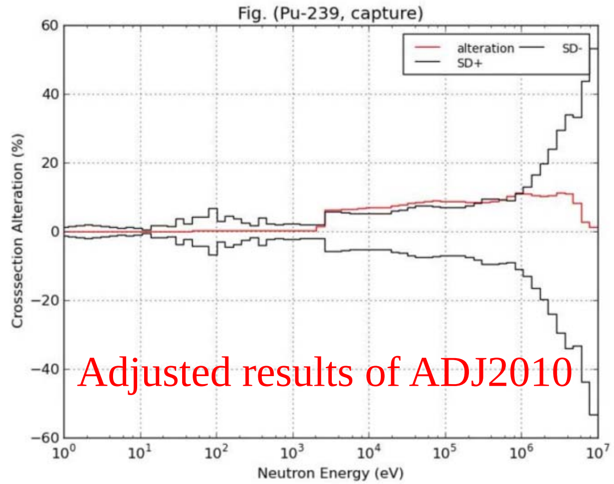


ENDF-7.1

Fig. Pu-239 Fission (ENDF/B-VII.1)



Pu-239 Capture (1/3)



<Energy Range>

2.5~10keV (lower part of unresolved resonance region)

<Observed Facts>

The **STD of ENDF-7.1** is **notably large in 2.5~10keV**, on the other hand, that of JENDL-4.0 is quite smooth above 2.5keV.

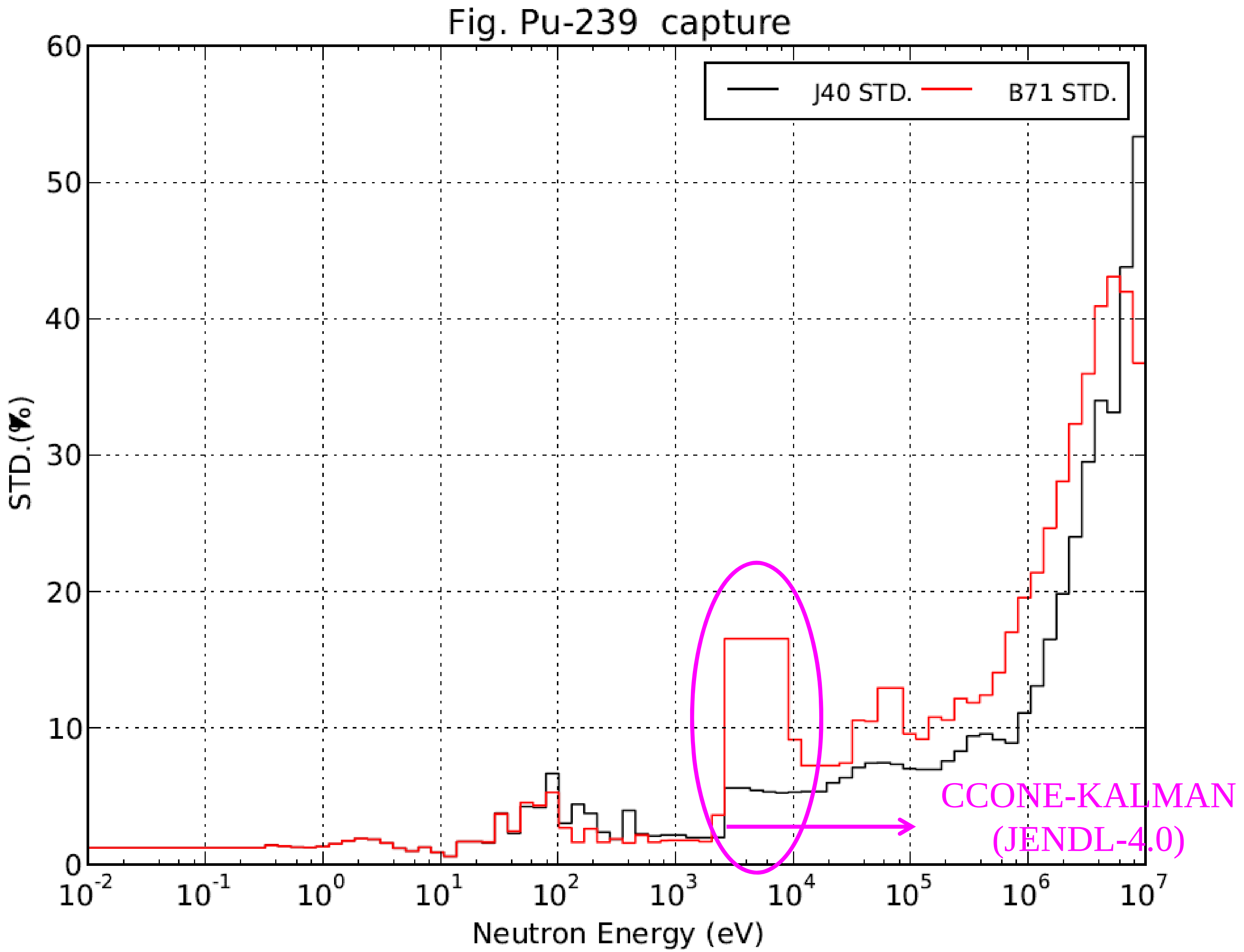
<Obtained Information and/or Comments>

Above 2.5keV, JENDL-4.0 adopted the results of the CCONE-KALMAN, not the simultaneous evaluation, therefore, the STD tends to be smooth in the high energy region[J-6]. However, there seems no explanation in the ENDF-7.1 comment file[E-3] to correspond to this discontinuity. In the US, there seems an opinion that the Pu-239 capture cross-section above 2.5keV should be 10% larger than ENDF-7.1[E-5], but no information on the relation with this covariance trend. Only for information, the adjusted result of ADJ2010 is shown in the figure above.

<Recommendations>

SG39 may **ask the ENDF evaluators** if there is **any physical reason** for this **discontinuity**.

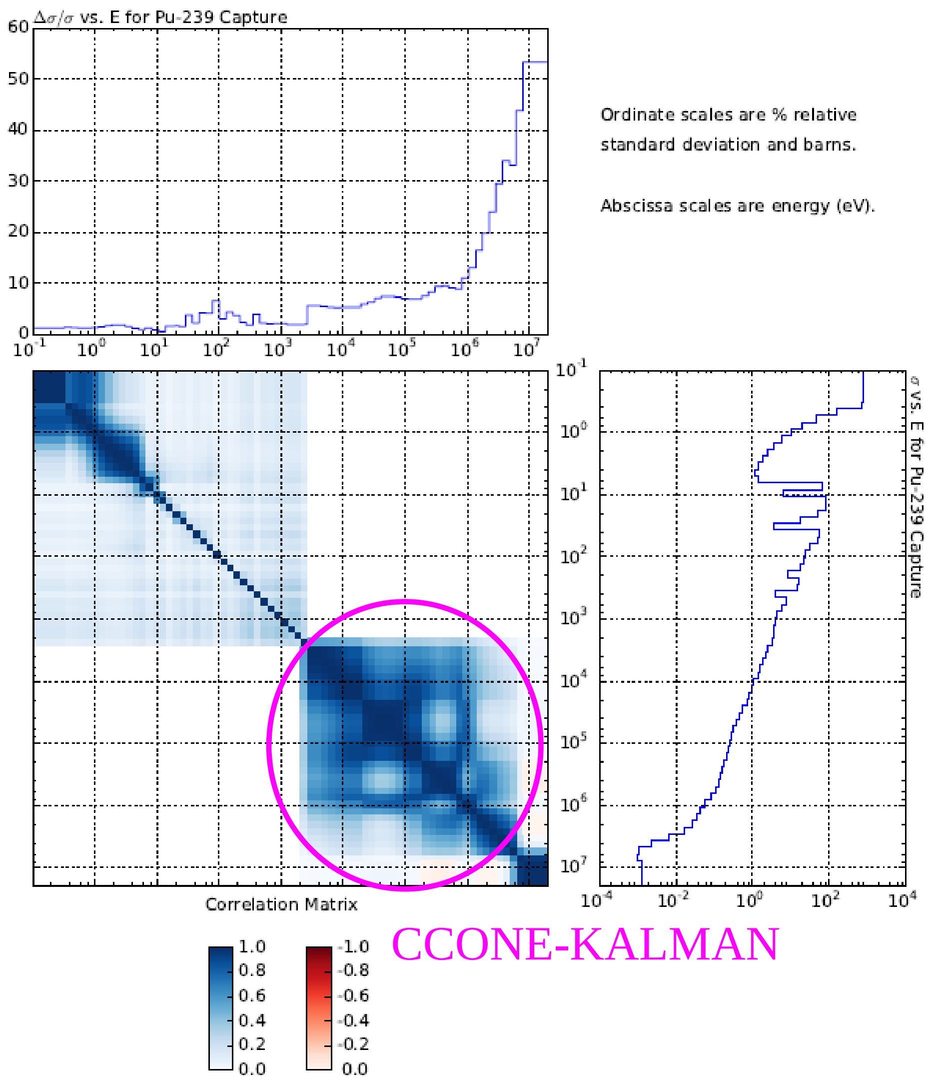
Pu-239 Capture (2/3)



Pu-239 Capture (3/3)

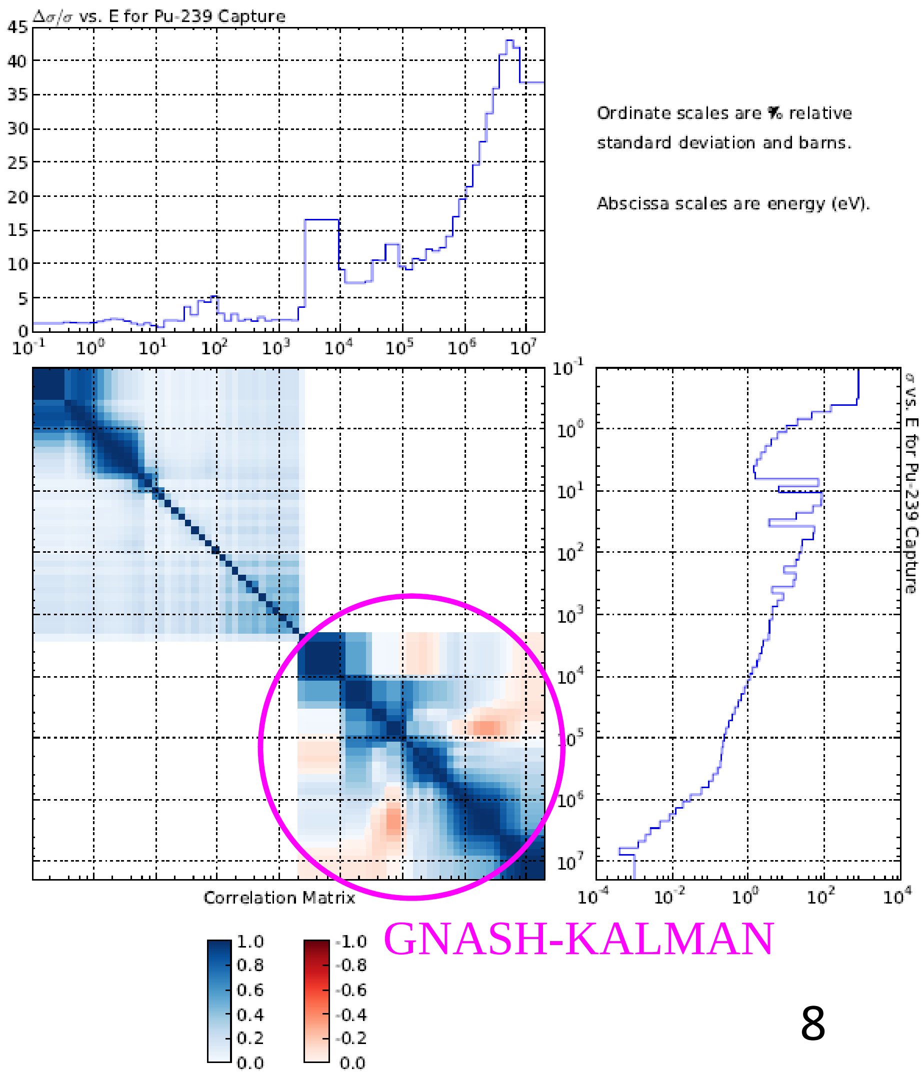
JENDL-4.0

Fig. Pu-239 Capture (JENDL-4.0)

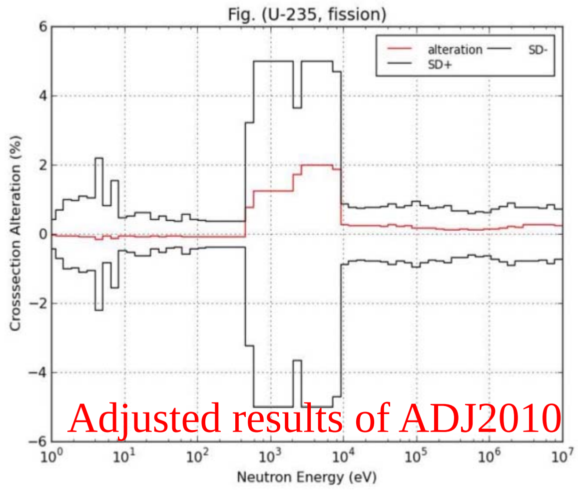


ENDF-7.1

Fig. Pu-239 Capture (ENDF/B-VII.1)



U-235 Fission (1/3)



<Energy Range>

500eV~10keV (resolved and unresolved resonance regions)

<Observed Facts>

The **STD of ENDF-7.1 in 500eV~2keV** is **extremely small**, on the other hand, **JENDL-4.0** shows the large value of **5%**. Further, **ENDF-7.1** has very **sharp peak around 2keV**.

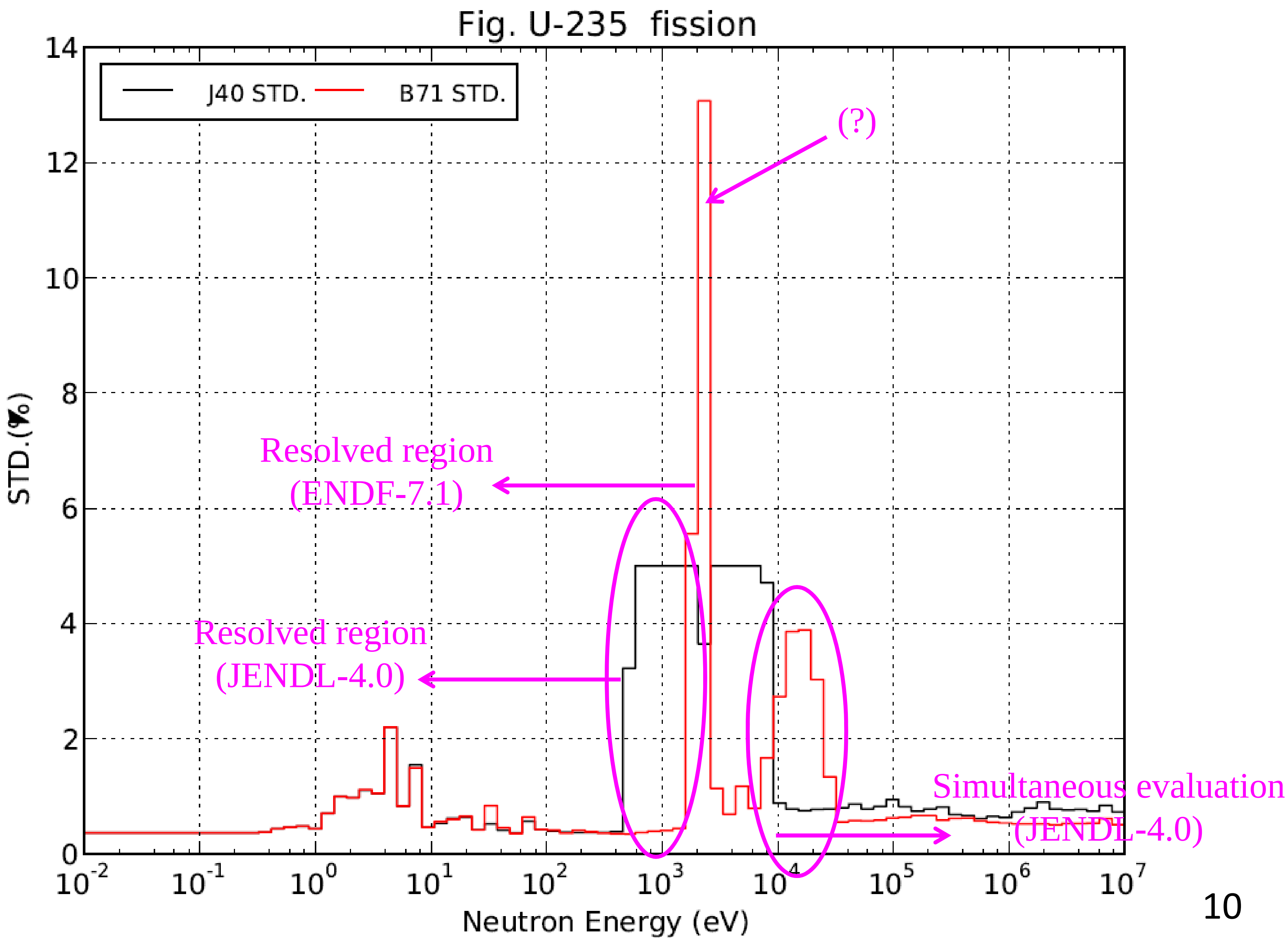
<Obtained information and/or Comments>

JENDL-4.0 adopted the resonance parameter values obtained from ORNL below 500eV**(J-1)**, and re-evaluated based on those of ENDF/B-VI.5 (=JENDL-3.3) n the range of 500eV~2.25keV. In 2.25~9keV, the CCONE code was used, and above 10keV, the simultaneous evaluation was adopted. JENDL-4.0 assumed the STD value of 5% in 500eV~9keV**(J-3)**, but the reason is unknown. The covariance of EENDF-7.1 was evaluated with GNASH-KALMAN**(E-2, p.20)**, but the strange STD peak appears around 2keV.

<Recommendations>

SG39 should **ask the JENDL evaluators** about the reason of **5% in the range of 500eV~9keV,** and the **ENDF evaluators** on the explanation of the **sharp peak around 2keV**, which might be a problem of NJOY.

