Ga-ele comparison:

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| File | Library | MT444; disdam | | | MT Ratio  14-MeV / 1-MeV | Comment |
| 19.95 MeV | 14.05 MeV | 0.98 MeV |
| Ga-ele\_TENDL…ASTM-DE…444 | TENDL-2019 | 60.560E3 | 54.682E3 | 29.257E3 | 1.87 | eV-b  used legacy eff with typo  no threshold treatment |
| Ga-ele\_TENDL…DK…444 | TENDL-2019 | 304.716E3 | 224.918 | 61.049E3 | 3.68 | eV-b |
|  |  |  |  |  |  |  |
| Ga-ele\_ENDFB6…ASTM-DE…444 | ENDF/B-VI | 60.487E3 | 56.488E3 | 29.770E3 | 1.975 | eV-b  used legacy eff – with typo  no threshold treatment |
| Ga-ele\_ENDFB6…ASTM-DE\_recreate\_legacy…444 | ENDF/B-VI | 60.708E3 | 56.66E3 | 29.823E3 | 1.90 | eV-b;  best recreation of legacy DE  used legacy eff – with typo  spKP threshold treatment |
| Ga-ele\_ENDFB6…DK…444 | ENDF/B-VI | 304.10E3 | 247.72E3 | 64.443E3 | 3.84 | eV-b  no threshold treatment |
| Ga-ele\_ENDFB6…spKP…\_recreate\_legacy.444 | ENDF/B-VI | 305.29E3 | 248.56E3 | 64.548E3 | 3.85 | eV-b;  best recreation of legacy DK  spKP threshold treatment |
|  |  |  |  |  |  |  |
| Ga-ele\_JEF2p2…DK…444 | JEF2.2 | 316.70E3 | 258.25E3 | 63.712E3 | 4.05 | eV-b  no threshold treatment  Howerton eval. From ENDL-78 |
|  |  |  |  |  |  |  |
| Ga-ele\_ENDL-78…DK…444 | ENDL-78 | --- | 258.25E3 | 63.712E3 | 4.05 | eV-b  no threshold treatment  upper eval. bound of 20 MeV but all groupr output stop at 15 due to index count error in eval. |
|  |  |  |  |  |  |  |
| Ga-natvi-fit.disdam | ENDF/B-VI | 108.43 | 104.24 | 56.642 | 1.84 | MeV-mb  Fit=efficiency applied  Typo found in legacy eff  Reflects renormalization of 1.786 |
| Ga-natvi.444 | ENDF/B-VI | 305.57 | 260.70 | 70.159 | 3.72 | MeV-mb |
| Ga.disdam | --- | 305.57 | 260.70 | 70.159 | 3.72 | MeV-mb ; Probably ENDF/B-VI |
|  |  |  |  |  |  |  |
| Ga-natv.444 | ENDF/B-V | 305.57 | 260.70 | 70.159 | 3.72 | MeV-mb |
| Ga-natv.disdam | ENDF/B-V | 305.57 | 260.70 | 70.159 | 3.72 | MeV-mb ; disdam=444 |
|  |  |  |  |  |  |  |
| Ga-nat-endlv.444 | ENDL-78 | 318.29 | 272.65 | 69.418 | 3.93 | MeV-mb; endl78.dat3  Howerton evaluation  Not sure what the “v” means here. Often “lendl-v” |
|  |  |  |  |  |  |  |
| Ga-natjef.444 | JEF | 318.29 | 272.65 | 69.418 | 3.93 | MeV-mb; tape3.asc  RCOM-Jul82; DIST-Jan92  JEF-2 is taken from ENDL-78 |
|  |  |  |  |  |  |  |
| Ga-ele\_ENDFB6…nopart\_DK…444 | ENDF/B-VI | 588.10E3 | 444.45E3 | 91.117E3 | --- | Special icntrl(8) flag; no partition function |
| Ga-natvi\_pka.444 | ENDF/B-VI | 588.80E3 | 470.78E3 | 99.453E3 | --- | Displacement kerma in eV-b  [x1E-3 to get MeV-mb]  Special pka flag |
| Ga-ele\_ENDFB6…DK…1 | ENDF/B-VI | 2.7025 | 3.2081 | 3.8707 | --- | Total cross section in b  Note: small difference seen at thermal energies |
| Ga-natvi\_pka.1 | ENDF/B-VI | 2.7026 | 3.2079 | 3.8709 | --- | Total cross section in b |
| Ga-natvi\_pka.recoil-E | ENDF/B-VI | 217.86 | 146.76 | 25.692 | --- | Appears to be recoil energy, really damage energy; MT444/MT2 x 1E-3 |

