AN ANALYSIS OF THE $^{239}$Pu NEUTRON CROSS SECTIONS FROM 20 keV TO 20 MeV

A. Prince, M.K. Drake, and P. Hlavac

April 1973

NATIONAL NEUTRON CROSS SECTION CENTER
BROOKHAVEN NATIONAL LABORATORY
UPTON, NEW YORK 11973
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*Present address: Science Applications Inc., La Jolla, California 92037.

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PLUTONIUM NEUTRON-PARTICLE CROSS SECTION

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PLUTONIUM-239 INELASTIC CROSS SECTIONS

**Figure 22**

- (a) $\sigma_{\text{ref}}$ 19-TH EXCITED STATE
- (b) $\sigma_{\text{ref}}$ 20-TH EXCITED STATE
- (c) $\sigma_{\text{ref}}$ 21-TH EXCITED STATE
- (d) $\sigma_{\text{ref}}$ 22-TH EXCITED STATE
- (e) $\sigma_{\text{ref}}$ 23-RO EXCITED STATE
- (f) $\sigma_{\text{ref}}$ CONTINUUM
PLUTONIUM-239 INELASTIC CROSS SECTIONS

Figure 20
has steadily increased and in most cases exceeds the accuracy of experimental differential data. A clear example of the latter is the proper interpretation of the inelastic scattering cross sections for Pu-239.

An earlier evaluation of $\sigma_{nn}$ and other reaction cross sections was presented at the Helsinki Conference, June 1970\textsuperscript{(1)} (hereafter referred to as P). This analysis was to form the basis for the high energy ($E > 100$ keV) cross sections for the Evaluated Nuclear Data File (ENDF/B) on Pu-239. A subsequent meeting of the Cross Section Evaluation Working Group (CSEWG) resulted in expressions of concern that the elastic cross sections in ENDF/B-II were lower than those in ENDF/B-I and the inelastic cross sections were higher.

As pointed out in P, previous calculations used in evaluating Pu-239 have employed a spherical optical potential with the various reaction cross sections being interpreted as arising only from compound nucleus formation. However, since this nuclide is known to exhibit a high degree of deformity, the scattering of neutrons cannot be described adequately by the conventional optical model, which does not consider the coupling between the incident neutron motion and the nuclear surface rotation. This coupling causes the direct excitation of the rotational levels by inelastic scattering.

While these previous analyses have provided fairly good agreement between calculated and experimental angular distributions, the magnitude of the diffraction minima and maxima has not been well produced. Earlier investigations\textsuperscript{(2,3)} have shown that neglecting the high degree of anisotropy exhibited by the direct inelastic component can lead to serious errors in the prediction of the differential elastic and inelastic cross sections. These errors manifest themselves in two major areas. In the low
Figure 17
PLUTONIUM-239
TOTAL INELASTIC
NEUTRON CROSS SECTION

ENERGY (MeV)

CROSS SECTION (\sigma)

THRESHOLD TO 1.0 MeV

Figure 18
PLUTONIUM-239
TOTAL INELASTIC
NEUTRON CROSS SECTION

ENERGY (MeV)

CROSS SECTION (\sigma)

1.0 TO 20.0 MeV
experimental constraints; namely, the total cross section $\sigma_{T}$, the potential scattering cross section $\sigma_{\text{pot}}$, and the s- and p-wave strength functions ($S_{0}$ and $S_{1}$).

Two additional pseudo-constraints $\sigma_{nf}$ and $\sigma_{\text{pY}}$ were also introduced in the statistical analysis such that the calculated values agreed to at least 5 to 7% of the most recent recommended values. The reason for the latter restriction is manifested in the fact that such an analysis would beget more confidence in the resulting inelastic processes.

These restrictions were very successful in providing a consistent set of parameters for performing calculations that produced very good agreement with all available experimental data from 10 keV to 20 MeV.

Theory

The differential cross sections for shape elastic scattering ($\sigma_{SE}$), the total reaction cross section ($\sigma_{R}$), and the direct inelastic scattering ($\sigma_{\text{rot}}$) were calculated using the Coupled Channel Code JUPITER I by Tamura(4).