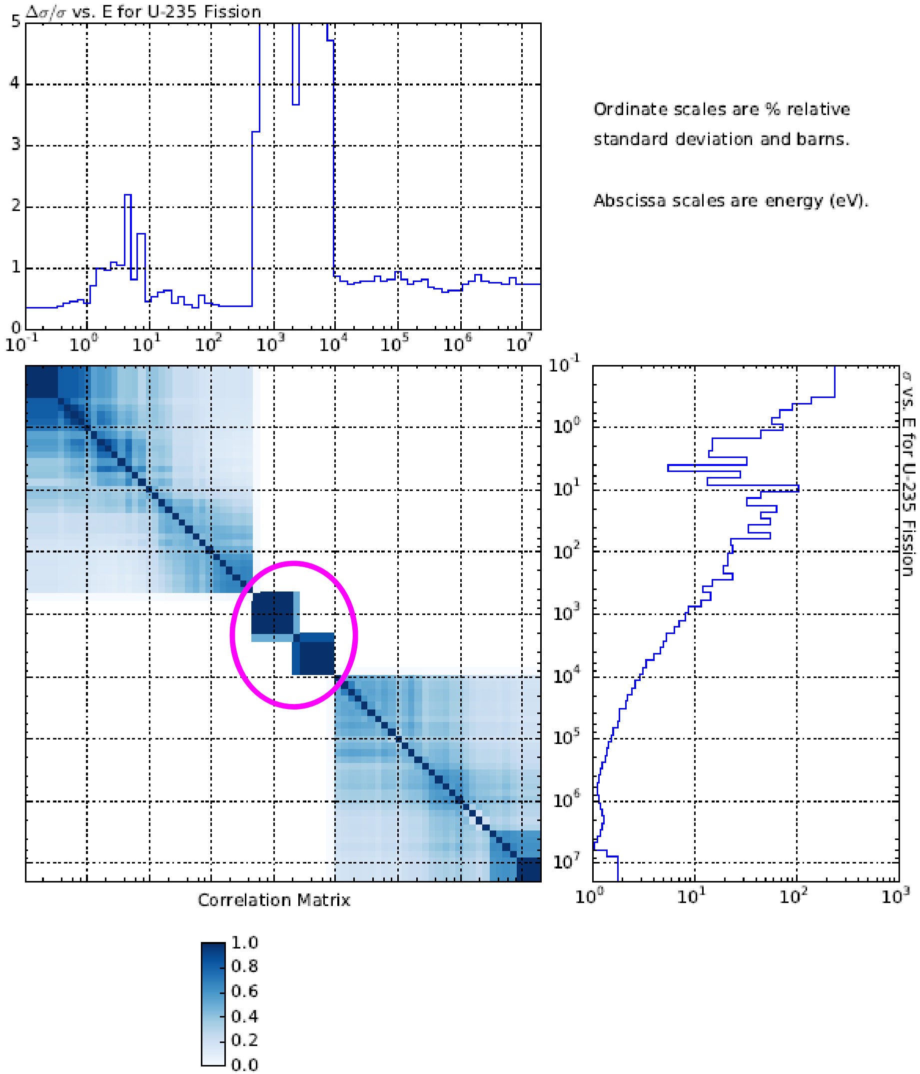
U-235 Fission (2/3)



U-235 Fission (3/3)

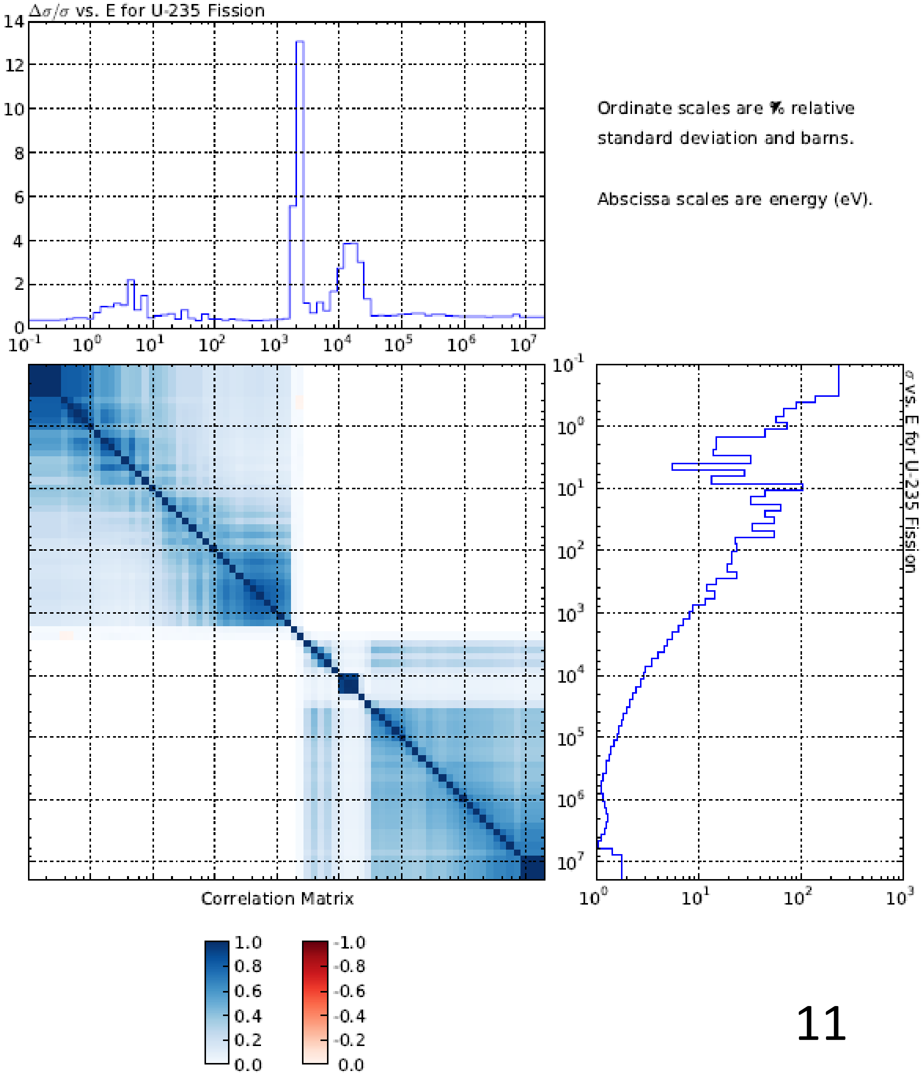
JENDL-4.0

Fig. U-235 Fission (JENDL-4.0)

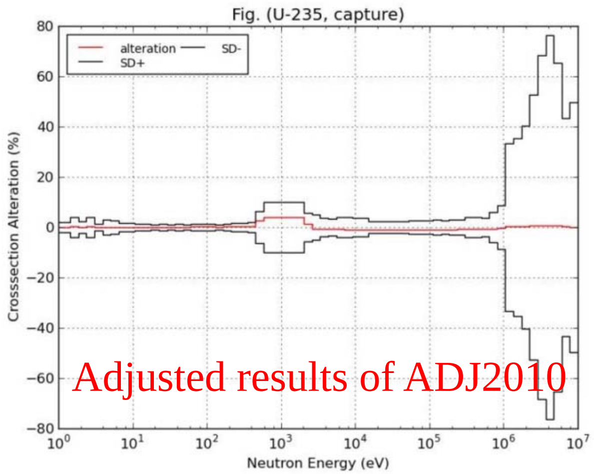


ENDF-7.1

Fig. U-235 Fission (ENDF/B-VII.1)



U-235 Capture (1/3)



<Energy Range>

500eV~30keV (unresolved resonance region of JENDL-4.0, resolved and unresolved regions of ENDF-7.1)

<Observed Facts>

The STD of **JENDL-4.0 in 500eV~2.25keV** is **10% constant and perfect correlation**, on the other hand, **ENDF-7.1 increases from a few % to 35%**. In **2.25~30keV**, ENDF-7.1 gives the STD of **35% with almost perfect correlation**, while JENDL-4.0 shows **several % with weak correlation**. Further, the **negative correlation** with high energy region was found in ENDF-7.1, on the contrary, no such trend in JENDL-4.0.

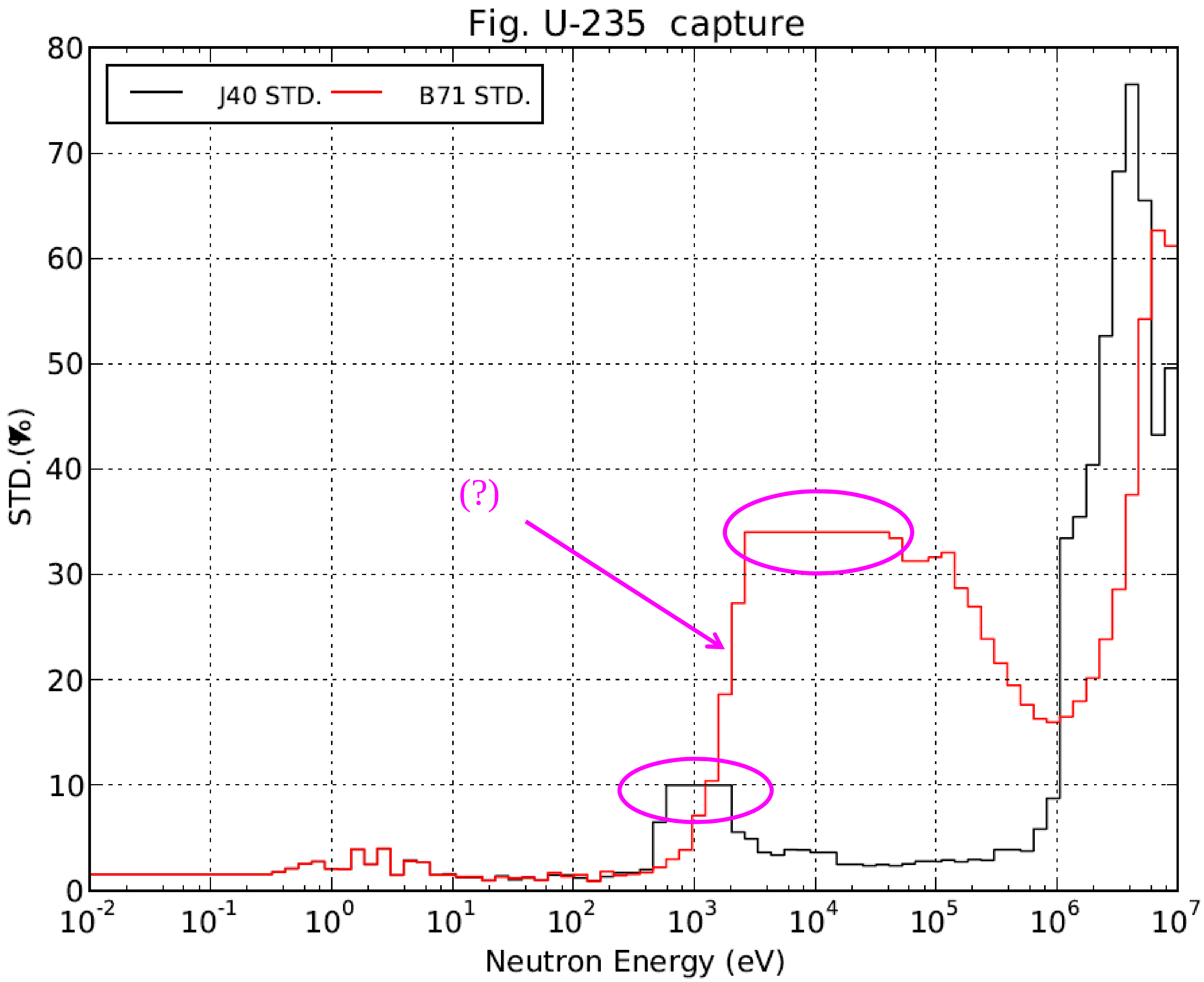
<Obtained Information and/or Comments>

The resonance parameters of JENDL-4.0 has the same explanation with U-235 fission, but the correction was added to make the cross-section close to that of JENDL-3.2 in 500eV~2.25keV[J-1, p.7], and the uncertainty was assumed as 10%[J-3]. Above 2.25keV, the covariance was obtained the least-square calculation based on the experimental values of the alpha values, that is, the ratio to U-235 fission. The resonance parameters of ENDF-7.1 below 2.25keV adopted the ORNL results, but the constant STD of 35% would reflect the recent LANL measurements. The reason of the slope from several % to 35% is unknown.

<Recommendations>

SG39 had better confirm the **reasons of the observed facts** to both **JENDL-4.0** and **ENDF-7.1 evaluators**.

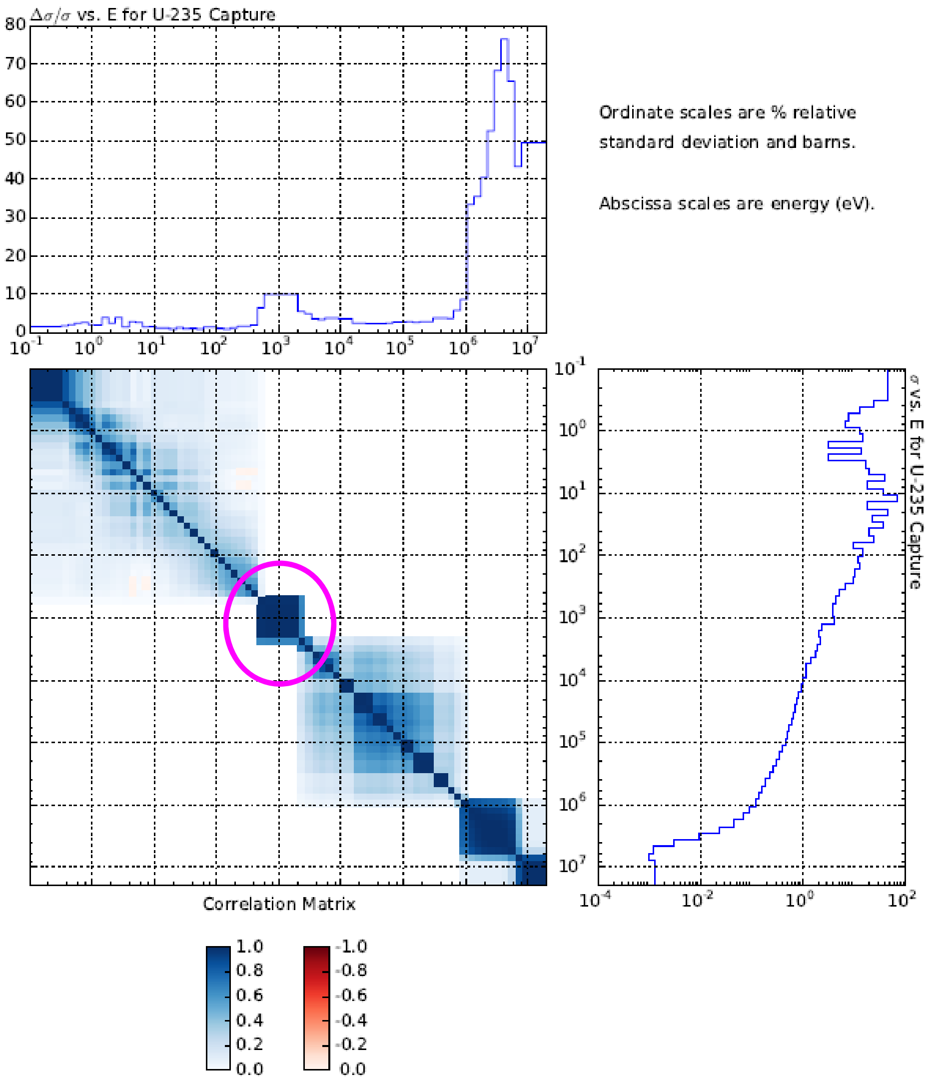
U-235 Capture (2/3)



U-235 Capture (3/3)

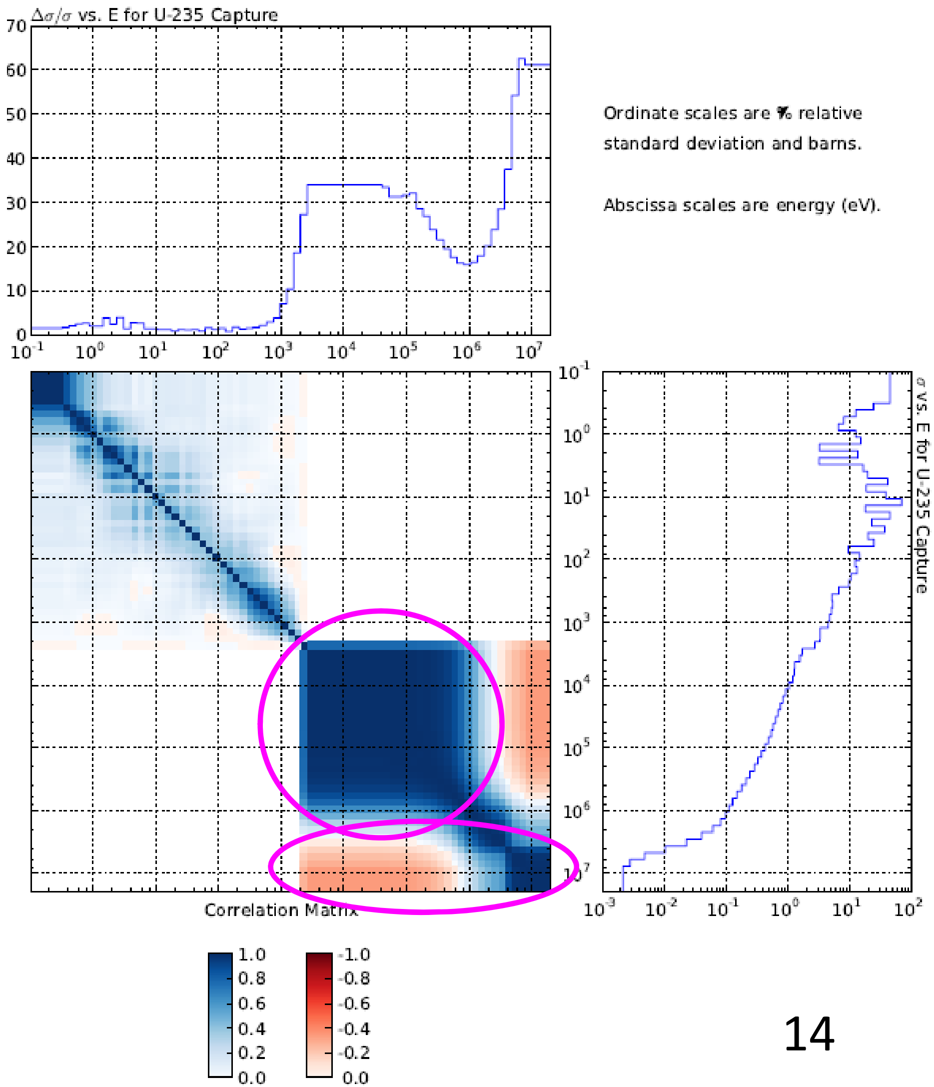
JENDL-4.0

Fig. U-235 Capture (JENDL-4.0)

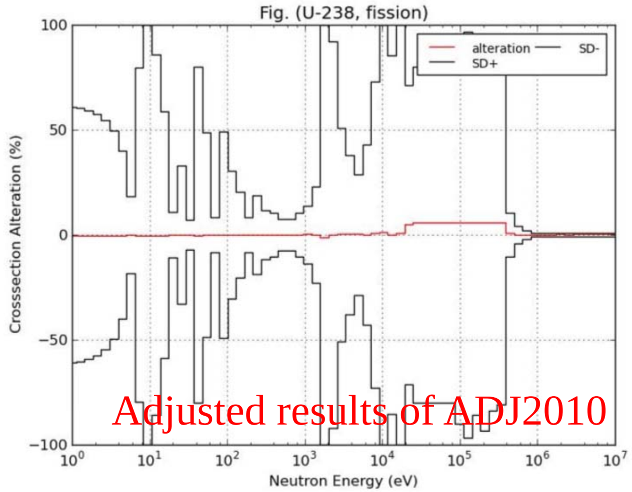


ENDF-7.1

Fig. U-235 Capture (ENDF/B-VII.1)



U-238 Fission (1/3)



<Energy Range>

1~10MeV (above threshold energy)

<Observed Fact>

In 1~10MeV, the **cross-section** and **STD** are **very similar** between **JENDL-7.0** and **ENDF-7.1**.