**Questions:**

1. Displacement kerma for ENDF/B-VI differs a little from legacy calculation; by about ~9% at 1-MeV. Why?

* Since legacy is larger, this difference cannot be due to difference between spKP (legacy) and DK (current).
* Values are very close near 20 MeV. So, look to a difference in the elastic cross section treatment.
* Legacy used a different/fewer number of elastic angular quadrature points.
* Legacy also erroneously applied a threshold of 25 eV rather than the desired 10 eV in one section of the elastic treatment (quadrature, not df) – but this also goes in the wrong direction.
* Legacy has different Robinson partition function parameters – not self atom and different mass.
* Restore NJOY91.38 and repeat calculations. Obtained a good compilation, but failed to get acceptable execution of old code. Work in progress to find out the cause of the error.

1. ASTM-DE values for baseline ENDF/B-VI case look very different! Why? Did my new efficiency function not get applied correctly? Solved. The reason is that the legacy efficiency curve reflected a typo in one high energy value: 200 keV was entered as 2000 keV during original development – which affected the results. Solution is to reproduce the original fitting efficiency – with the typo.
2. Note: Legacy “fit” applies the efficiency as well as the renormalization factor listed as 2.2 in standard. The code appears to apply a normalization of 1.786. This normalization was only used to match the DK with the DE at 1-MeV to support the 1-MeV(GaAs)-Eqv value of 70 MeV-mb. See later discussion of GaAs as reflected in ASTM E722 that has a potential explanation for this difference.
3. Use legacy GaAs DK response to convert paper LET damage constants from [ms-1/(DK(GaAs))] to per [ms-1/(n/cm2)].
4. Pass legacy data files over to Nick. (Done)
5. Use NJOY-2016 to calculate the JEF-2 and ENDL DK. (Done)
6. Why is Ga-natvi\_pka.444 not equal to Ga-natvi.444? For my logic that this is the recoil energy times the cross section, they should be the same. Maybe this is because, in the original work, I turned off the damage partition function. This would have meant that the results did, in fact, reflect the recoil energy, and not just the damage energy. Check this out by reproducing the results for Ga-nat ENDF/B-VI evaluation by using a unity function for the damage partition function. Done – confirmed. Partition function was inhibited in these calculations. Option for user-input of damage partition function activated in coding. Some acceptable difference (~8%) seen in average recoil spectrum, but this could be explained by the difference between the spKP and the DK in the methodology, i.e., more low energy recoils are included in the DK calculation.
7. Annotate comments on evaluation source. Done.
8. Compare Ga-natvi\_pka.1 with new NJOY-2016 calculation – this is supposed to be the total cross section. Close, agree for elastic (1-MeV) and at high energy, difference at low energy. So, difference must be in (n,g) reaction. Why? Could temperature broadening be the difference? Current used broadr to 293.6. Legacy used reconr at 300. Check complete – difference persists!
9. Plot variation/ratio in legacy DK and total cross section for ENDF/B-VI case.

Total xsec ratio (current/legacy):



The source of the (n,g) cross section difference is not clear. It is possible that the differences is due to use of a difference release version of the ENDF/B-VI library – there were 6. I do not know which version was used in the legacy calculations. However, I did not think that this evaluation changed in the various releases.

spKP ratio (current/legacy):

|  |  |
| --- | --- |
| 1. Difference (log) | 1. Difference (linear) |

|  |  |
| --- | --- |
| 1. spKP (log) | 1. spKP (linear) |

The jagged difference at high energy looks suspect.

The difference near the displacement threshold can be explained by changes in the coding – error in legacy model for treatment of threshold in elastic channel integration.

The differences in the basic spKP damage energies show that the jagged nature is associated with the legacy calculations. I assume that the newest version of NJOY corrected previous interpolation issues.

There is only marginal benefit in trying to isolate the exact source of the differences in the legacy NJOY91.38 version.

DE ratio (current:ASTM-DE;spKP;x1.786/legacy):

|  |  |
| --- | --- |
| 1. Difference (log) | 1. Difference (linear) |

|  |  |
| --- | --- |
| 1. ASTM-DE (log) | 1. ASTM-DE (linear) |

1. Add 14-MeV metrics. (Done)
2. Extract table entries to look at the 14-MeV/1-MeV variation in magnitude. (Done)
3. HEATR coding changed to resolve conflict between NRT threshold implementation and efficiency term. Also now use log-log efficiency interpolation rather than the precious linear-log – done to be consistent with precious implementation.
4. Note typo found in legacy efficiency curve points that were interpolated. The 200 keV point appears in the table as 2000 keV. So, high recoil efficiency interpolation was affected by legacy work.
5. To match the previous work with the ENDF/B-VI cross sections, we should use the spKP threshold treatment. Add this entry to the table we above where the baseline DK and DE results did not apply any threshold treatment.