In the phenomenological description it is assumed that the whole interaction to which the neutron is subjected may be described by an optical-model potential $V(r,\theta,\phi)$ which is complex and includes spin orbit coupling. Its radial dependence is of the Saxon-Woods form and its derivative. $V(r,\theta,\phi)$ is assumed to be, in general, non-spherical and is defined as(4):
Figure 14

Figure 15

- 36 -
as to incorporate the more recent methods in the analysis of continuum particle emission. The following description is based on the procedures outlined in Ref. (5); for a more complete analysis the reader should consult this work.

From Moldauer (6,7) the reaction cross section for incident channel c and outgoing channel c' (c = n, f) may be written as:

\[
\langle \sigma_{cc'} \rangle = \frac{\pi^2}{c} \left[ \frac{\langle \theta_{\lambda c}' \rangle \langle \theta_{\lambda c} \rangle}{\langle \theta_{\lambda} \rangle} W_{cc'} - \frac{\delta_{cc'}}{4} Q_{c} \langle \theta_{\lambda c} \rangle^2 \right]
\]

(1)

where

\[
\theta_{\lambda} = \sum_{\alpha} \langle \theta_{\lambda \alpha} \rangle \quad \alpha = \text{all open channels.}
\]

(2)

\[
W_{cc'} = \frac{\langle \theta_{\lambda c} \theta_{\lambda c}' \rangle}{\langle \theta_{\lambda} \rangle} \cdot \frac{\langle \theta_{\lambda c} \rangle \langle \theta_{\lambda c} \rangle}{\langle \theta_{\lambda} \rangle} .
\]

(3)

and

\[
\langle \theta_{\lambda c} \rangle = T_{c} + \frac{1}{Q_{c}} \left[ 1 - \sqrt{1 - Q_{c} T_{c}} \right]^2 .
\]

(4)

\( T_{c} \) is the optical model penetrability for channel c, and \( Q_{c} \) is the statistical parameter with range \( 0 \leq Q_{c} \leq 2 \).

In previous calculations using ABACUS-NEARREX(9) the quantity \( Q_{c} \) was treated as a constant where its dependence on \( \langle \theta_{\lambda c} \rangle \) was ignored. However, as was discovered in several instances during the analysis in P and also reported by(10), such a treatment can lead to negative values for the compound elastic cross section for some partial waves when many channels are open and \( Q_{c} \) is not taken sufficiently small.
Figure 11

90° INELASTIC SCATTERING CROSS-SECTIONS FOR Pu$^{239}$

- $(0.057 + 0.075)$ MeV
- $0.286$ MeV
- $0.331$ MeV

CAVANAGH et al AERE-R5972 (1969)

CALCULATED
Lane and Lynn (12) and Brown (13).

The fission cross section was interpreted in terms of the Hill-Wheeler (14) model with

\[ \langle \theta^{J^\pi} \rangle = \frac{N^{J^\pi}}{2\pi}, \]

where \( N^{J^\pi} \) is the effective number of fission channels and is dependent upon the penetrability factor \( P_i \) by

\[ N^{J^\pi} = \sum P_i \]

and

\[ P_i = \frac{1}{1 + \exp \left[ \frac{2\pi(E_{fi} - E)}{\hbar\omega} \right]} \]

\( E_{fi} \) is the fission threshold, and \( \hbar\omega \) the characteristic energy of the barrier curvature.

Combining the coupled-channel calculations with the statistical model produced the following interaction cross sections:

- \( \sigma_T \) = total cross section
- \( \sigma_{SE} \) = shape elastic cross section
- \( \sigma_{CE} \) = compound elastic cross section
- \( \sigma_{el} \) = \( \sigma_{SE} + \sigma_{CE} \) total elastic
- \( \sigma_R \) = reaction cross section
- \( \sigma_C \) = compound formation cross section
- \( \sigma_{nn'}(\text{comp.}) \) = compound inelastic cross section
- \( \sigma_{nn'}(\text{rot.}) \) = direct inelastic cross section.