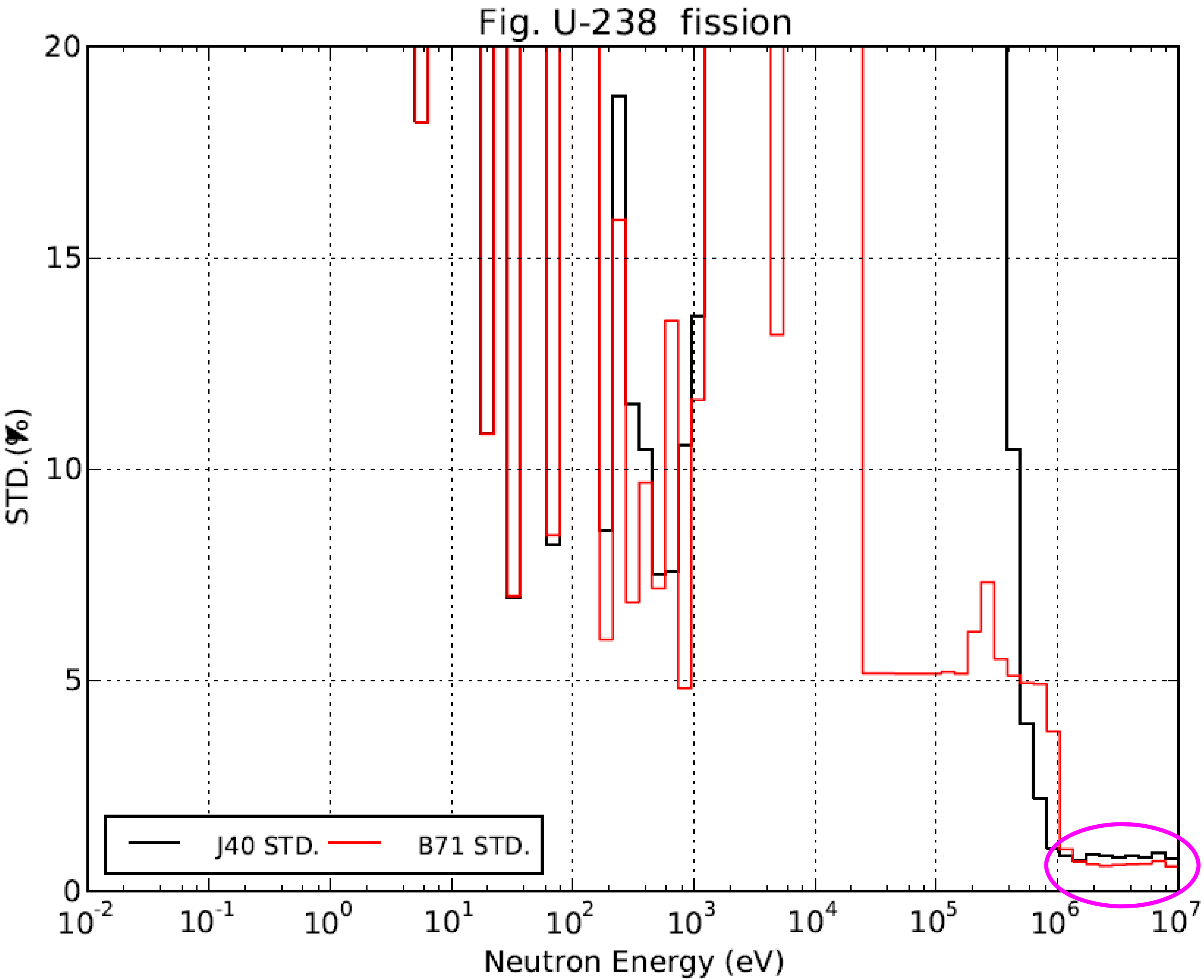
<Obtained Information and/or Comments>

JENDL-4.0 adopted the results of the simultaneous evaluation**(J-1)**, on the other hand, the covariance of ENDF-7.1 applied the evaluation by GNASH-KALMAN**(E-3)**. The similar results from the different evaluation method might come from the ample experimental data of U-238 fission.

<Recommendations>

No comments.

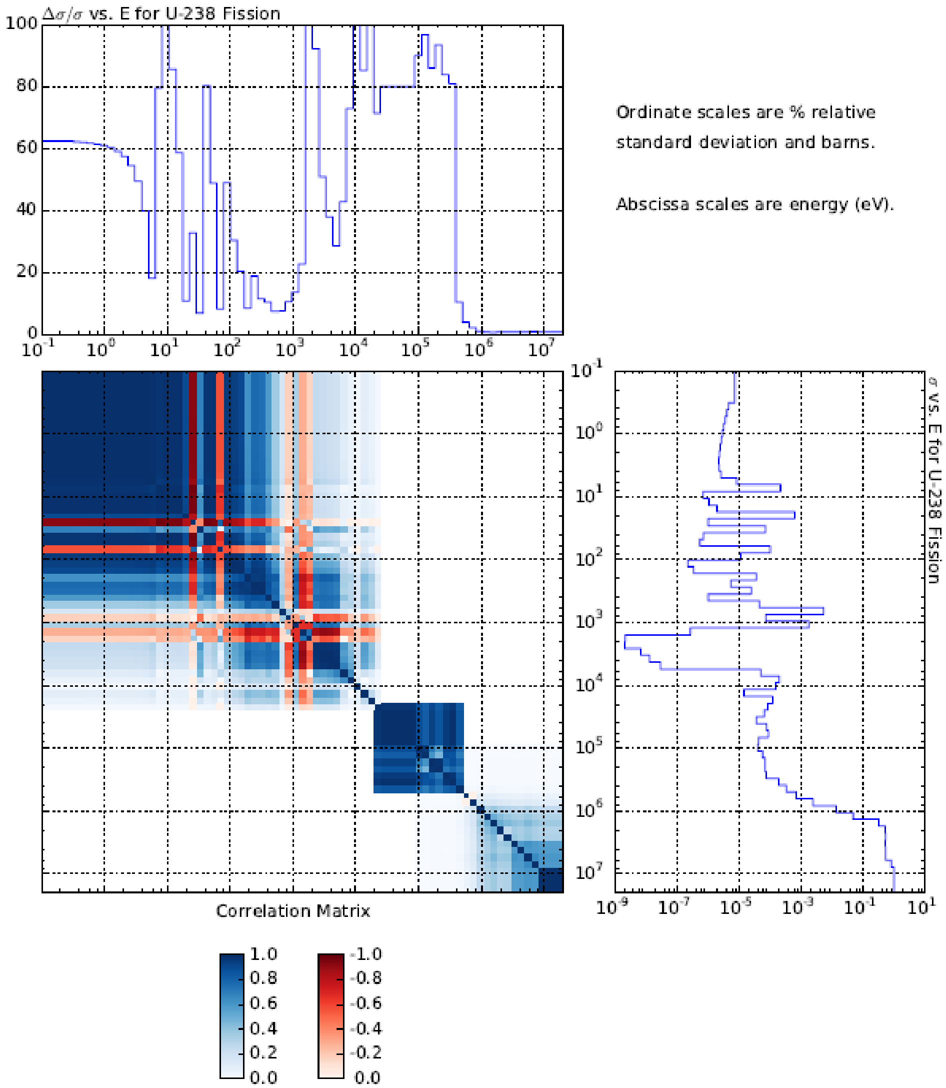
U-238 Fission (2/3)



U-238 Fission (3/3)

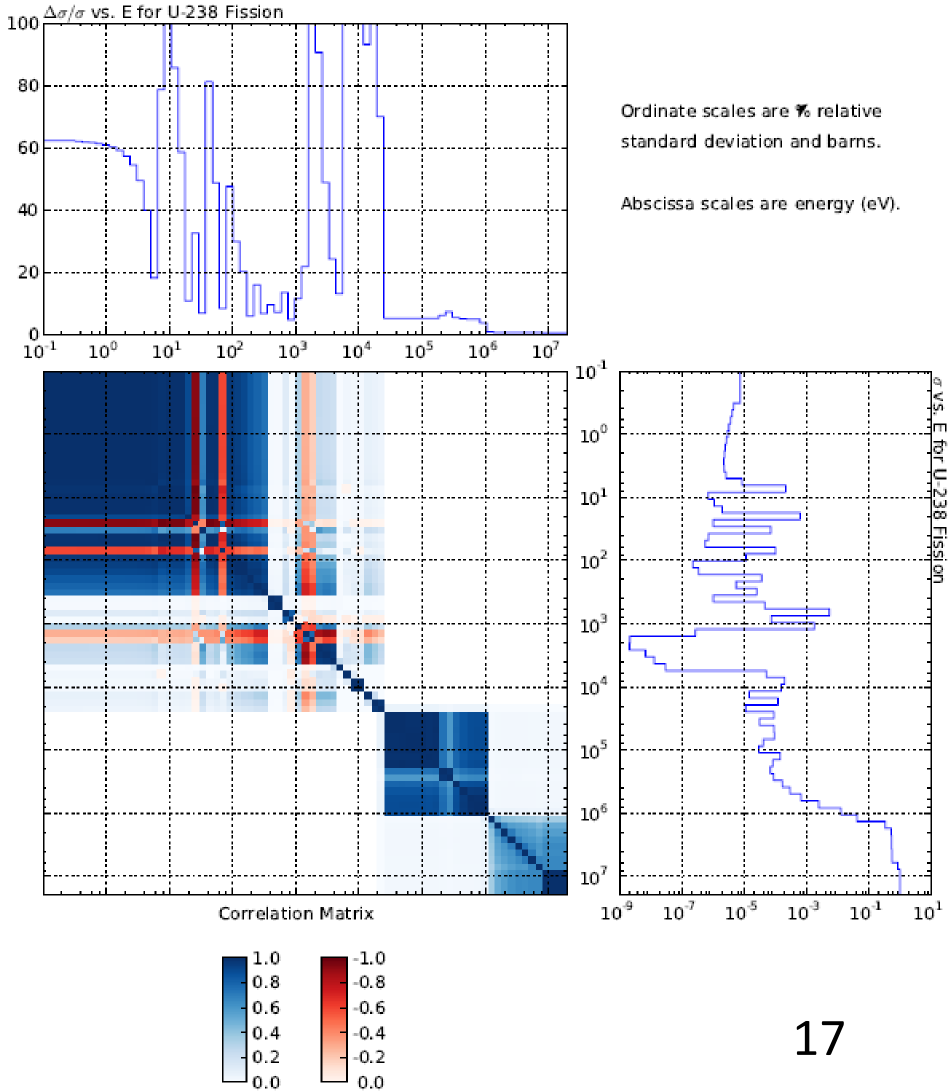
JENDL-4.0

Fig. U-238 Fission (JENDL-4.0)

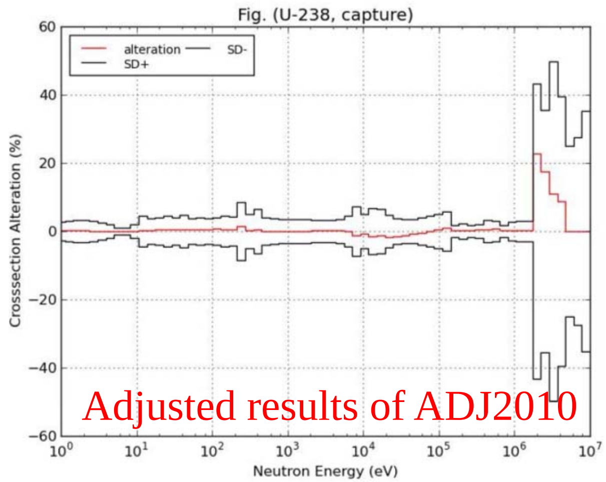


ENDF-7.1

Fig. U-238 Fission (ENDF/B-VII.1)



U-238 Capture (1/3)



<Energy Range>

1) **below 20keV** (resolved resonance region)
2) **20~150keV** (unresolved resonance region)

<Observed Facts>

1) The covariance **below 20keV** is **almost identical** between JENDL-4.0 and ENDF-7., but the **spikes of STD** appears only in **JENDL-4.0**.

2) In the unresolved region of **20~100keV**, the **STD of JENDL-4.0** is significantly **larger** than that of **ENDF-7.1**, and **vice versa in 100~150keV**.

<Obtained Information and/or Comments>

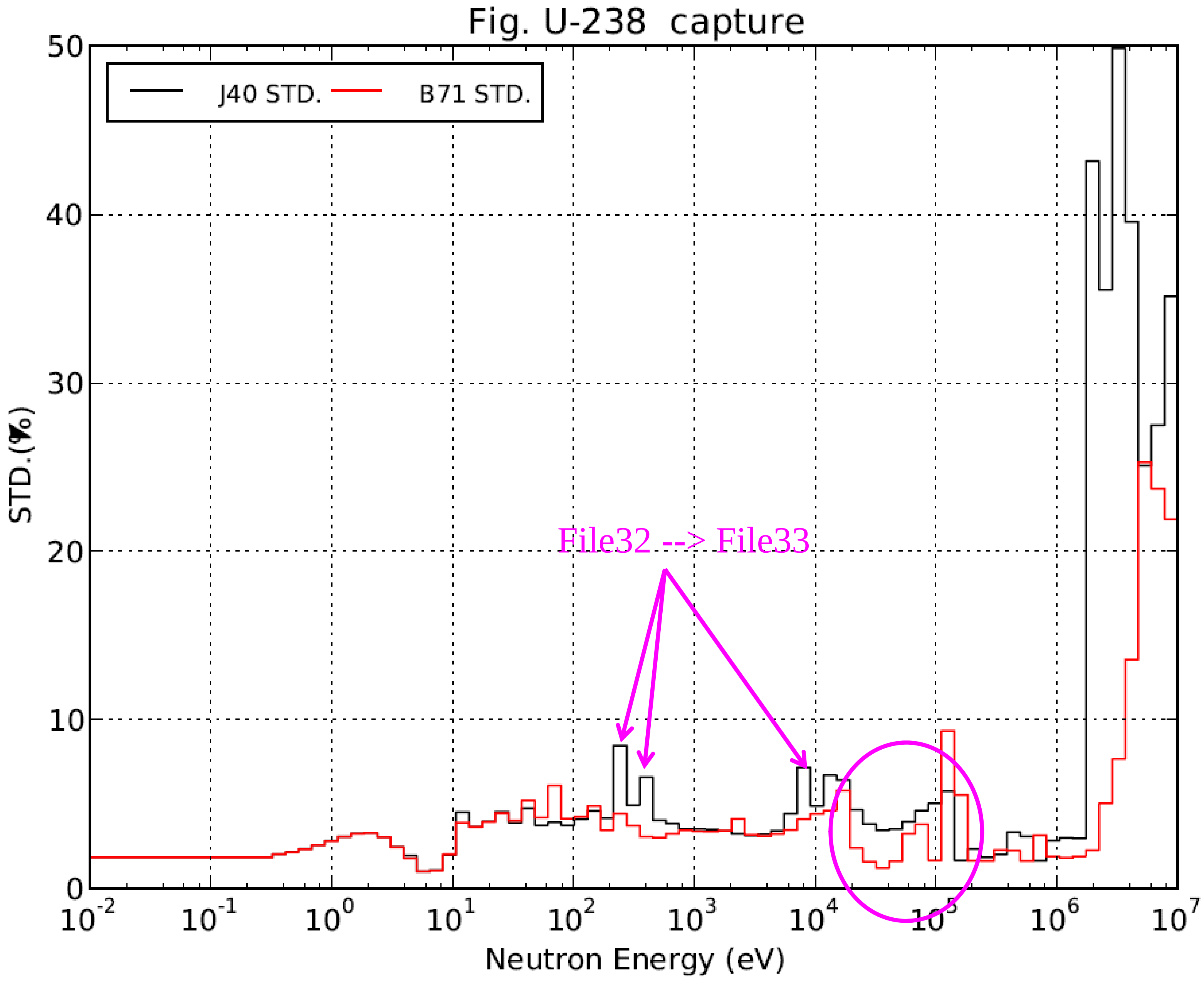
1) Both JENDL-4.0[J-3] and ENDF-7.1[E-2, p.20] adopted the same resonance parameters obtained from ORNL, and converted it to File 33. The process from File 32 to File 33 has some arbitrariness such as energy boundaries, therefore, some differences are possible even if the resonance parameters are identical[J-6].