**Recap logic for legacy Ga cross section recommendation:**

1. ENDF/B-VI

Za3100; eval-may80, Howerton, elemental evaluation

1. ENDF/B-V – same as ENDF/B-VI, so, defer to that evaluation

nt507; eval-may88, Howerton

1. JEF-2 – adopted ENDL-78, so defer to that evaluation

Tape3.asc; RCOM-July82

1. ENDL-78

Endl78.dat3; RCOM-July82; MAT=7840, elemental evaluation

1. CENDL-2 – did not include a Ga evaluation
2. JENDL-3.2 – not available during the legacy work

Ga-69/Ga-71 as well as an elemental evaluation in jendl305.asc; eval-Mar94

So, acceptable evaluations were ENDF/B-VI and ENDL-78. Both evaluations were performed by Howerton. The ENDF/B-VI evaluation was the later evaluation. Photon data was included in MF12. (n,p), (n,a), and (n,2n) reaction channels were included.

Conclusion, based on what was available the ENDF/B-VI elemental Ga evaluation was used.

One issue to be examines is the status of the energy balance in ENDF/B-VI? Given the options, this would not affect the decision, but does affect the fidelity of the selection.

**Logic for current cross section is discussion**

This is addressed in more detail in a different summary report.

The decision came down to either ENDF/B-VIII.0 or TENDL-2019. Based on the availability of the MF6 energy/angle data and treatment of the photon production in MF12, the recommendation was to use the TENDL-2019. The cons here were that the TENDL-2019 represented a purely calculated cross section and did not reflect a comparison with available EXFOR experimental data.

**GaAs Reconstruction:**

1. Table 2 shows some of the recovered files for GaAs.

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| File | Library | MT444; disdam | | | MT Ratio  14-MeV / 1-MeV | Comment |
| 19.95 MeV | 14.05 MeV | 0.98 MeV |
| ga-natvi.disdam | ENDF/B-VI | 305.57 | 260.70 | 70.159 | 3.72 | MeV-mb |
| as-75endl.disdam | ENDL-78 | 313.39 | 255.69 | 49.965 | 5.117 | MeV-mb |
| GaAs\_recreation\_spKP.444 | Sum of above | 309.48 | 258.195 | 60.062 | 4.30 | MeV-mb |
|  |  |  |  |  |  |  |
| Gaas-mix.disdam | --- | 309.480 | 258.195 | 60.062 | 4.30 | MeV-mb |
|  |  |  |  |  |  |  |
| Ga-natvi-fit.disdam | ENDF/B-VI | 108.43 | 104.24 | 56.642 | 1.84 | MeV-mb  Fit=efficiency applied  Typo found in legacy eff  Reflects renormalization of 1.786 |
| as-75endl-fit.disdam | ENDL-78 | 115.68 | 104.650 | 55.616 | 1.88 | MeV-mb  Fit=efficiency applied  Typo found in legacy eff  Reflects renormalization of 1.786 |
| GaAs\_recreation\_ASTM-DE.444 | Sum of above | 112.055 | 104.445 | 56.129 | 1.8608 |  |
|  |  |  |  |  |  |  |
| gaas-fit\_10ev-vax.disdam | --- | 112.0555 | 104.4463 | 56.1231 | 1.861 | Equal to sum of ASTM-DE |
|  |  |  |  |  |  |  |
| gaas\_astm.E722 | --- | 137.1559 | 127.8423 | 68.6947 | 1.861 | Standard uses efficiency normalization of 2.2 |
|  |  |  |  |  |  |  |
| GaAs\_recreation\_ASTM-DE\_normalized.444 | --- | 138.029 | 128.657 | 69.1324 | 1.861 | ASTM-DE sum corrected by 2.2/1.786 =1.2318 to address change in normalization of 1-MeV point.  Ratio is 0.9936, difference within the accuracy of the 2.2 value selected for normalization. A renormalization of 2.186 would fit difference. |

1. The E722 standard reflects the adjusted/new normalization of the efficiency function – from 1.786 to 2.2. This adjustment only applies to the ASTM-DE – not the DK.
2. Thus, we do have a good energy-dependent function for the DK – represented by the sum of the legacy Ga and As files. This response can be used to interpret the damage constants found in the paper.
3. We have validated the SNL-NJOY-2016 ability to reconstruct the previous analysis that produced the results reflected in E722 for GaAs.