Computer code THRESH (15) which is an empirical model embodying the evaporation theory of Weisskopf was used to calculate the \( \sigma_n, 2n', \sigma_n, 3n' \), \( \sigma_{np}, \sigma_{nd}, \sigma_{nt} \), and \( \sigma_{ny} \) cross sections.
Figure 9

SCATTERING CROSS SECTION FOR $^{239}$Pu

$E=4.0$ MeV

- COPPOLA & KNITTER, Z PHYS. 232 (1970) 266
- BATCHELOR & WYLD, AWRE 0-55/69 (1969)

\[
\begin{align*}
\sigma_s &= 4.93 \text{ b} \\
\mu &= 7.57 \times 10^{-1} \\
\xi &= 2.04 \times 10^{-3} \\
\sigma_{el} &= 4.11 \text{ b} \\
\mu &= 8.65 \times 10^{-1} \\
\xi &= 1.13 \times 10^{-3}
\end{align*}
\]
The thresholds for the n,2n, n,3n, and charged particle emission were taken from Ref. (21) and are given below:

<table>
<thead>
<tr>
<th>Reaction</th>
<th>E_{\text{thresh.}} (MeV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>n-2n</td>
<td>5.68</td>
</tr>
<tr>
<td>n-3n</td>
<td>12.71</td>
</tr>
<tr>
<td>n-p</td>
<td>-0.06</td>
</tr>
<tr>
<td>n-d</td>
<td>3.96</td>
</tr>
<tr>
<td>n-t</td>
<td>3.18</td>
</tr>
<tr>
<td>n-He^3</td>
<td>3.68</td>
</tr>
<tr>
<td>n-He^4</td>
<td>-11.79</td>
</tr>
</tbody>
</table>

In order to ascertain the quality of the resultant calculation and perhaps to gain a clearer insight into the apparent enigmatic features of the inelastic and elastic scattering processes in Pu-239, it was decided to carry out the calculations which would include the exact energies described in the most recent differential measurements of the microscopic data. These include the following, Knitter and Coppola (22), Cavanagh, et al. (23), Batchelor and Wyld (24), Coppola and Knitter (25), and A. B. Smith (26).

Calculations and Comparison with Experiment

The total cross section for Pu-239 in the energy range 0.001 MeV ≤ E ≤ 0.1 MeV is shown in Fig. 1 and is compared with the experimental data of Uttley (17). Along with the calculated values of this work is the evaluation due to Barre, et al. (28). In both cases the agreement with Uttley's experimental points is very good, deviating only slightly around 50 keV.

The s- and p-wave strength functions at 1 keV were calculated to be 1.19 x 10^{-4} and 1.71 x 10^{-4}, respectively, which may be compared
the data of Smith (ANL) and Hearon (NBS) (received after the completion of this evaluation).

In Figure 3, the evaluated total cross section is shown to be in excellent agreement with empirical data of Smith (ANL), Heaton et al. (NBS), and Foster and Glasgow, (34) however, the data of Cabe is about 5% higher than the others.

In Figures 4 and 5, the calculated values of the fission cross sections are compared with the experimental data available in the SCISRS data library, and the recommended data of the CSEWG Task Force. It is clearly seen that the calculational results are, in general, within 0.1 to 0.2 barns of the recommended values and well within the accuracy of the experimental data. The wide dispersion in the experimental data points illustrates another region wherein model calculations could possibly aid in unraveling the inconsistencies that exist in the experimental data.

The radiative capture cross section was also calculated for the 0.01 to 1.0 MeV region and up to about 0.5 MeV (discrete inelastic) region, the COMNUC code provided surprisingly good results when compared with the recommended ENDF/B III capture cross section. It should be remembered that the ENDF/B III evaluated cross sections were based on the previously mentioned fission data and recent experimental $\sigma$ values. Thus, any errors in either of these quantities will be manifested in the recommended capture cross section. Above 0.5 MeV, the calculated capture cross section was somewhat larger than the recommended cross
Figure 5
A comparison of the differences that become evident when the high degree of anisotropy of these low lying levels is ignored is given in Table IV, where the Legendre coefficients* at 4.0 MeV were calculated from the angular distributions shown in Figure 9. The average cosine of the scattering angle in the Lab system, $\mu_L$, and the average logarithmic energy decrement per elastic collision, $\xi$, are given in Figure 9 and at the bottom of Table IV. The contribution of the compound elastic and inelastic (first two levels) at 4.0 MeV are of the order $10^{-5}$ mb/sr and are therefore ignored in Figure 9 and Table IV. Note that including the anisotropic contributions changes the scattering cross section by about 20% while $\mu_L$ and $\xi$ are changed by 14% and 45% respectively.