2) The U-238 capture in the energy range of 20~150keV greatly affects the breeding ratio or burnup reactivity loss of fast reactors, therefore, these differences are very important. The covariance of JENDL-4.0 resonance parameters was evaluated with ASREP-KALMAN in 1997[J-4, p.13], but the details are not recorded.

<Recommendations>

SG39 should ask the **reason of item 2)** to both **JENDL-4.0** and **ENDF-7.1 evaluators**.

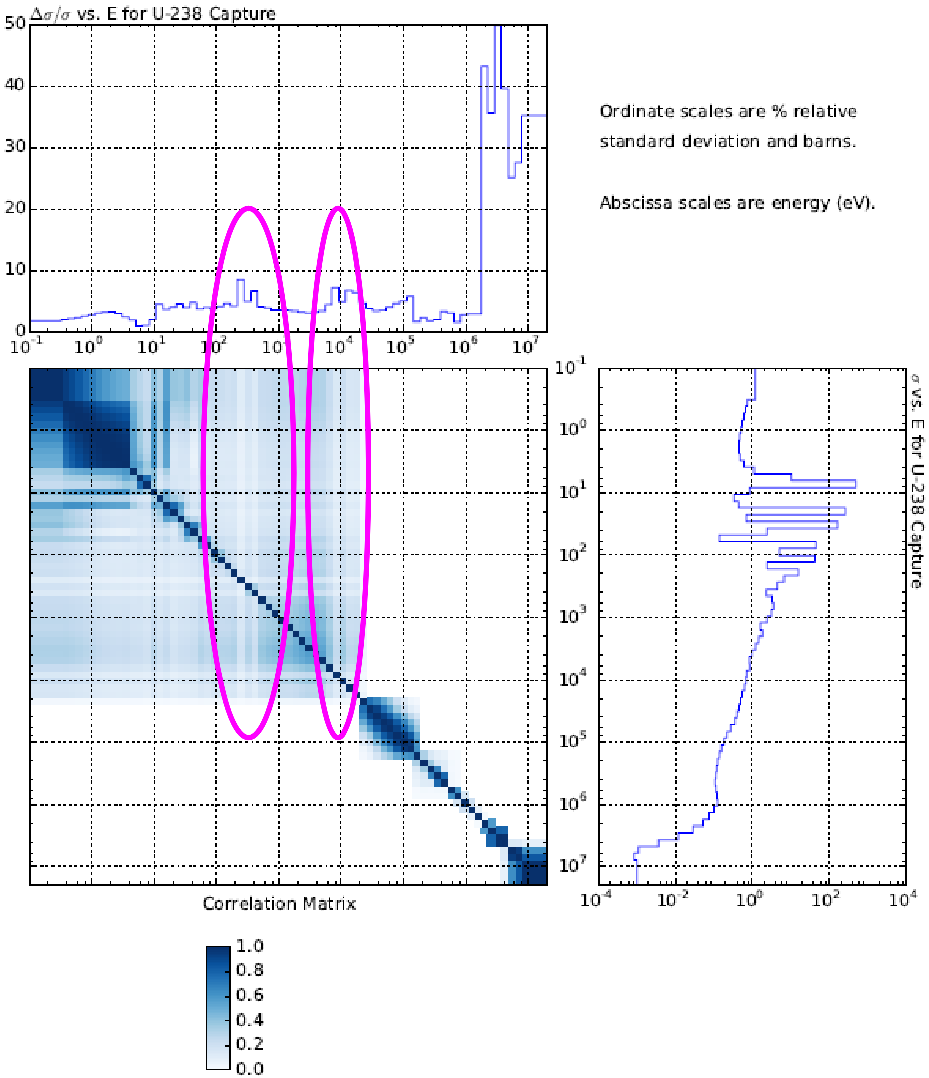
U-238 Capture (2/3)



U-238 Capture (3/3)

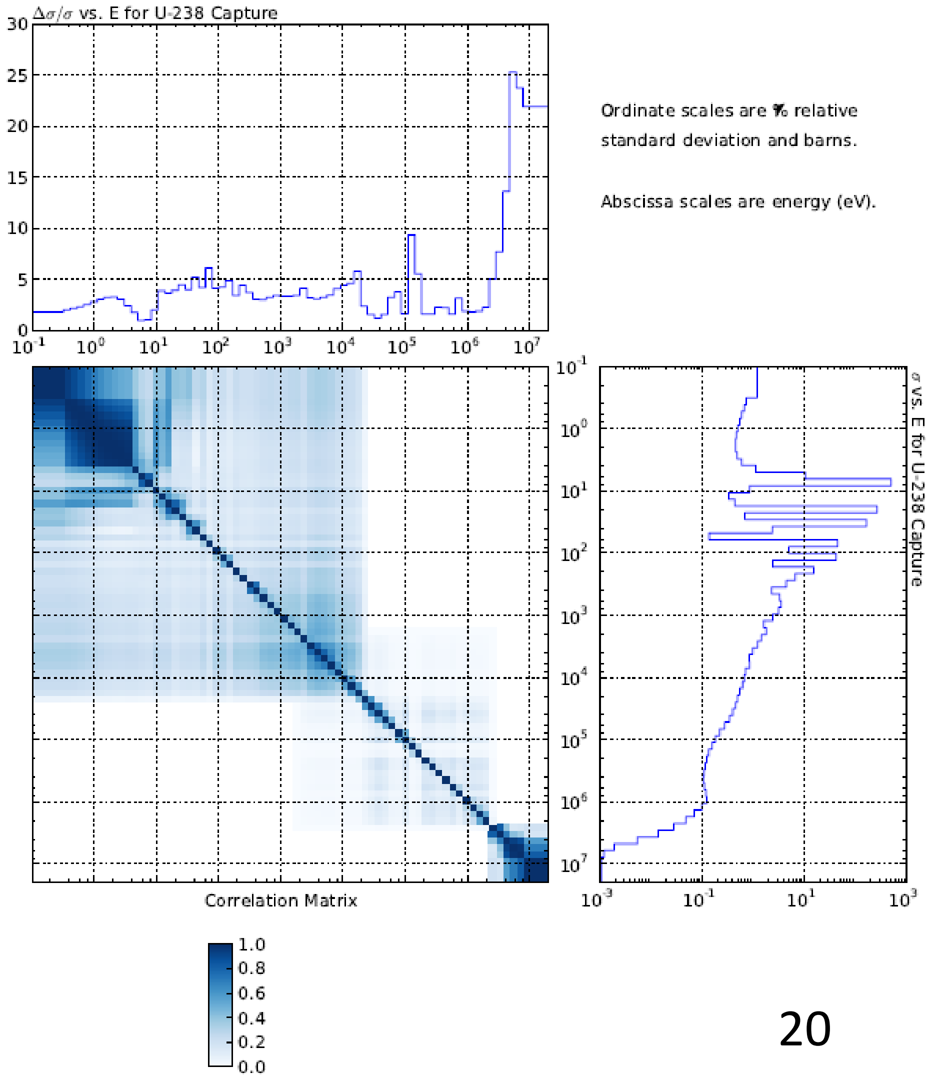
JENDL-4.0

Fig. U-238 Capture (JENDL-4.0)

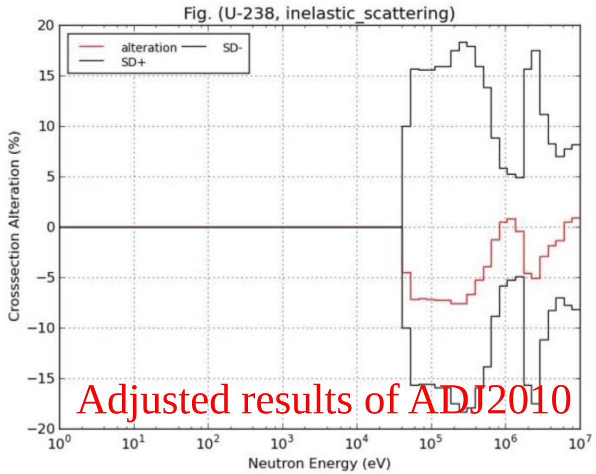


ENDF-7.1

Fig. U-238 Capture (ENDF/B-VII.1)



U-238 Inelastic (1/3)



<Energy Range>

Above 100keV (with meaningful cross-section values)

<Observed Facts>

The total inelastic **cross-sections** of **JENDL-4.0** and **ENDF-7.1** seems **quite similar**, but the **STD values and the shapes** are **completely different**.

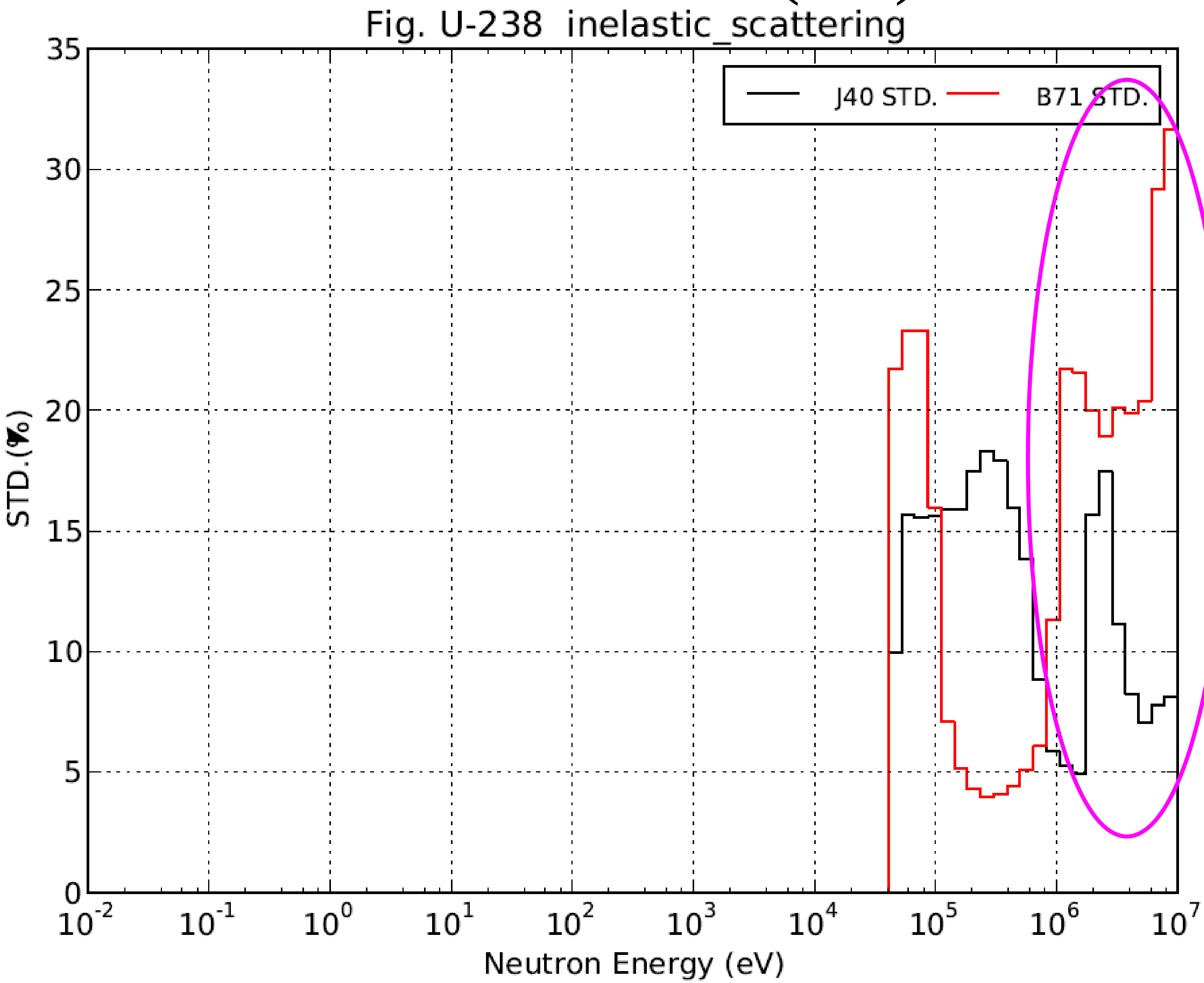
<Obtained Information and/or Comments>

A possibility was considered where the level-wise evaluation of both libraries are different but the total evaluation was similar. However, the total of inelastic cross-section is simply summation of each level-wise unlike the relation between the total and the elastic cross-section case, therefore, the idea is not the reason of the differences**[J-6]**.

<Recommendations>

SG39 had better **consult** both **JENDL-4.0** and **ENDF-7.1 evaluators**.

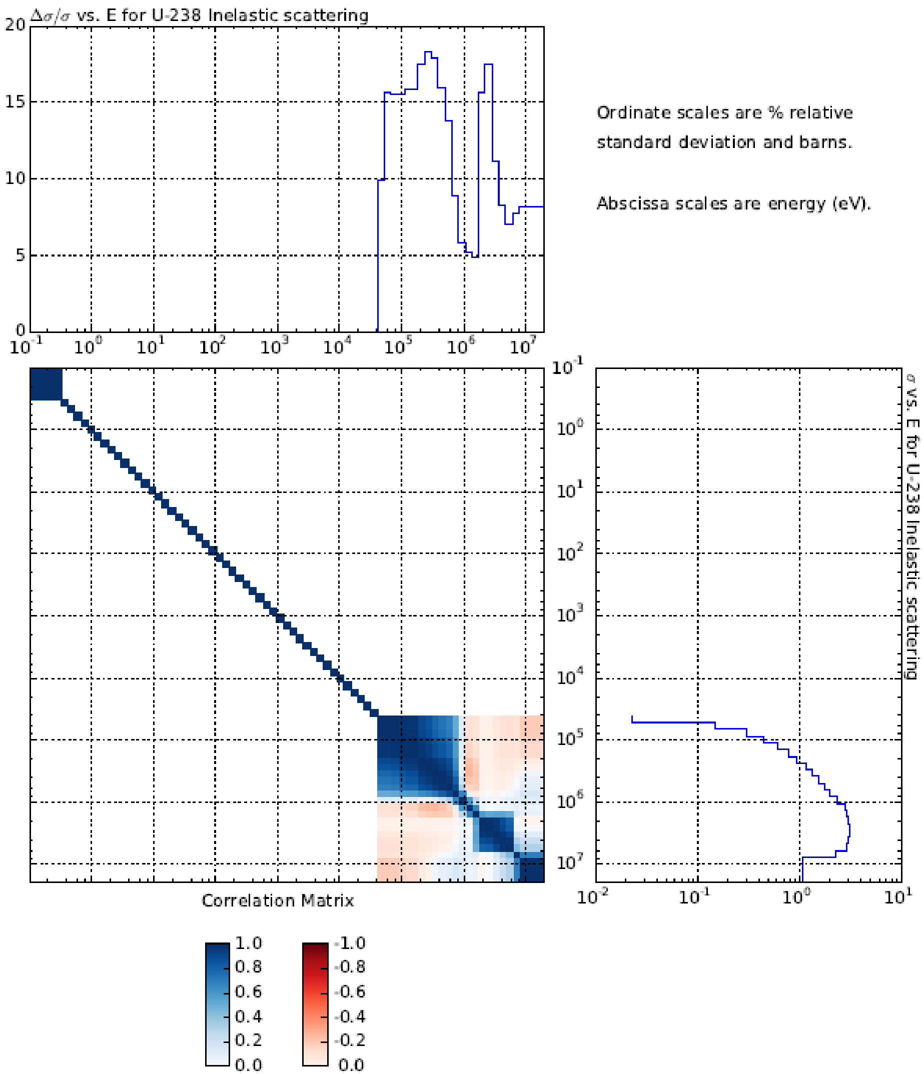
U-238 Inelastic (2/3)



U-238 Inelastic (3/3)

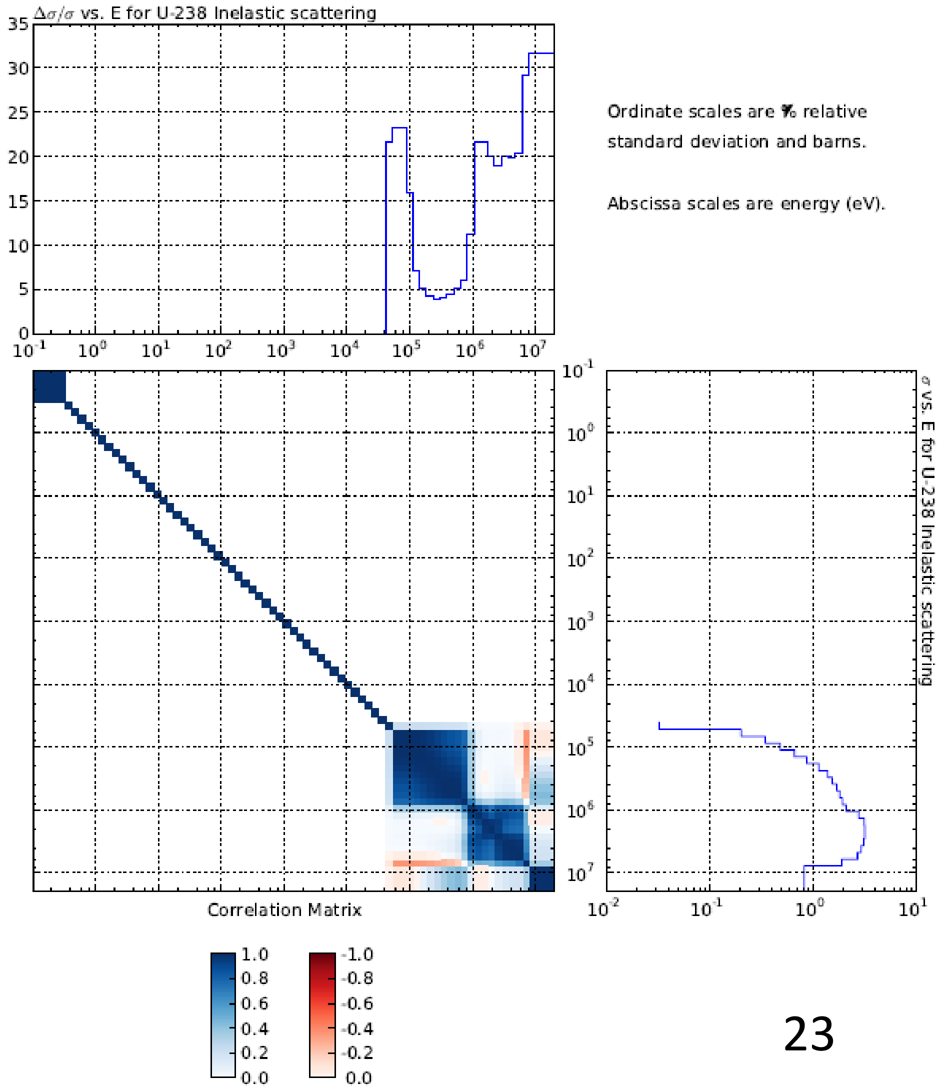
JENDL-4.0

Fig. U-238 Inelastic scattering (JENDL-4.0)

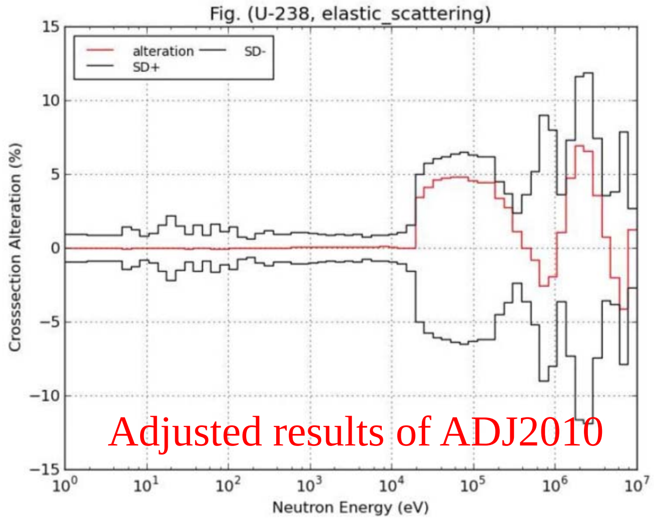


ENDF-7.1

Fig. U-238 Inelastic scattering (ENDF/B-VII.1)



U-238 Elastic (1/3)



<Energy Range>

Above 20keV (unresolved resonance and continuous energy regions)

<Observed Facts>

The STD values and shapes are rather similar in both libraries, but the energy regions with **large negative correlations** were found in **JENDL-4.0**, but **NOT in ENDF-7.1**.