As-75 comparison:

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| File | Library | MT444;disdam | | | MT Ratio  14-MeV / 1-MeV | Comment |
| 19.95 MeV | 14.05 MeV | 0.98 MeV |  |
| As-75\_ENDFB-VIII…ASTM-DE…444 | ENDF/B-VIII.0 |  |  |  |  | eV-b |
| As-75\_ENDFB-VIII…DK…444 | ENDF/B-VIII.0 |  |  |  |  | eV-b |
|  |  |  |  |  |  |  |
| As-75\_ENDL-84…ASTM-DE…444 | ENDL-84 |  |  |  |  | eV-b  used legacy eff – with typo  no threshold treatment |
| As-75\_ENDL-84…ASTM-DE\_recreate\_legacy…444 | ENDL-84 |  |  |  |  | eV-b;  best recreation of legacy DE  used legacy eff – with typo  spKP threshold treatment |
| As-75\_ENDL-84…DK…444 | ENDL-84 |  |  |  |  | eV-b  no threshold treatment |
| As-75\_ENDL-84…spKP…\_recreate\_legacy.444 | ENDL-84 |  |  |  |  | eV-b;  best recreation of legacy DK  spKP threshold treatment |
|  |  |  |  |  |  |  |
| As-75\_JENDL-4…DK…444 | JENDL-4.0 |  |  |  |  | eV-b  used since recent evaluation |
|  |  |  |  |  |  |  |
| As-75\_ENDFB-VI…DK…444 | ENDF/B-VI |  |  |  |  | eV-b |
|  |  |  |  |  |  |  |
| As-75\_JEF2…DK…444 | JEF 2 |  |  |  |  | eV-b  used for comparison with legacy |
|  |  |  |  |  |  |  |
| As-75endl-fit.disdam | ENDL-84 | 115.68 | 104.65 | 55.616 | 1.882 | MeV-mb  Fit=efficiency applied |
| As-75endl.disdam | ENDL-84 | 313.39 | 255.69 | 49.965 | 5.117 | MeV-mb |
| As-75endl.444 | ENDL-84 | 313.39 | 255.69 | 49.965 | 5.117 | MeV-mb |
|  |  |  |  |  |  |  |
| As-75jef.disdam | JEF-2 | 693.95 | 632.90 | 70.783 | 8.941 | MeV-mb; tape3.asc  Taken from ENDF/B-V |
| As-75jef.444 | JEF-2 | 693.95 | 632.90 | 70.783 | 8.941 | MeV-mb; tape3.asc  Taken from ENDF/B-V |
|  |  |  |  |  |  |  |
| As-75v.disdam | ENDF/B-V | 694.58 | 631.68 | 70.785 | 8.924 |  |
| As-75v.444 | ENDF/B-V | 694.58 | 631.68 | 70.785 | 8.924 |  |
|  |  |  |  |  |  |  |
| As-75vi.disdam | ENDF/B-VI | 694.58 | 631.68 | 70.785 | 8.924 |  |
| As-75vi.444 | ENDF/B-VI | 694.58 | 631.68 | 70.785 | 8.924 |  |
|  |  |  |  |  |  |  |
| As-75\_ENDFB6…nopart\_DK…444 | ENDF/B-VI |  |  |  | --- | Special; no partition function |
| As-75vi\_pka.444 | ENDF/B-VI | 1391.5E3 | 1176.3E3 | 98.797E3 | --- | Displacement kerma in eV-b  [x1E-3 to get MeV-mb] |
| As-75vi\_pka.1 | ENDF/B-VI | 3.1128 | 3.7277 | 4.0788 | --- | Total cross section in b |
| As-75vi\_pka.recoil-E | ENDF/B-VI | 447.03 | 31.556 | 24.222 | --- | Appears to be recoil energy, MT444/MT1 x 1E-3 |
|  |  |  |  |  |  |  |
| As-75\_ENDL-78…nopart\_DK…444 | ENDL-78 |  |  |  | --- | Special; no partition function |
| As-75endl\_pka.444 | ENDL-78 | 563.2E3 | 439.30E3 | 89.318E3 | --- |  |
| As-75endl\_pka.1 | ENDL-78 | 3.0541 | 3.4483 | 5.0243 | --- |  |
| As-75endl\_pka.recoil-E | ENDL-78 | 184.41 | 127.4 | 17.777 | --- | Appears to be recoil energy, MT444/MT1 x 1E-3 |

Questions:

1. ENDL is very different in DK than ENDF/B-VI(ENDF/B-V) and JEF – at 1-MeV and at 20-MeV. ENDL appears to be the issue. When the response is unfolded using the experimental data, this difference will be important in the deduced damage efficiency function, i.e., the unfolded damage efficiency function has a strong correlation with the cross sections (and the derived DK).
   1. The difference is only large in the high energy region, i.e., 1-MeV elastic is close, but the (n,p) or (n,a) recoil energies must be way off – by 2X too low (when comparted to ENDF/B-VI).
      1. At 20 MeV; (n,p): threshold 0.46 MeV; ENDL-84=3.5E-2; ENDF/B-VIII.0=2.77818E-2. This is 25% higher.
      2. At 20 MeV; (n,a), threshold = 1.1 MeV; ENDL-84=5.0E-3; ENDF/B-VIII.0=9.078966E-3. This is 50% low.
      3. I conclude that the difference in the modeling of the (n,a) reaction is the major contributor to the observed difference.
   2. Since no MF6 file existed in this evaluation, the problem may be based on the NJOY modeling of the kinematics in the absence of a high-fidelity photon spectrum.
2. Annotate comments on evaluation source (Done)

**Recap logic for As-75 legacy cross section recommendation:**

For source files, look in:

<https://www.oecd-nea.org/dbforms/data/eva/evatapes/>

<https://www-nds.iaea.org/public/download-endf/>

1. ENDF/B-VI

Za33075; eval-apr74, Schenter&Schmittroth,

Same as ENDF/B-V

no MF6 or MF12 photon file. The lack of a photon file has a big effect on the (n,g) capture displacement kerma and on the energy balance. The evaluation failed to include any (n,p), (n,2n), or (n,a) reaction channel.

1. ENDF/B-V

tape541.asc; EVAL-Apr74, Schrender&Schmittroth

1. JEF-2 – taken from ENDF/B-V (MAT=9071).

RCOM-Jul82, tape3.asc

This evaluation has a MT102 (n,g) capture reaction as well as MT103 (n,p), MT104 (n,d), MT105 (n,t), MT106 (n,3He), MT107 (n,a), and MT111 (n,2p) reaction channels.

There is no MF6 or MF12 photon production file.

1. ENDL-84

GaAs paper states that MAT=8302 was used. But I cannot find this MAT in the ENDL-78 files. Neither can I find any As-75 evaluation there.

ENDL-82 may be available from RSIC as DLC-103 (based on comments from a Williams paper). See <https://rsicc.ornl.gov/codes/dlc/dlc1/dlc-103.html> Based on the MAT number, I suspect that As-75 is not part of ENDL-82, but was first introduced in ENDL-83.

The evaluation was found in the ENDL-84 evaluations: <https://www-nds.iaea.org/public/download-endf/ENDL-84/> These files were titles “ENDL84V.DAT”.

DIST-83; Howerton

Included MT103 and MT107 reaction channels. Also included the MF12 photon characterization.

1. CENDL-2 – did not include a As evaluation
2. JENDL-3.1 – available as individual files from: <https://wwwndc.jaea.go.jp/jendl/jendl.html>

EVAL-Mar90;

Includes MF103, MF104, MF105, MF106, MF107

No MF12 photon production nor a MF6 file.

1. JENDL-3.2 – the library was not available during the legacy work.

As-75 is on jendl305.asc; eval-Mar90

Based on JENDL Fusion file by Kosako and Chiba in 1994.

Includes MF103, MF104, and MF107 but did not have a MF6 or MF12 file. .

So, potential evaluations were ENDF/B-VI, JEF-2, JENDL-3.1, and ENDL-84. The ENDF/B-VI evaluation was rejected because it lacked charged particle reaction channels. Photon data was only included for the ENDL-84 evaluation in MF12 – so it was the recommended file. This file also included the important (n,p) and (n,a) reaction channels. We note that this evaluation was done by Howerton, and so was the ENDF/B-VI evaluation used for Ga-ele – so they were well matched.

Conclusion, based on what was available at the time, the ENDL-84 As-75 evaluation was selected.

Actions for Nick:

1. Complete the As-75 table like the above Ga-ele table. This table should compare the historical/legacy data with new processed files using NJOY-2016. Use the older versions of the various libraries to make comparisons with the legacy decisions on what library to use. Use the new versions of the libraries to look for trends in the behavior with the library.
2. Look at the damage constants in the 1991 paper. Look carefully at the units. These units support a direct plotting of the data versus the recoil energy – as seen in the sloped line in the Figure. Use the legacy data files to convert the units in the damage constant to a more useful unit – a unit that does not depend upon the nuclear data file used.