Figure 10 provides a rather vivid description of the interpretation of the experimental scattering data. The dashed curve shown what is referred to as "pure elastic" scattering ($\sigma_{el}=\sigma_{SE}+\sigma_{CE}$). The dash-dot curve includes contributions from direct and compound inelastic excitation of the 8 keV level and should be compared with A. B. Smith's data up to at least 1.1 MeV. To describe the data of Knitter and Coppola(22), one must consider the contributions from the first 3 levels above the ground state. From Figure 10 it is obvious that such evaluatory considerations do produce rather satisfactory agreement with the experimental data.

Figure 11 shows the differential inelastic scattering of Cavanagh, et al.(23) at 90° for a combination of the 57 and 76 keV levels and separate excitations for the 286 and 331 keV levels respectively. It is

*The Legendre coefficients in Table IV are for illustrative purpose only. In ENDF/B VII, 20 Legendre coefficients are used to describe the elastic angular distribution, with $\mu = 0.8759$ and $\xi = 0.00105$, $\sigma_{SE} = 3.98$ b, $\sigma_{CE} = 0.0$ b.
Figure 3

W - priv. Comm
C - conference
Conclusion

Since the accuracy requirements for Pu-239 in analyzing fast reactors has become more demanding, it was necessary to apply the most sophisticated theoretical concepts in the evaluation.

In order to explain the experimental angular distribution data, the effects of deformation leading to the direct rotational excitation had to be considered.

It was also important that the various compound nucleus reactions, $\sigma_{nn}$, $\sigma_{nf}$, $\sigma_{nf}$, etc. be analyzed in a consistent manner so as to properly define their competitive characteristics.

These factors coupled with comparison with the most recent experimental data have produced what is hoped to be a very important intermediary for a logical evaluation which should prove to be adequate in the analysis of fast reactors which use Pu-239 as fuel.

All calculations used in this evaluation were completed by February 1972.
TOTAL B POTENTIAL SCATTERING CROSS SECTIONS FOR $^{239}$Pu

Figure 1


TABLE IV: Legendre Coefficients ($f_k$) for Scattering at 4.0 MeV

<table>
<thead>
<tr>
<th>$k$</th>
<th>$f_k$</th>
<th>$f_k$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>1.00000</td>
<td>1.00000</td>
</tr>
<tr>
<td>1</td>
<td>8.64369x10^{-1}</td>
<td>7.55472x10^{-1}</td>
</tr>
<tr>
<td>2</td>
<td>7.17507x10^{-1}</td>
<td>6.04563x10^{-1}</td>
</tr>
<tr>
<td>3</td>
<td>5.70527x10^{-1}</td>
<td>4.73420x10^{-1}</td>
</tr>
<tr>
<td>4</td>
<td>4.43269x10^{-1}</td>
<td>3.62664x10^{-1}</td>
</tr>
<tr>
<td>5</td>
<td>3.24059x10^{-1}</td>
<td>2.74031x10^{-1}</td>
</tr>
<tr>
<td>6</td>
<td>2.04351x10^{-1}</td>
<td>1.68689x10^{-1}</td>
</tr>
<tr>
<td>7</td>
<td>9.88382x10^{-2}</td>
<td>8.21425x10^{-2}</td>
</tr>
<tr>
<td>8</td>
<td>3.72463x10^{-2}</td>
<td>3.33180x10^{-2}</td>
</tr>
<tr>
<td>9</td>
<td>8.51738x10^{-3}</td>
<td>6.80190x10^{-3}</td>
</tr>
<tr>
<td>10</td>
<td>9.75251x10^{-4}</td>
<td>7.82202x10^{-4}</td>
</tr>
<tr>
<td>11</td>
<td>-2.27483x10^{-5}</td>
<td>-1.85806x10^{-5}</td>
</tr>
<tr>
<td>12</td>
<td>3.29123x10^{-6}</td>
<td>2.10669x10^{-6}</td>
</tr>
<tr>
<td>13</td>
<td>3.16028x10^{-6}</td>
<td>1.83861x10^{-6}</td>
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<tr>
<td>14</td>
<td>3.62436x10^{-6}</td>
<td>2.08059x10^{-6}</td>
</tr>
</tbody>
</table>

\[
\sigma_{sE} = 2\pi \int_{-1}^{1} \frac{d\sigma_{sE}}{d\Omega} \, d\mu = 4.11 \text{b} \\
\sigma_s = 2\pi \int_{-1}^{1} \frac{d\sigma_s}{d\Omega} \, d\mu = 4.93 \text{b}
\]

\[
\bar{\mu}_L = 0.8647 \\
\bar{\mu}_L = 0.7567 \\
\xi = 0.001128 \\
\zeta = 0.002037
\]
### TABLE II