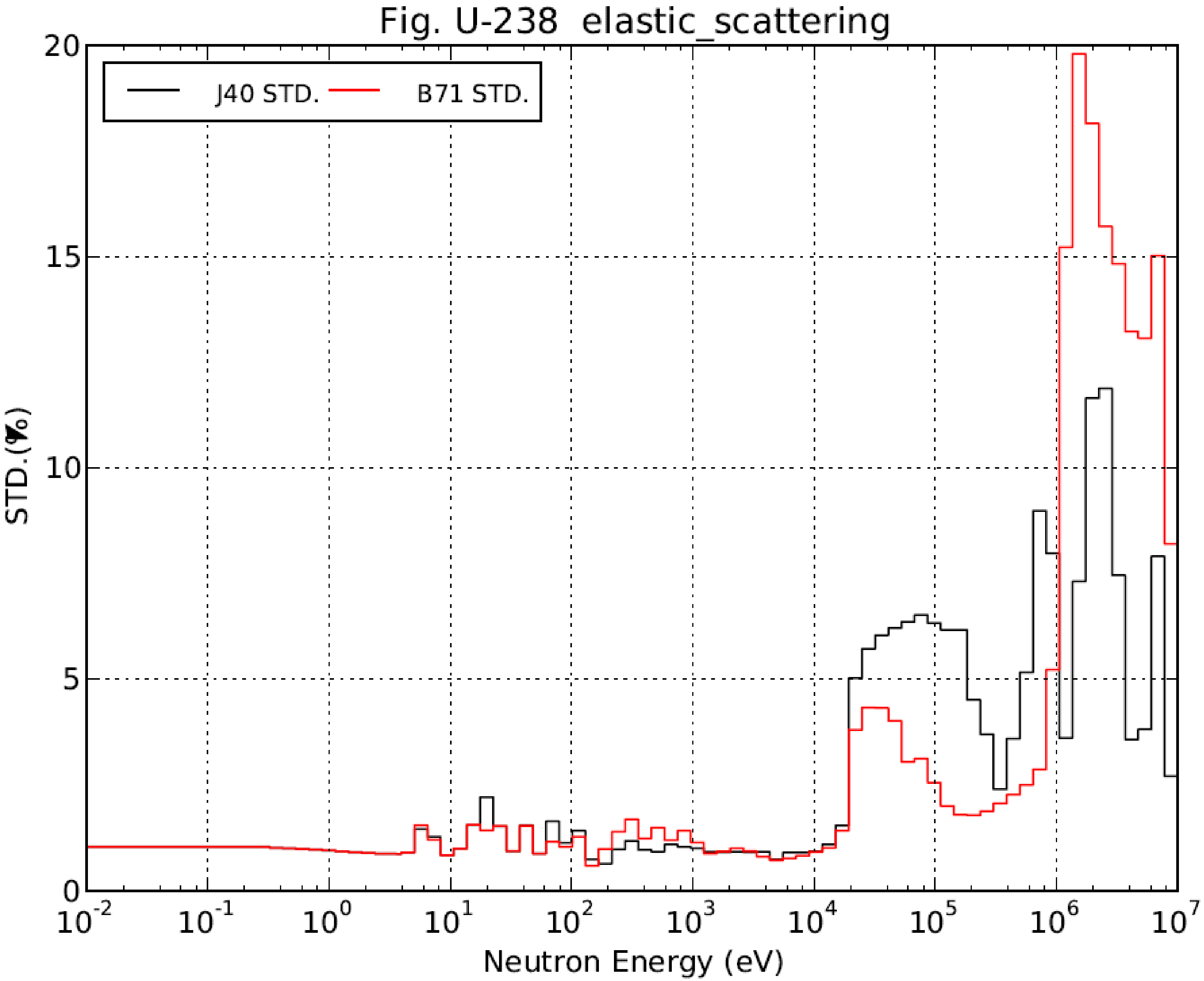
<Obtained Information and/or Comments>

The covariance of JENDL-4.0 was evaluated by CCONE-KALMAN[J-3], and that of ENDF-7.1 by GNASH-KALMAN[E-3], while both applied the relation of "Elastic=Total - Nonelastic" to evaluate the central cross-section values[J-3, E-3].

<Recommendations>

SG39 may ask the **possible reason of the correlation differences** to both **JENDL-4.0** and **ENDF-7.1 evaluators**.

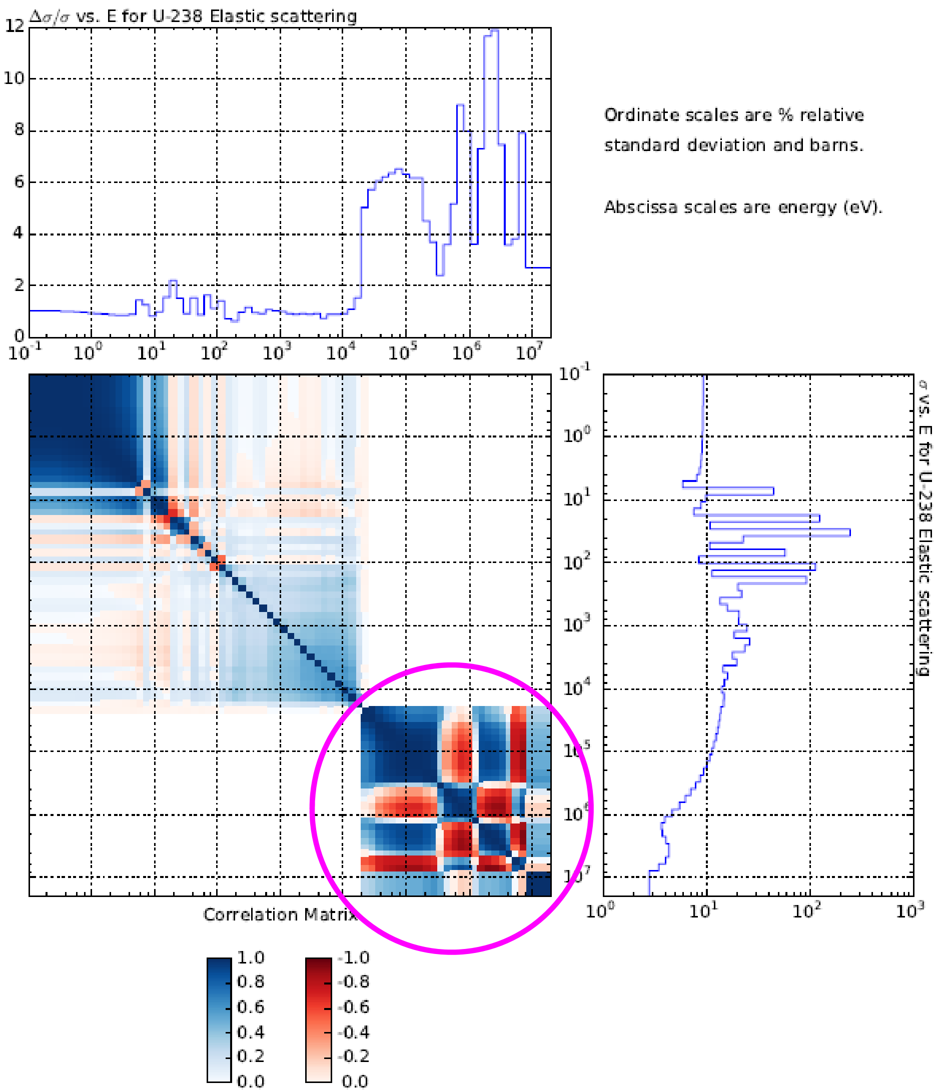
U-238 Elastic (2/3)



U-238 Elastic (3/3)

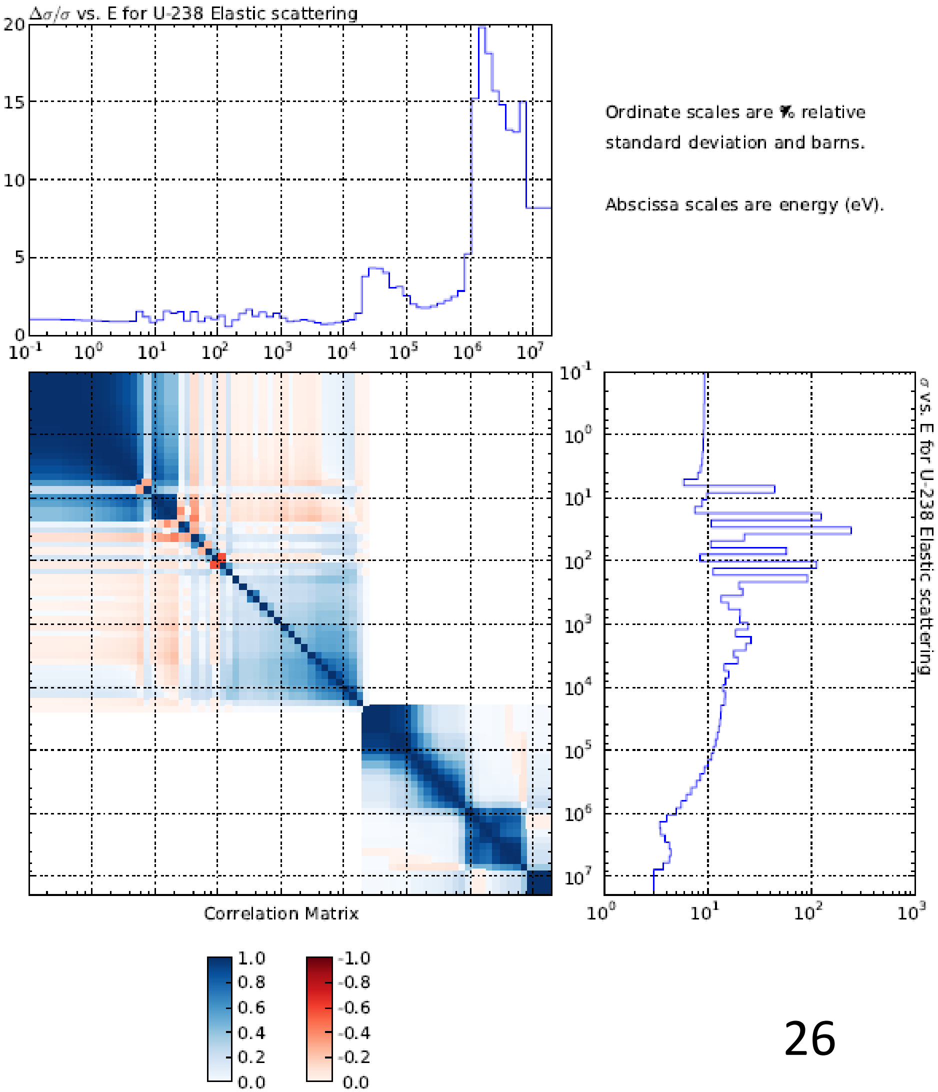
JENDL-4.0

Fig. U-238 Elastic scattering (JENDL-4.0)

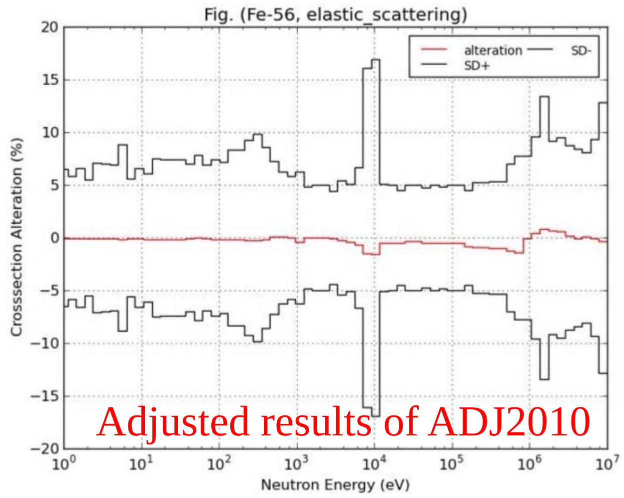


ENDF-7.1

Fig. U-238 Elastic scattering (ENDF/B-VII.1)



Fe-56 Elastic (1/3)



<Energy Range>

Below 850keV (resolved resonance region)

<Observed Facts>

The covariance of ENDF-7.1 in the energy region of 100~300eV and 300eV~30keV shows the complete correlation respectively, but the the STD values are rather similar around 6~8%. Above 30keV, the STDs of both libraries are utterly different. Further, a sharp peak near 10keV appears in JENDL-4.0, but not in ENDF-7.1.

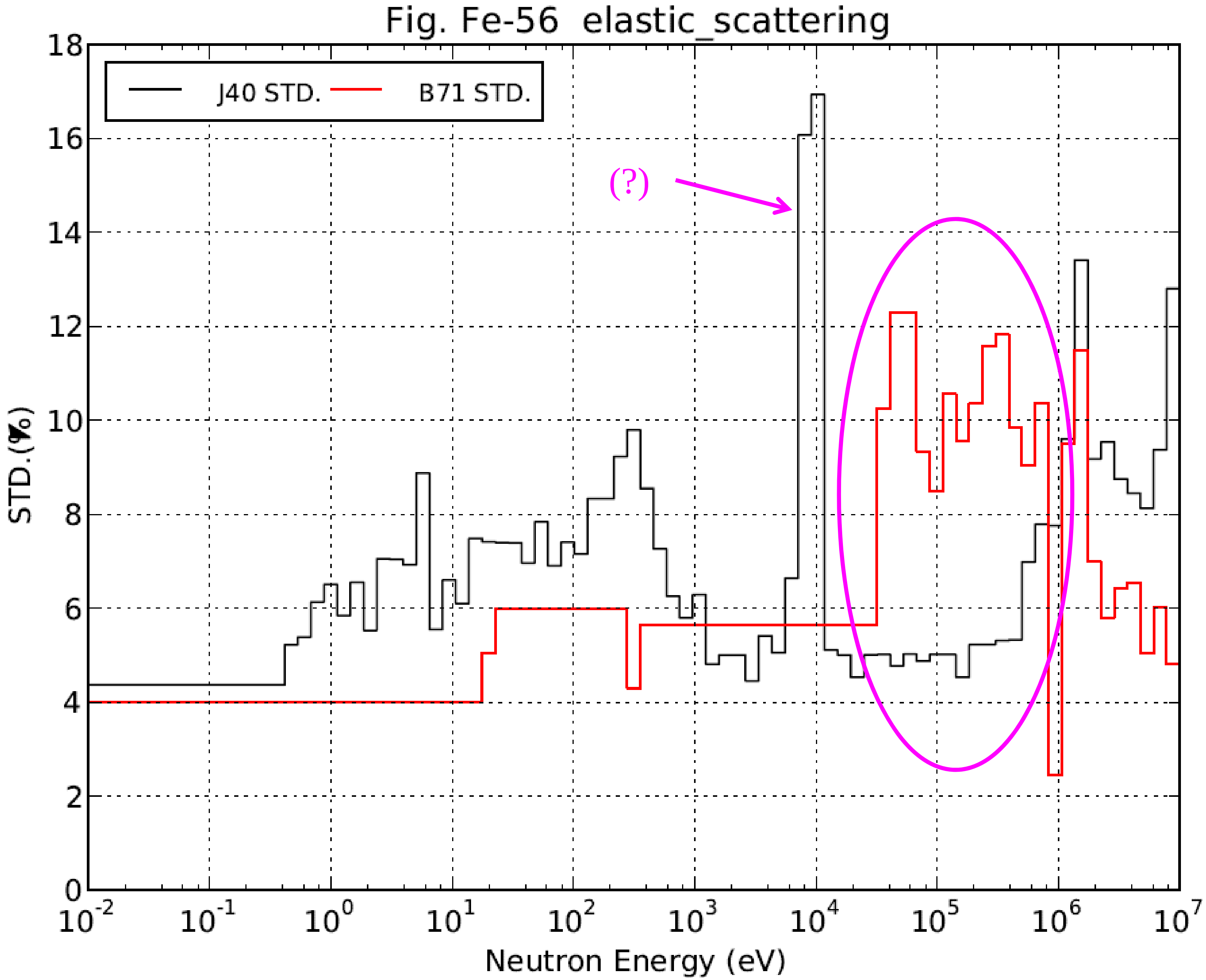
<Obtained Information and/or Comments>

The central cross-sections are almost identical, since they are based on the common resonance parameters evaluated by Froehner in 1990s[J-5]. The covariance of ENDF-7.1 was Kernel approximation with the resonance parameter uncertainty of Mugahabghab[E-2, p.15], while JENDL-4.0 adopted the least-square calculation of Fe-56 experimental data, and corrected the covariance based on the difference of the least-square central values and JENDL-4.0[J-3].

<Recommendations>

SG39 may **ask the reasonableness** of the covariance data to both **JENDL-4.0** and **ENDF-7.1 evaluators**.

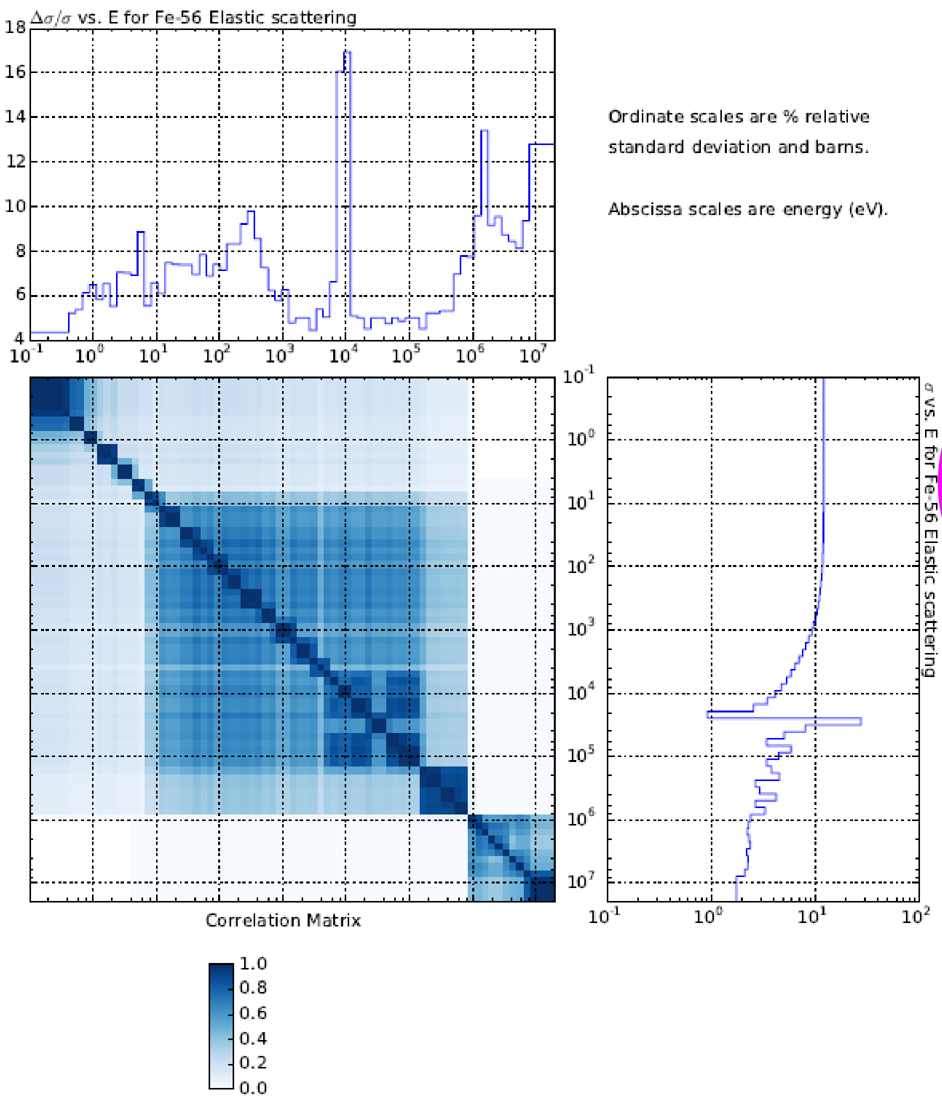
Fe-56 Elastic (2/3)



Fe-56 Elastic (3/3)

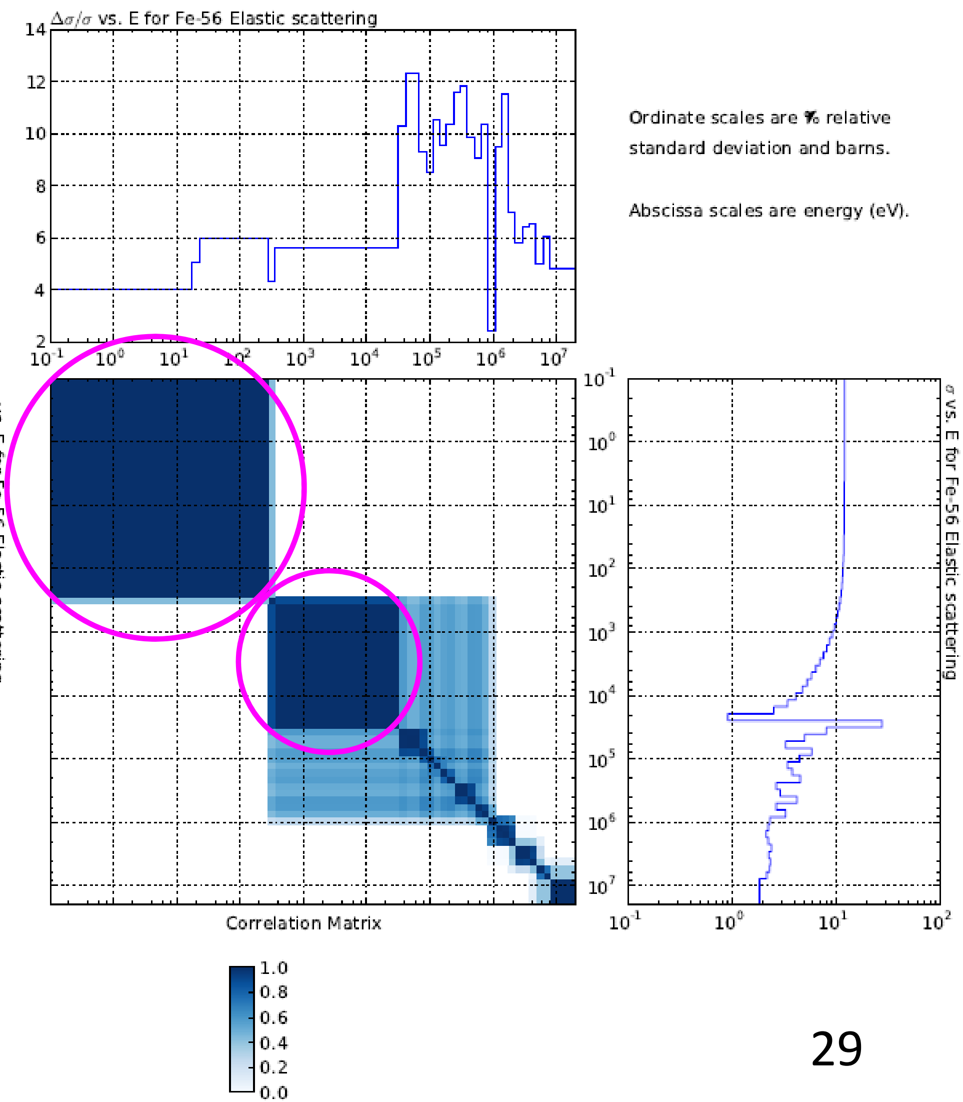
JENDL-4.0

Fig. Fe-56 Elastic scattering (JENDL-4.0)

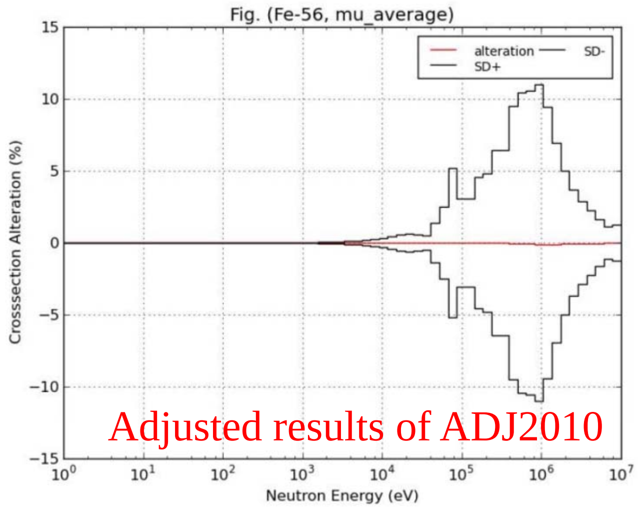


ENDF-7.1

Fig. Fe-56 Elastic scattering (ENDF/B-VII.1)



Fe-56 Mu-bar (1/3)



<Energy Range>

Above 10keV (upper part of resolved resonance region)

<Observed Facts>

In **JENDL-4.0**, the **maximum value of STD** is **10%**, on the other hand, **30%** in **ENDF-7.1**. The **negative correlation** appears in **JENDL-4.0**, **NOT in ENDF-7.1**. Further, The correlation factors are **1.0 below 50keV** in ENDF-7.1.

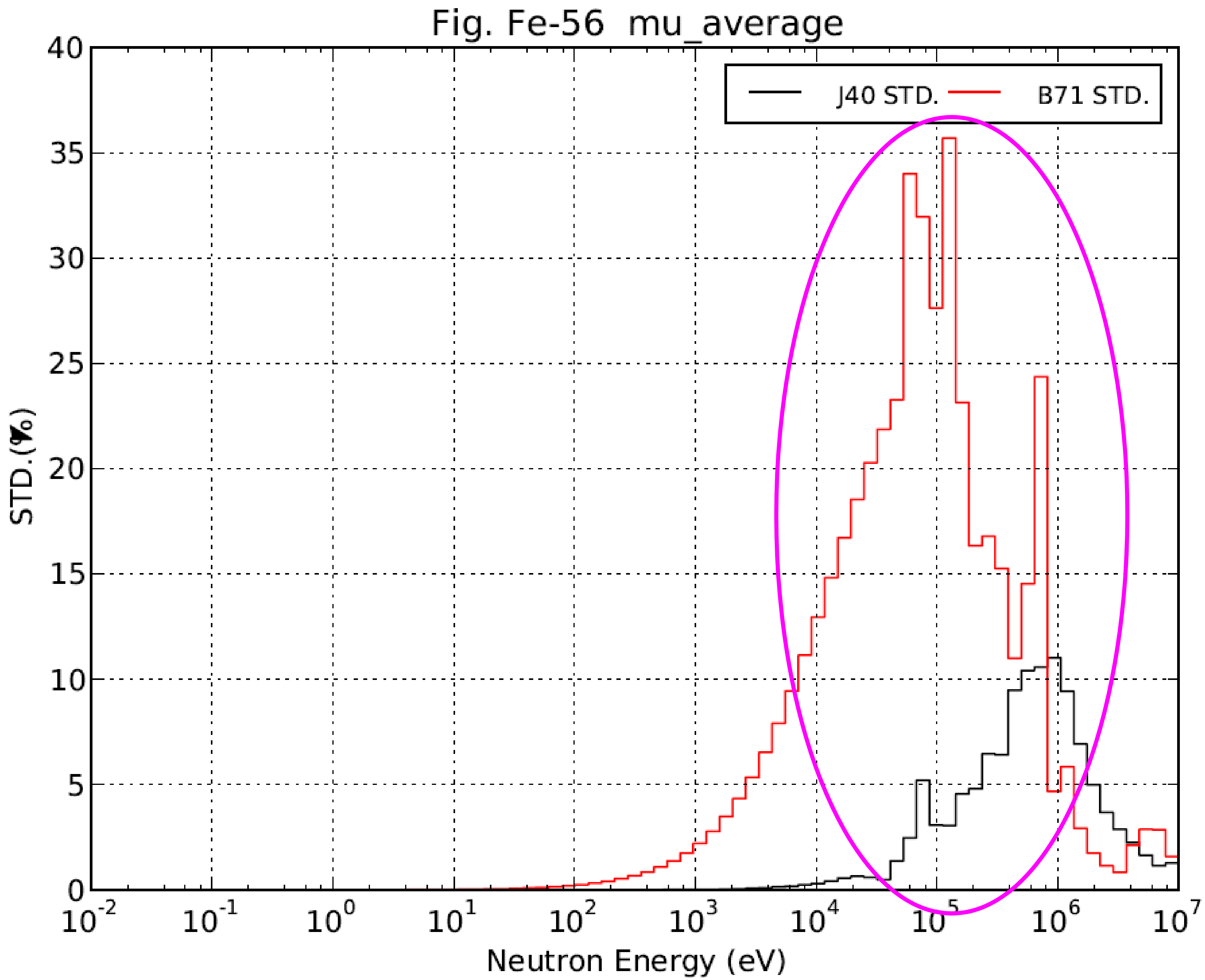
<Obtained Information and/or Comments>

The covariance of JENDL-4.0 was evaluated with ELIESE3-KALMAN in 1997**[J-4, p.8]**. That of ENDF-7.1 may be Kernel approximation as well as that of the elastic cross-section**[E-2, p.15]**. The reason of large differences are unknown.

<Recommendations>

SG39 should **ask the reason** of the large differences to both **JENDL-4.0** and **ENDF-7.1 evaluators**. Besides, **ENDF-7.1** has only the mu-bar covariance for Na-23, Fe-56 and minor actinides, but that of **other isotopes such as U-238** is also **necessary** for the reactor application.

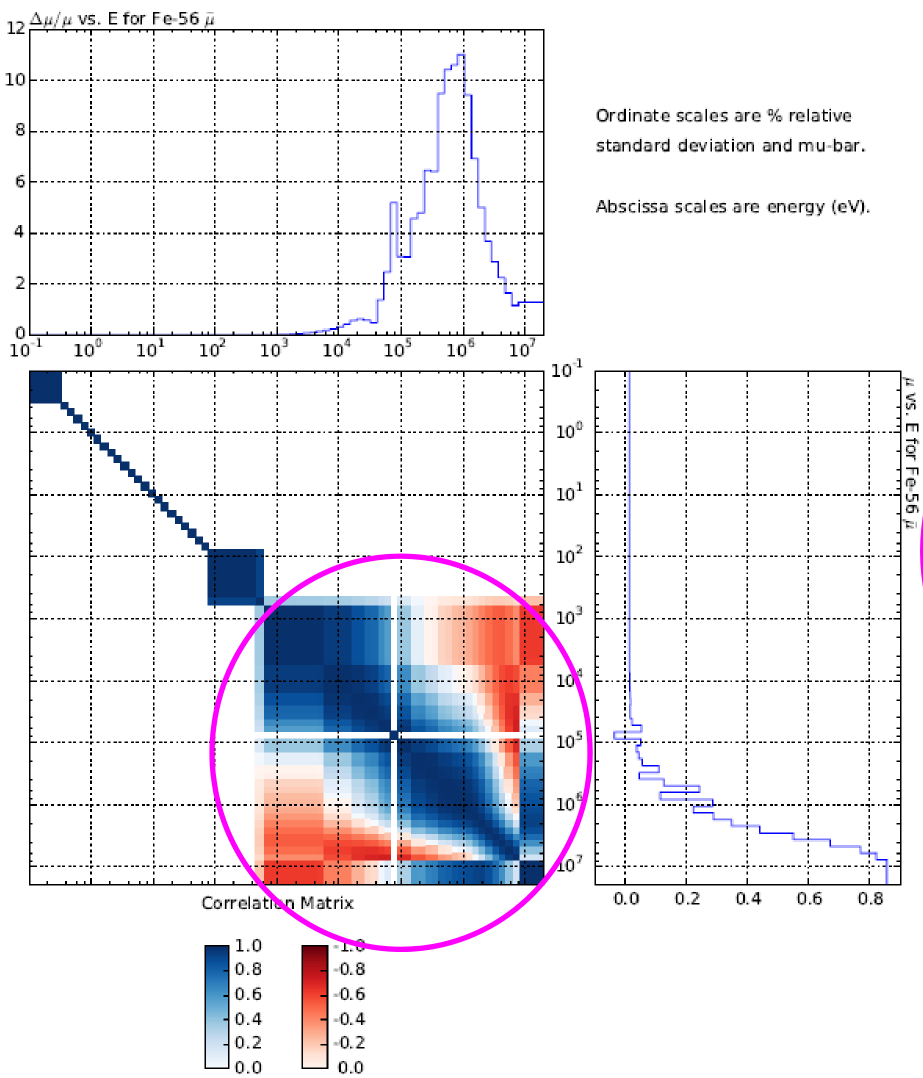
Fe-56 Mu-bar (2/3)



Fe-56 Mu-bar (3/3)