Energy Level Scheme

<table>
<thead>
<tr>
<th>Level</th>
<th>I^π</th>
<th>Excitation (MeV)</th>
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<tr>
<td>0</td>
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<tr>
<td>1</td>
<td>3/2^+</td>
<td>0.0080</td>
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<tr>
<td>2</td>
<td>5/2^+</td>
<td>0.0570</td>
</tr>
<tr>
<td>3</td>
<td>7/2^+</td>
<td>0.0760</td>
</tr>
<tr>
<td>4</td>
<td>9/2^+</td>
<td>0.1640</td>
</tr>
<tr>
<td>5</td>
<td>11/2^+</td>
<td>0.1930</td>
</tr>
<tr>
<td>6</td>
<td>5/2^-</td>
<td>0.2860</td>
</tr>
<tr>
<td>7</td>
<td>7/2^+</td>
<td>0.3300</td>
</tr>
<tr>
<td>8</td>
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<td>7/2^-</td>
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<td>5/2^-</td>
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<tr>
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<tr>
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<tr>
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<td>15</td>
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<td>16</td>
<td>3/2^-</td>
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<td>17</td>
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<td>Level</td>
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<tr>
<td>0</td>
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</tr>
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<td>0.8000</td>
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<td>0.8490</td>
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TABLE IV: Legendre Coefficients ($f_l$) for Scattering at 4.0 MeV

<table>
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<th>$l$</th>
<th>$f_{lE}$</th>
<th>$f_{lT}$</th>
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</thead>
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<td>1.0000</td>
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<td>1</td>
<td>8.64369x10^-1</td>
<td>7.55472x10^-1</td>
</tr>
<tr>
<td>2</td>
<td>7.17507x10^-1</td>
<td>6.04563x10^-1</td>
</tr>
<tr>
<td>3</td>
<td>5.70527x10^-1</td>
<td>4.73420x10^-1</td>
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<tr>
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<td>3.24059x10^-1</td>
<td>2.74031x10^-1</td>
</tr>
<tr>
<td>6</td>
<td>2.04351x10^-1</td>
<td>1.68689x10^-1</td>
</tr>
<tr>
<td>7</td>
<td>9.88382x10^-2</td>
<td>8.21425x10^-2</td>
</tr>
<tr>
<td>8</td>
<td>3.72463x10^-2</td>
<td>3.33180x10^-2</td>
</tr>
<tr>
<td>9</td>
<td>8.51738x10^-3</td>
<td>6.80190x10^-3</td>
</tr>
<tr>
<td>10</td>
<td>9.75251x10^-4</td>
<td>7.82202x10^-4</td>
</tr>
<tr>
<td>11</td>
<td>-2.27483x10^-5</td>
<td>-1.85806x10^-5</td>
</tr>
<tr>
<td>12</td>
<td>3.29123x10^-6</td>
<td>2.10669x10^-6</td>
</tr>
<tr>
<td>13</td>
<td>3.16028x10^-6</td>
<td>1.83861x10^-6</td>
</tr>
<tr>
<td>14</td>
<td>3.62436x10^-6</td>
<td>2.08059x10^-6</td>
</tr>
</tbody>
</table>

\[
\sigma_{SE} = 2\pi \int_{-1}^{1} \frac{d\sigma_{SE}}{d\Omega} d\mu = 4.11 b \\
\sigma_s = 2\pi \int_{-1}^{1} \frac{d\sigma_s}{d\Omega} d\mu = 4.93 b \\
\bar{\mu}_L = 0.8647 \\
\bar{\mu}_L = 0.7567 \\
\xi = 0.001128 \\
\xi = 0.002037 \]


TOTAL POTENTIAL SCATTERING
CROSS SECTIONS FOR $^{239}\text{Pu}$

Figure 1
Conclusion

Since the accuracy requirements for Pu-239 in analyzing fast reactors has become more demanding, it was necessary to apply the most sophisticated theoretical concepts in the evaluation.