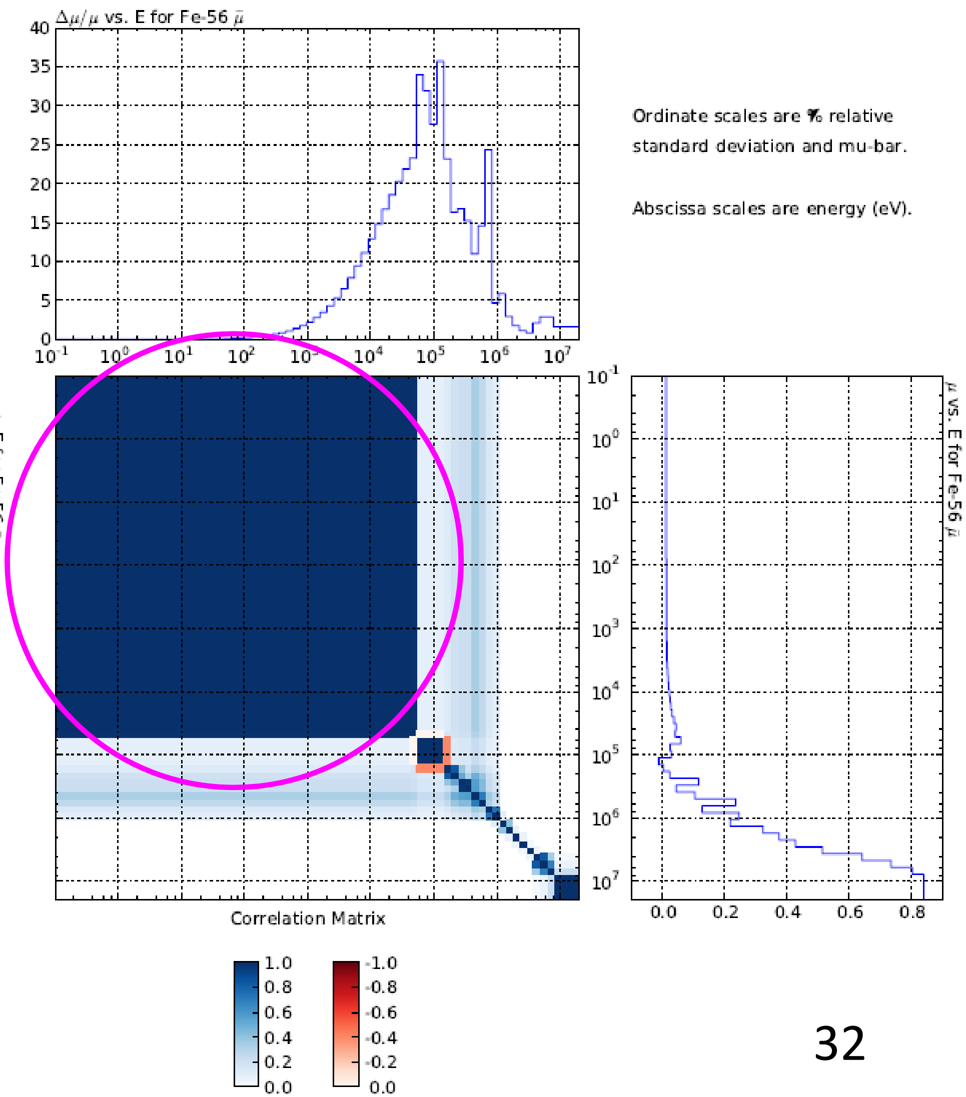
JENDL-4.0

Fig. Fe-56 $\bar{\mu}$ (JENDL-4.0)

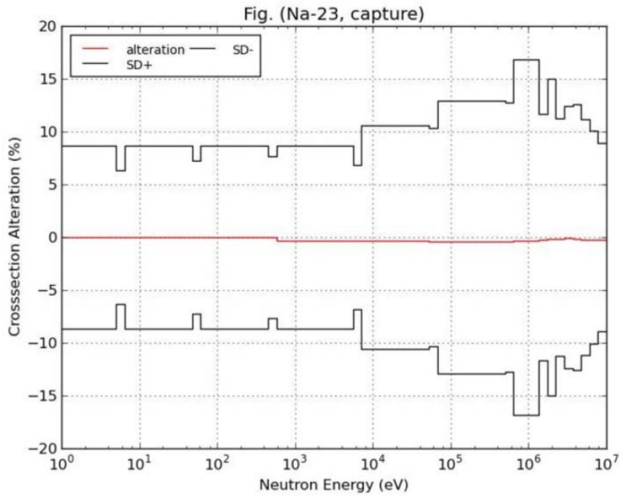


ENDF-7.1

Fig. Fe-56 $\bar{\mu}$ (ENDF/B-VII.1)



Na-23 Capture (1/3)



<Energy Range>

600eV~600keV (upper part of resolved resonance, and continuous energy region (only JENDL-4.0))

<Observed Facts>

In **JENDL-4.0**, the **STD** value is approximately **10%**, on the other hand, **100% in ENDF-7.1**, although the cross-section values are very small, the order of **milli-barn**.

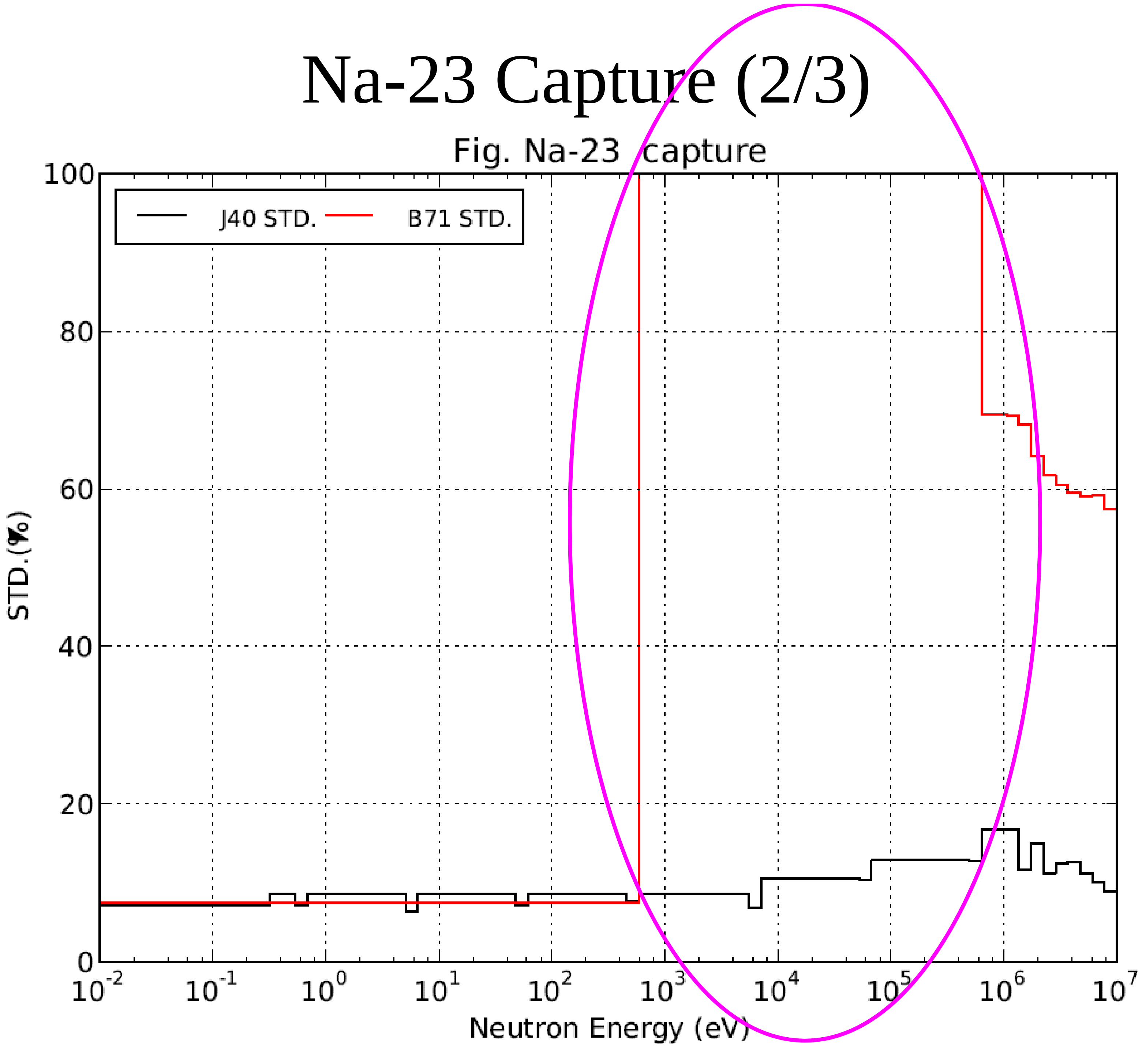
<Obtained Information and/or Comments>

The covariance of JENDL-4.0 was evaluated from the experimental values with the least-square fitting[J-3]. ENDF-7.1 adopted the results of EMPIRE-KALMAN[E-2, p.14]. The 100% STD of ENDF-7.1 might be the a priori guess which was not changed due to the large experimental uncertainty.

<Recommendations>

Though this reaction is not important for the reactor application, there would be some concerns from sodium activation viewpoint. It is **better** to **ask the reason** of the **STD differences** between **10% and 100%** to both **JENDL-4.0** and **ENDF-7.1 evaluators**.

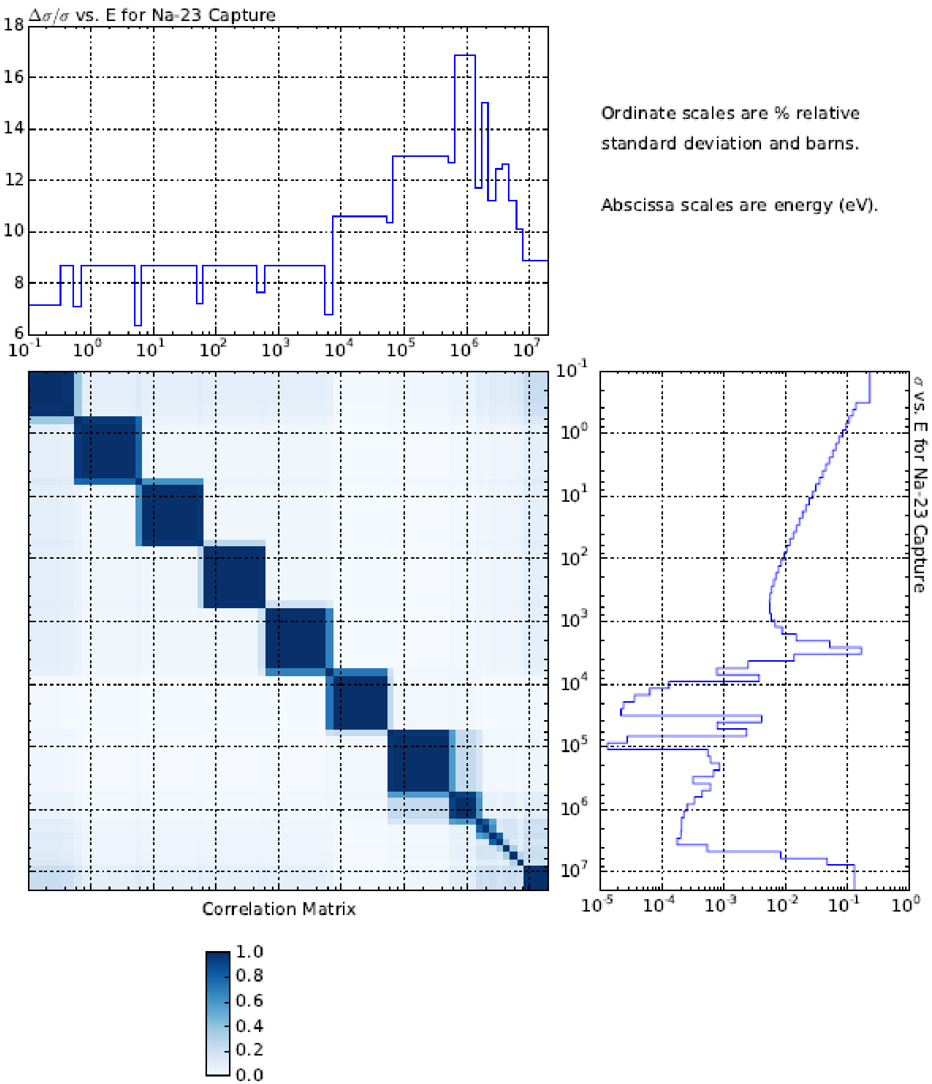
Na-23 Capture (2/3)



Na-23 Capture (3/3)

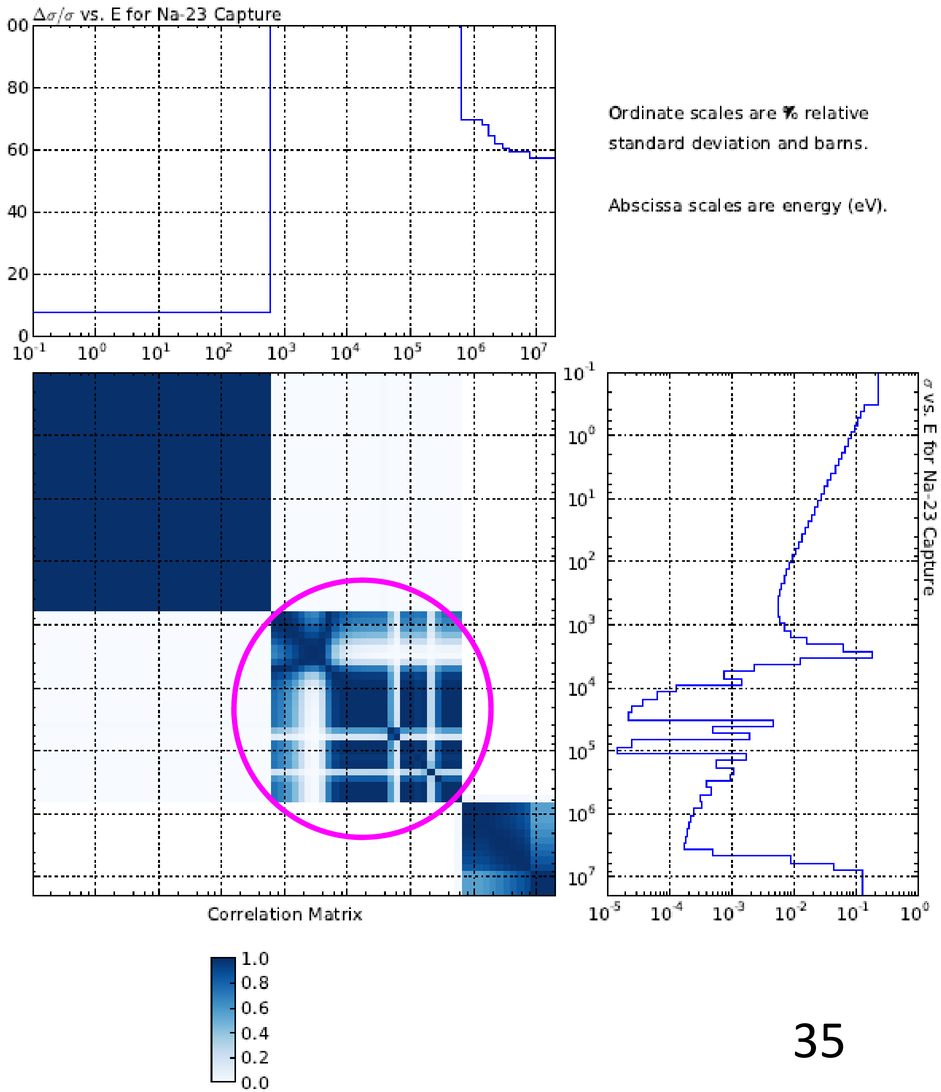
JENDL-4.0

Fig. Na-23 Capture (JENDL-4.0)

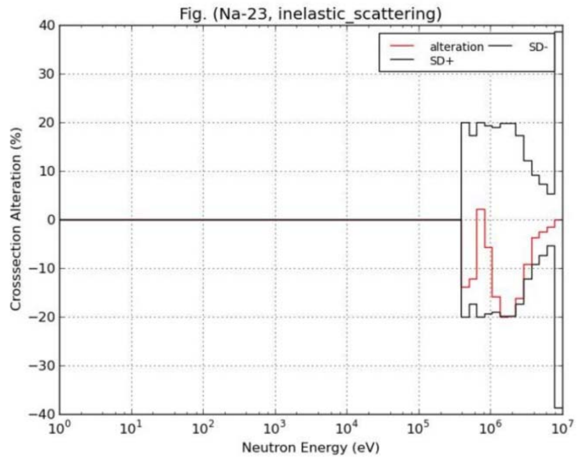


ENDF-7.1

Fig. Na-23 Capture (ENDF/B-VII.1)



Na-23 Inelastic (1/3)



<Energy Range>

Above 1MeV (with meaningful cross-section values)

<Observed Facts>

The **STD of ENDF-7.1** monotonously decreases from **17% at 1MeV** to **5% at 6MeV**, on the other hand, that of **JENDL-4.0** keeps constant value of **20% until 3MeV**, and monotonously decreases to 5% at 6MeV. Consequently, the **STD difference** of two libraries are **more than double** in the important **2~3 MeV** region.

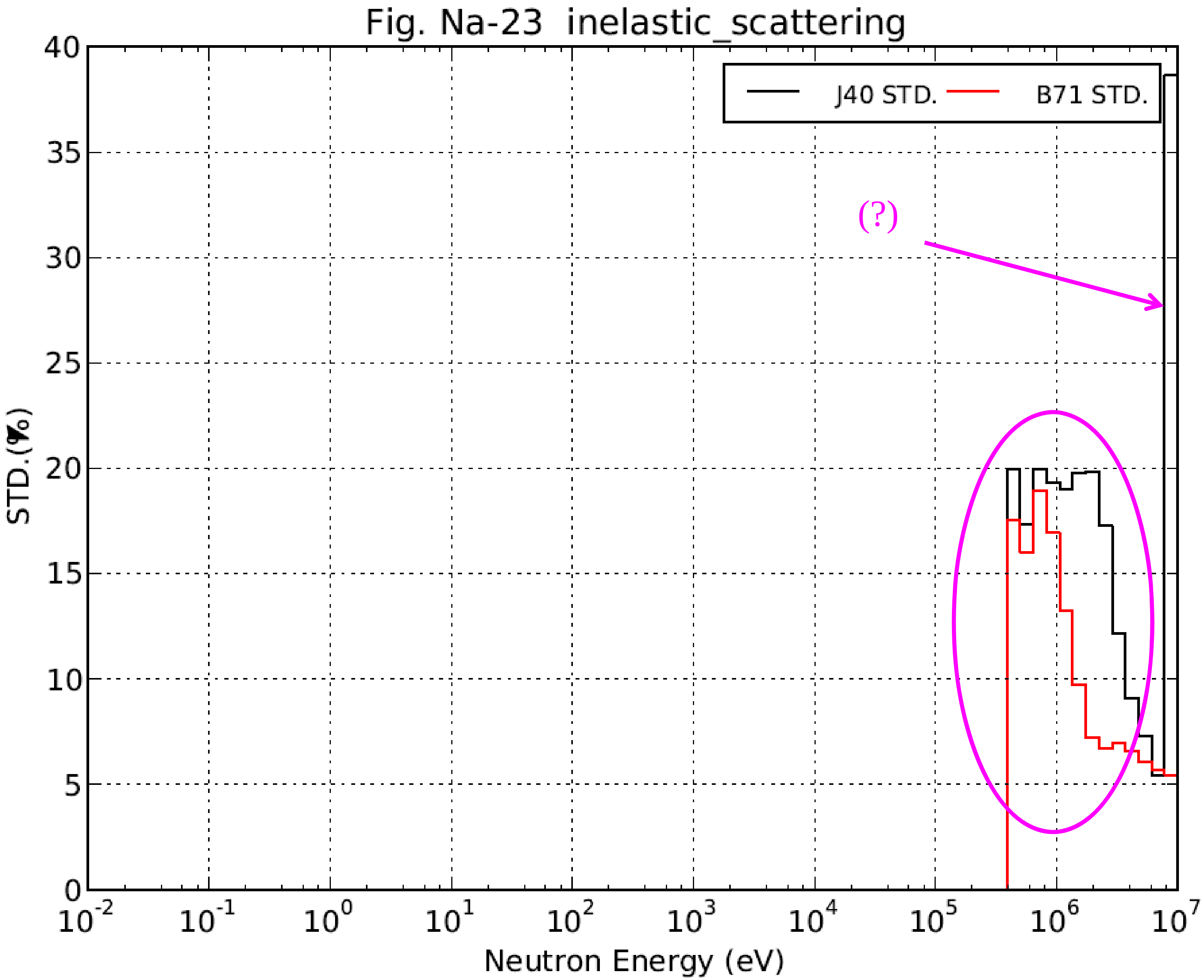
<Obtained Information and/or Comments>

The cross-section of ENDF-7.1 was evaluated with EMPIRE-excitation pre-equilibrium model using the RIPL library[E-4, p.8], while that of JENDL-7.0 adopted the results of TNG code (1986), and the first excitation level was multiplied by a factor of 1.25[J-3], according to an analytical result of an integral experimental related to neutron penetration in thick sodium layers at ORNL. The covariance of two libraries are evaluated with KALMAN[J-3, E-4], but no information related to the large STD differences.

<Recommendations>

SG39 had better **ask the physical reason** of the **large STD differences** to both **JENDL-4.0** and **ENDF-7.1 evaluators**.

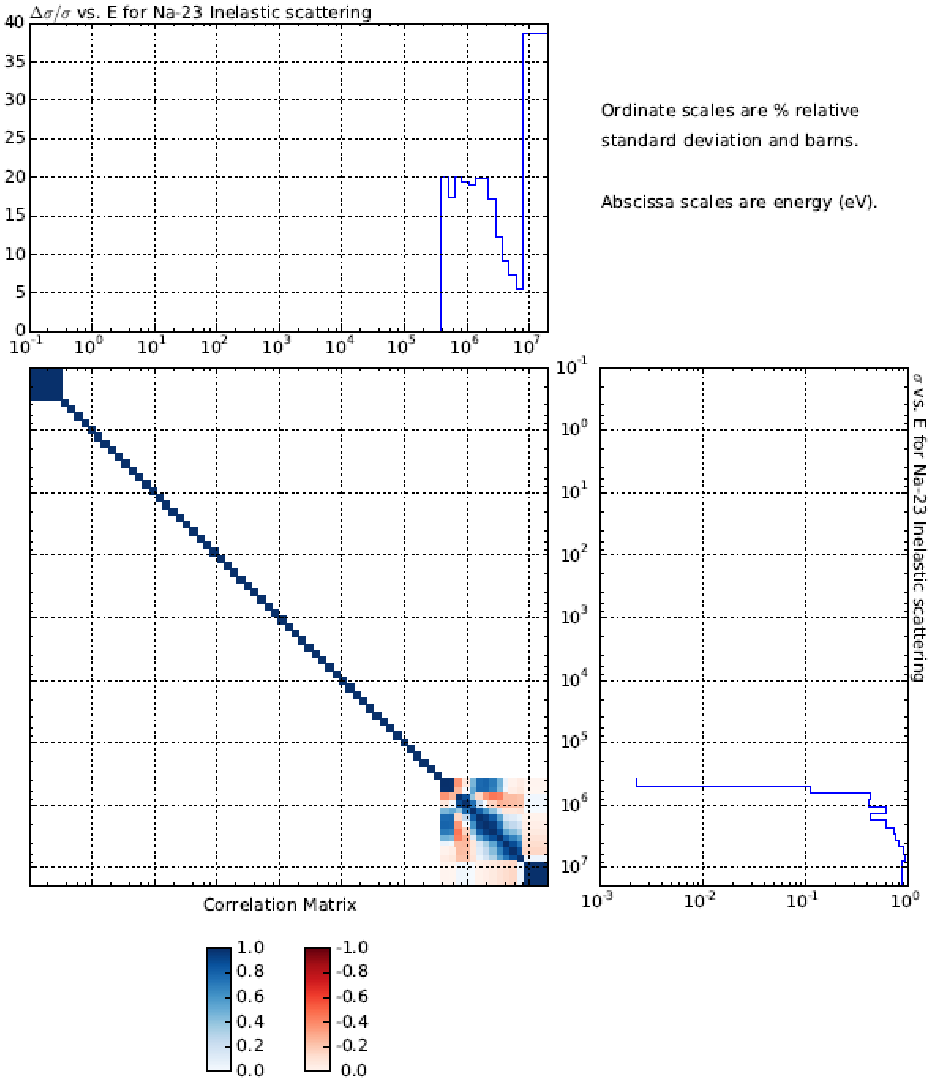
Na-23 Inelastic (2/3)



Na-23 Inelastic (3/3)

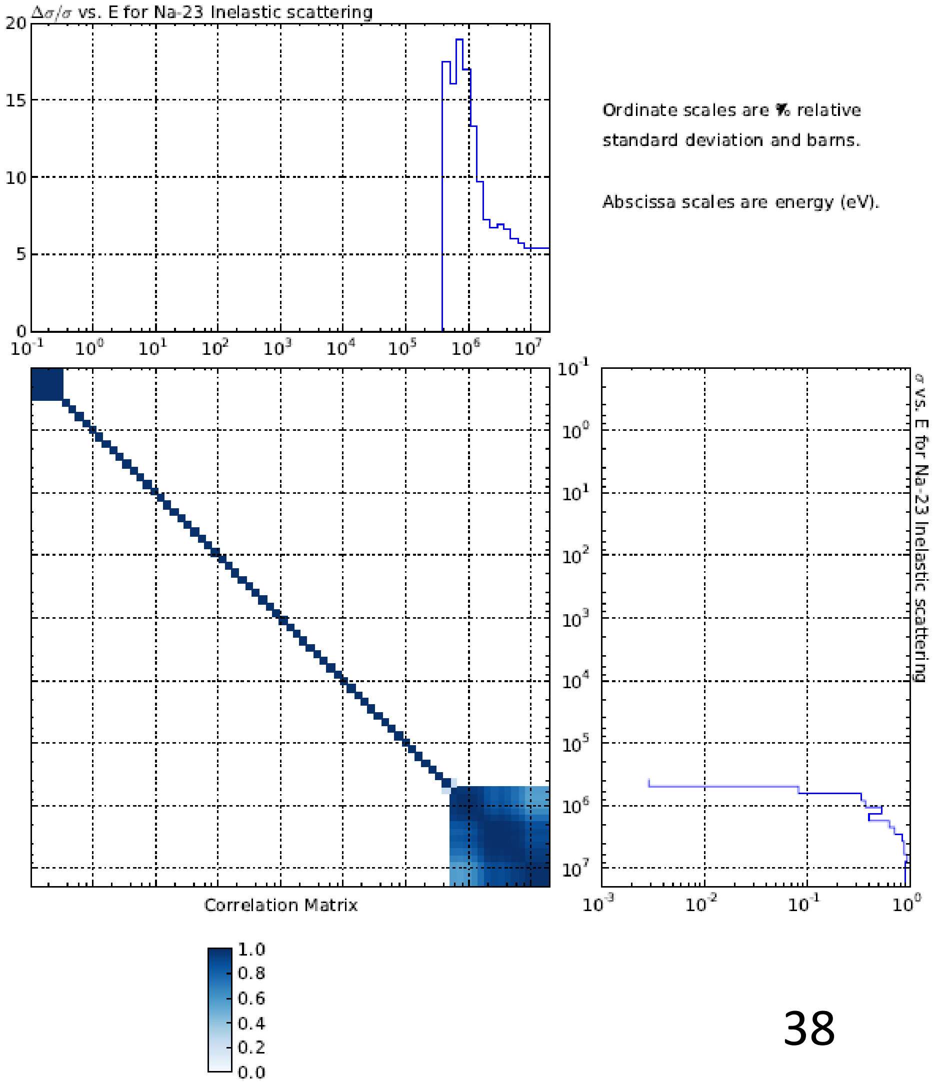
JENDL-4.0

Fig. Na-23 Inelastic scattering (JENDL-4.0)

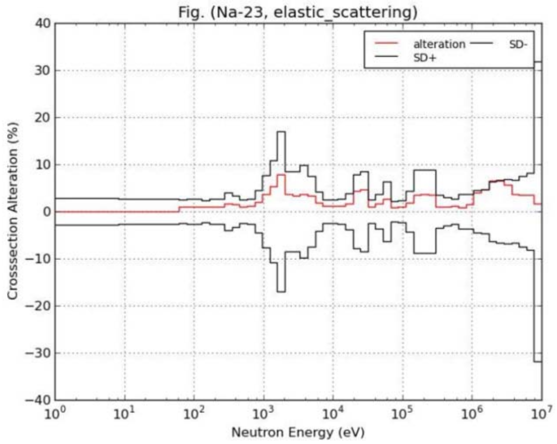


ENDF-7.1

Fig. Na-23 Inelastic scattering (ENDF/B-VII.1)



Na-23 Elastic (1/3)



<Energy Range>

Around 2keV (with a giant resonance peak)

<Observed Facts>

In **JENDL-4.0**, the **STD at the resonance peak** takes the **maximum value of 17%,** on the other hand, that of **ENDF-7.1** the minimum value of 1%. Further, the correlation with other energy region is seen in JENDL-4.0, but not in ENDF-7.1.

<Obtained Information and/or Comments>

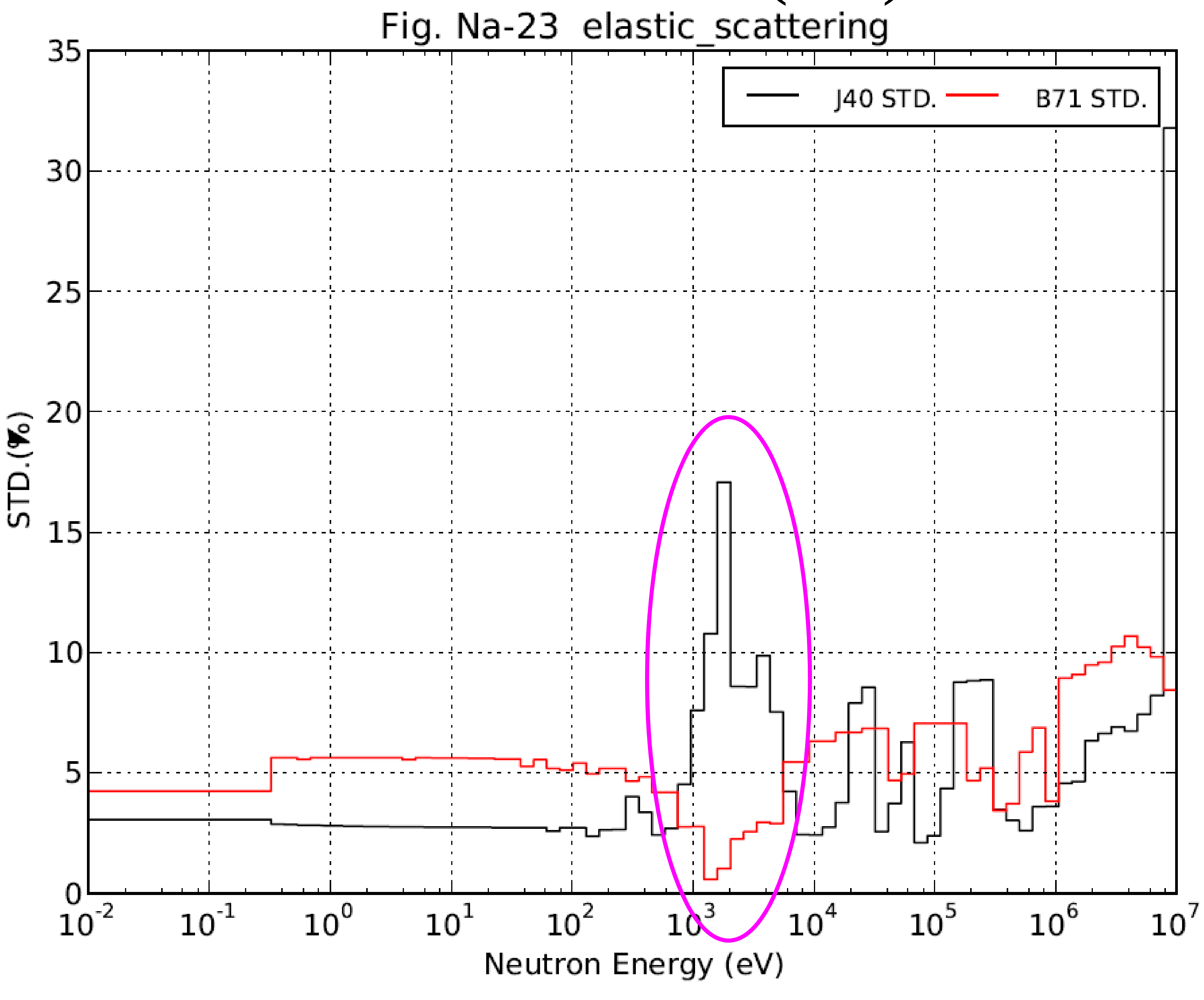
The physical reason of the large covariance differences between two libraries can be found in the SG33 final report, p.38.

"In this energy range, there appears a giant resonance peak which significantly affects the sodium-voiding reactivity in sodium-cooled fast reactor cores. As shown in Figure 15, the shape of standard deviation (STD) is extremely different between two libraries, that is, the minimum STD value occurs at the cross-section peak energy in C-2.0, in contrast, the maximum appears there in J-4.0. It can be concluded that the trend of C-2.0 seems more natural, since the larger cross-sections would be more accurate due to the small statistical error in the measurement. The correlations are also quite different. In the C-2.0 covariance, the 2 keV peak has no correlations with other energy3, while J-4.0 is partially positive everywhere above 100 eV. The covariance of C-2.0 is evaluated by the EMPIRE/KALMAN combination, where the prior resonance model parameter uncertainties are derived from Mughabghab, on the other hand, J-4.0 applies the GMA code with some corrections to meet the measured cross-sections with the evaluated ones of J-4.0 which is based on the multi-level Breit-Wigner formula with rather old resonance parameter values recommended by BNL in 1981. The cross-section difference between ENDF/B-VII.0 and J-4.0 is -17~+4% around 2 keV, therefore, the difference of STDs might be reasonable considering the corrections given to J-4.0 covariance."

<Recommendations>

No comments.

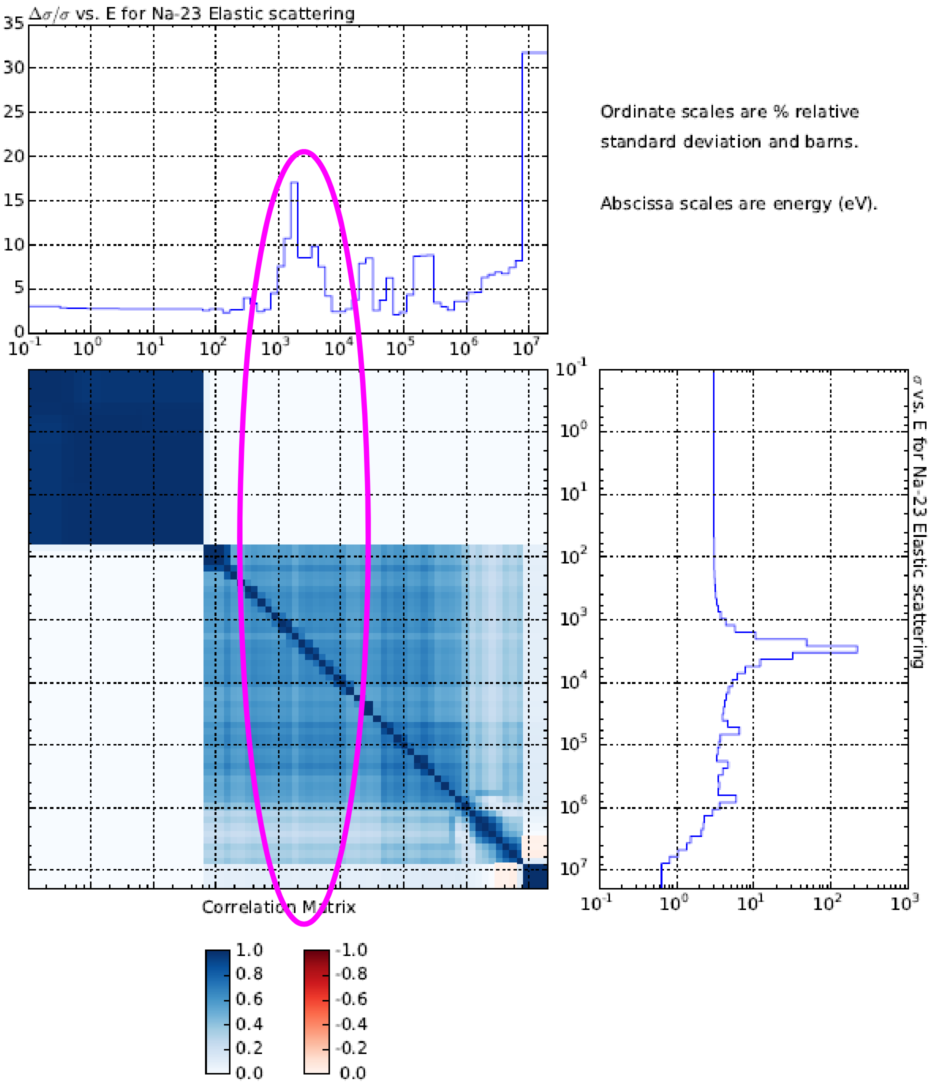
Na-23 Elastic (2/3)



Na-23 Elastic (3/3)

JENDL-4.0

Fig. Na-23 Elastic scattering (JENDL-4.0)



ENDF-7.1

Fig. Na-23 Elastic scattering (ENDF/B-VII.1)