In order to explain the experimental angular distribution data, the effects of deformation leading to the direct rotational excitation had to be considered.

It was also important that the various compound nucleus reactions, $\sigma_{nn}$, $\sigma_{nf}$, $\sigma_{ny}$, etc. be analyzed in a consistent manner so as to properly define their competitive characteristics.

These factors coupled with comparison with the most recent experimental data have produced what is hoped to be a very important intermediary for a logical evaluation which should prove to be adequate in the analysis of fast reactors which use Pu-239 as fuel.

All calculations used in this evaluation were completed by February 1972.
Figure 3

\( \text{Neutron Energy (MeV) Lab} \)

\( \text{Cross-Section [ barns] } \)
A comparison of the differences that become evident when the high
degree of anisotropy of these low lying levels is ignored is given in
Table IV, where the Legendre coefficients* at 4.0 MeV were calculated
from the angular distributions shown in Figure 9. The average cosine
of the scattering angle in the Lab system, $\mu_L$, and the average logarithmic
energy decrement per elastic collision, $\xi$, are given in Figure 9 and
at the bottom of Table IV. The contribution of the compound elastic and
inelastic (first two levels) at 4.0 MeV are of the order $10^{-5}$ mb/sr
and are therefore ignored in Figure 9 and Table IV. Note that including
the anisotropic contributions changes the scattering cross section by
about 20% while $\mu_L$ and $\xi$ are changed by 14% and 45% respectively.

Figure 10 provides a rather vivid description of the interpretation
of the experimental scattering data. The dashed curve shown what is
referred to as "pure elastic" scattering ($\sigma_{el} = \sigma_{SE} + \sigma_{CE}$). The dash-dot
curve includes contributions from direct and compound inelastic excitation
of the 8 keV level and should be compared with A. B. Smith's data up to
at least 1.1 MeV. To describe the data of Knitter and Coppola(22), one
must consider the contributions from the first 3 levels above the ground
state. From Figure 10 it is obvious that such evaluatory considerations
do produce rather satisfactory agreement with the experimental data.

Figure 11 shows the differential inelastic scattering of Cavanagh,
et al. (23) at 90° for a combination of the 57 and 76 keV levels and
separate excitations for the 286 and 331 keV levels respectively. It is

*The Legendre coefficients in Table IV are for illustrative purpose only.
In ENDF/B III, 20 Legendre coefficients are used to describe the
elastic angular distribution, with $\mu = 0.8759$ and $\epsilon = 0.00105$, $\sigma_{SE} = 3.98$ b,
$\sigma_{CE} = 0.0$ b.
the data of Smith (ANL) and Hearon (NBS) (received after the completion of this evaluation).

In Figure 3, the evaluated total cross section is shown to be in excellent agreement with empirical data of Smith (ANL), Heaton et al. (NBS), and Foster and Glasgow, however, the data of Cabe is about 5% higher than the others.

In Figures 4 and 5, the calculated values of the fission cross sections are compared with the experimental data available in the SCISRS data library, and the recommended data of the CSEWG Task Force. It is clearly seen that the calculational results are, in general, within 0.1 to 0.2 barns of the recommended values and well within the accuracy of the experimental data. The wide dispersion in the experimental data points illustrates another region wherein model calculations could possibly aid in unraveling the inconsistencies that exist in the experimental data.

The radiative capture cross section was also calculated for the 0.01 to 1.0 MeV region and up to about 0.5 MeV (discrete inelastic) region, the COMMUC code provided surprisingly good results when compared with the recommended ENDF/B III capture cross section. It should be remembered that the ENDF/B III evaluated cross sections were based on the previously mentioned fission data and recent experimental $\sigma$ values. Thus, any errors in either of these quantities will be manifested in the recommended capture cross section. Above 0.5 MeV, the calculated capture cross section was somewhat larger than the recommended cross section.
The thresholds for the \( n,2n \), \( n,3n \), and charged particle emission were taken from Ref. (21) and are given below:

<table>
<thead>
<tr>
<th>Reaction</th>
<th>( E_{\text{thresh}} ) (MeV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>( n-2n )</td>
<td>5.88</td>
</tr>
<tr>
<td>( n-3n )</td>
<td>12.71</td>
</tr>
<tr>
<td>( n-p )</td>
<td>-0.06</td>
</tr>
<tr>
<td>( n-d )</td>
<td>3.96</td>
</tr>
<tr>
<td>( n-t )</td>
<td>3.18</td>
</tr>
<tr>
<td>( n-\text{He}^3 )</td>
<td>3.68</td>
</tr>
<tr>
<td>( n-\text{He}^4 )</td>
<td>-11.79</td>
</tr>
</tbody>
</table>

In order to ascertain the quality of the resultant calculation and perhaps to gain a clearer insight into the apparent enigmatic features of the inelastic and elastic scattering processes in Pu-239, it was decided to carry out the calculations which would include the exact energies described in the most recent differential measurements of the microscopic data. These include the following, Knitter and Coppola (22), Cavanagh, et al. (23), Batchelor and Wyld (24), Coppola and Knitter (25), and A. B. Smith (26).

**Calculations and Comparison with Experiment**

The total cross section for Pu-239 in the energy range \( 0.001 \text{ MeV} \leq E \leq 0.1 \text{ MeV} \) is shown in Fig. 1 and is compared with the experimental data of Uttley (17). Along with the calculated values of this work is the evaluation due to Barre, et al. (28). In both cases the agreement with Uttley's experimental points is very good, deviating only slightly around 50 keV.

The \( s\)- and \( p\)-wave strength functions at 1 keV were calculated to be \( 1.19 \times 10^{-4} \) and \( 1.71 \times 10^{-4} \), respectively, which may be compared
Figure 9
Lane and Lynn (12) and Brown (13).

The fission cross section was interpreted in terms of the Hill-Wheeler (14) model with

$$\langle E_{\lambda\pi}^{J\pi} \rangle = \frac{N_{J\pi}^2}{\pi},$$

where $N_{J\pi}^2$ is the effective number of fission channels and is dependent upon the penetrability factor $P_i$ by

$$N_{J\pi}^2 = \sum P_i$$

and

$$P_i = \frac{1}{1 + \exp \left[ \frac{2\pi(E_{f1}^{J\pi} - E)}{\hbar\omega} \right]}.$$  

$E_{f1}$ is the fission threshold, and $\hbar\omega$ the characteristic energy of the barrier curvature.

Combining the coupled-channel calculations with the statistical model produced the following interaction cross sections:

- $\sigma_T$ = total cross section
- $\sigma_{SE}$ = shape elastic cross section
- $\sigma_{CE}$ = compound elastic cross section
- $\sigma_{el}$ = $\sigma_{SE} + \sigma_{CE}$ total elastic
- $\sigma_R$ = reaction cross section
- $\sigma_C$ = compound formation cross section
- $\sigma_{nn}^{(comp.)}$ = compound inelastic cross section
- $\sigma_{nn}^{(rot.)}$ = direct inelastic cross section.

Computer code THRESH (15) which is an empirical model embodying the evaporation theory of Weisskopf was used to calculate the $\sigma_{n,2n}$, $\sigma_{n,3n}$, $\sigma_{np}$, $\sigma_{nd}$, $\sigma_{nt}$, and $\sigma_{n\gamma}$ cross sections.
Figure 11

90° INELASTIC SCATTERING CROSS-SECTIONS FOR Pu$_{239}$

- (0.057 + 0.075) MeV
- 0.286 MeV
- 0.331 MeV

CAVANAGH et al
AERE - R5972 (1969)

CALCULATED

- (0.057 + 0.076)$_{comp}$
- + (0.057)$_{rot}$

- (0.057 + 0.075)$_{comp}$

0.286
0.331
as to incorporate the more recent methods in the analysis of continuum particle emission. The following description is based on the procedures outlined in Ref. (5); for a more complete analysis the reader should consult this work.

From Moldauer(6,7) the reaction cross section for incident channel c and outgoing channel c' (c ≡ nτj) may be written as:

\[ \langle \sigma_{cc'} \rangle = \pi^2 \frac{\langle \theta_{\lambda c}, \theta_{\lambda c'} \rangle}{\langle \theta_{\lambda} \rangle} \left( \frac{\delta_{cc'} - \frac{\delta_{cc'}}{4} Q_c \langle \theta_{\lambda c} \rangle^2}{w_{cc'}} \right) \]  

(1)

where

\[ \theta_{\lambda} = \sum_{\alpha} \langle \theta_{\lambda \alpha} \rangle \quad \alpha = \text{all open channels.} \]  

(2)

\[ w_{cc'} = \frac{\langle \theta_{\lambda c}, \theta_{\lambda c'} \rangle}{\langle \theta_{\lambda} \rangle} \]  

(3)

and

\[ \langle \theta_{\lambda c} \rangle = T_c + \frac{1}{Q_c} \left[ 1 - \sqrt{1 - \frac{Q_c T_c}{\gamma} \gamma^2} \right]. \]  

(4)

\( T_c \) is the optical model penetrability for channel c, and \( Q_c \) is the statistical parameter with range \( 0 \leq Q_c \leq 2 \).

In previous calculations using ABACUS-NARREEX(9) the quantity \( Q_c \) was treated as a constant where its dependence on \( \langle \theta_{\lambda c} \rangle \) was ignored. However, as was discovered in several instances during the analysis in P and also reported by(10), such a treatment can lead to negative values for the compound elastic cross section for some partial waves when many channels are open and \( Q_c \) is not taken sufficiently small.
Figure 14

Figure 15
experimental constraints; namely, the total cross section \( \sigma_T \), the
potential scattering cross section \( \sigma_{pot} \), and the s- and p-wave strength
functions (\( S_0 \) and \( S_1 \)).

Two additional pseudo-constraints \( \sigma_{nf} \) and \( \sigma_{np} \) were also introduced
in the statistical analysis such that the calculated values agreed to
at least 5 to 7% of the most recent recommended values. The reason for
the latter restriction is manifested in the fact that such an analysis
would beget more confidence in the resulting inelastic processes.

These restrictions were very successful in providing a consistent
set of parameters for performing calculations that produced very good
agreement with all available experimental data from 10 keV to 20 MeV.

Theory

The differential cross sections for shape elastic scattering (\( \sigma_{SE} \)),
the total reaction cross section (\( \sigma_R \)), and the direct inelastic scattering
(\( \sigma_{(rot)} \)) were calculated using the Coupled Channel Code JUPITER I by
Tamura (4).

In the phenomenological description it is assumed that the whole
interaction to which the neutron is subjected may be described by an
optical-model potential \( V(r,\theta,\phi) \) which is complex and includes spin orbit
coupling. Its radial dependence is of the Saxon-Woods form and its
derivative. \( V(r,\theta,\phi) \) is assumed to be, in general, non-spherical and
is defined as (4):
Figure 17

PLUTONIUM-239 TOTAL INELASTIC NEUTRON CROSS SECTION

Figure 18

PLUTONIUM-239 TOTAL INELASTIC NEUTRON CROSS SECTION
has steadily increased and in most cases exceeds the accuracy of experimental differential data. A clear example of the latter is the proper interpretation of the inelastic scattering cross sections for Pu-239.

An earlier evaluation of $\sigma_{nn}$ and other reaction cross sections was presented at the Helsinki Conference, June 1970 (1) (hereafter referred to as P). This analysis was to form the basis for the high energy ($E > 100$ keV) cross sections for the Evaluated Nuclear Data File (ENDF/B) on Pu-239. A subsequent meeting of the Cross Section Evaluation Working Group (CSEWG) resulted in expressions of concern that the elastic cross sections in ENDF/B-II were lower than those in ENDF/B-I and the inelastic cross sections were higher.

As pointed out in P, previous calculations used in evaluating Pu-239 have employed a spherical optical potential with the various reaction cross sections being interpreted as arising only from compound nucleus formation. However, since this nuclide is known to exhibit a high degree of deformity, the scattering of neutrons cannot be described adequately by the conventional optical model, which does not consider the coupling between the incident neutron motion and the nuclear surface rotation. This coupling causes the direct excitation of the rotational levels by inelastic scattering.

While these previous analyses have provided fairly good agreement between calculated and experimental angular distributions, the magnitude of the diffraction minima and maxima has not been well produced. Earlier investigations (2,3) have shown that neglecting the high degree of anisotropy exhibited by the direct inelastic component can lead to serious errors in the prediction of the differential elastic and inelastic cross sections. These errors manifest themselves in two major areas. In the low
PLUTONIUM-239 INELASTIC CROSS SECTIONS

Figure 20
PLUTONIUM-239 INELASTIC CROSS SECTIONS

Figure 22
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NOTICE

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