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LLNL-TR-729076

Total and Compound Formation Cross Sections for Americium Nuclei: Recommendations for Coupled-Channels Calculations

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April 13, 2017

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This work performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

Total and compound formation cross sections for americium nuclei: Recommendations for coupled-channels calculations

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(Dated: April 11, 2017)

Calculations for total cross sections and compound-nucleus (CN) formation cross sections for americium isotopes are described, for use in the 2017 NA-22 evaluation effort. The code ECIS 2006 was used in conjunction with Frank Dietrich's wrapper 'runtemplate'.

I. ACTINIDE CALCULATIONS

A. General considerations

Coupled-channels (CC) calculations are required to obtain the compound-formation cross sections for neutrons impinging on various actinide nuclei, as well as to obtain neutron transmission coefficients for Hauser-Feshbach calculations. The calculations described here are carried out with the code ECIS06 [3]. For convenience, a wrapper ('runtemplate'), written by F.S. Dietrich, is used to prepare the input and to parse the output of ECIS.

Traditional CC calculations for deformed target employ only a few states (3 to 5) for these types of applications. Since it was recently shown that a larger number of states is required to ensure convergence [1] [Dietrich et al, PRC85 (2012) 044611], in various regions of the nuclear chart, the calculations were repeated with 8-14 states. Two actinide potentials were considered, Flap 2.2 by Dietrich [2], and Soukh by Soukhovitskii *et al.* [5]. Flap 2.2 was developed with a small set of coupled states [2] and it was recently recommended that an updated version be developed. The Soukhovitskii potential is based on a larger number of coupled states and is expected to be somewhat more accurate. Some estimates of deformation lengths, based on experimental data and CC analyses exist for ^{238}U and ^{232}Th, and systematics are being developed by Dietrich and Thompson (2012). Here, various sets of deformation parameters were considered.

II. THE AM CASE

For both surrogate applications and Hauser-Feshbach calculations, ECIS runs were carried out. Total cross sections, s-wave (S_0) and p-wave (S_1) neutron strength functions, as well as (R') were calculated and compared to experimental values, where available. Compound-formation cross sections were calculated for Surrogate applications, and neutron transmission coefficients were determined as input for Hauser-Feshbach calculations. Since the latter are needed for a variety of Am isotopes, a more careful study was carried out of various aspects of the calculations (convergence with number of coupled rotational states, effect of deformation, effect of level energies, effect of approximations to the levels in the coupled rotational band).

The focus here is on the n+^{241}Am case, which involves a stable target.

In the recent paper by Dietrich [1], it was determined that a large number of rotational states (14 in the ^{239}U case) are required to achieve converged results. Here, I investigate the convergence by considering 5, 6, 9, 12, and 15 coupled states. Dietrich *et al.* also found that the target spin (and K value) has essentially no effect on the calculated (total) cross section, *i.e.* instead of carrying out the calculation for a band of experimentally-observed levels, it is sufficient to construct a rotational band with $J = 0, K = 0$, as long as the effective moment of inertia is approximately the same. I confirm this here.

Various optical potentials exist for actinides. Dietrich's FLAP 2.2 is in the process of being revised, since the parameters were determined prior to the realization that a large number of states has to be coupled. I use the recommended OMP by Soukhovitskii *et al.* [4] and vary the deformation parameters β_2 and β_4 to achieve agreement with measured strength functions and total cross sections.

I carried out two types of calculations: I used experimentally-determined levels in the $K = 5/2$ rotational band in a coupled-channels calculation to determine the total cross section. I extracted the parameter c from the energies of these levels and the formula $E_{ex} = c[I(I+1)-K(K+1)]$ where $K = 5/2$ and the spins I and energies E are listed in Table III. That $c = 0.00568$ value was then used to construct a new, artificial rotational band with $K = 0$ and $0^+, 2^+, 4^+ \ldots$. Total cross sections obtained with CC calculations using this artificial band were compared to the calculation with the actual levels.

Comparing the latter calculations with varying numbers of coupled states and to the calculations with half-integer states, I find:

- The calculations using the artifical even-J bands are converged when 9 states are coupled; there is no difference when using 12 states, as can be seen in Fig. 1.
- The calculations confirm that the members of the gs band can be approximated by an even-even band with K=0, as can be seen in Figure 2. The actual K value (5/2 here) does not play a role, nei-

ther do the actual spins. I get perfect agreement when both calculations couple states up to 1.5 MeV, which involves 9 states of the even-J band ($0^+, 2^+, 4^+ \ldots 16^+$), up to E_{ex}=1.545 MeV, or 15 states of the half-integer band ($5/2^- \ \ldots \ 33/2^-$), up to E_{ex} = 1.562 MeV. It seems that either approach is appropriate, as long as states up the the same excitation energy are coupled.

- Varying the energies of the levels within the artificial rotational bands had no visible effect on the calculated total cross section (not shown).

- Changing the deformation of the target nucleus had an effect in particular on the low-energy cross section (below about 1 MeV) and on the calculated average resonance parameters. I considered deformations recommended in RIPL-3, from HFB calculations (β_2=0.290, β_4=0.140) and from FRDM95 calculations (β_2=0.223, β_4=0.087, β_6=-0.022, but setting β_6=0). I found that the calculated s-wave and p-wave strength functions did not agree very well with experimental data when the HFB results were used (see Table III). The FRDM95 values gave better agreement with experiment. I explored further options, including the optimal deformation found by Capote *et al.* in a recent study of actinide optical potentials (β_2=0.209, β_4=0.070). After further variations, I selected the values β_2=0.212, β_4=0.073. Results for various sets of deformation parameters are shown in Figure 3 (top panel).

- Overall, the results for the β_2=0.212, β_4=0.073 case agree well with available data and are of similar quality as results from recent evaluations. Above 0.01 MeV, only data from Phillips (1997) is available. The experimental uncertainties are between 0.2% at E_n = 0.45 MeV and 1.5% at E_n = 20 MeV. The calculated total cross section is shown along with evaluated cross sections and data in Figure 3 (bottom panel). The selected parametrization gives results that are slightly above the data for 2-5 MeV (by about 4%) and above 15 MeV (by about 5%), and excellent agreement with the data (within 2%) for energies below 2 MeV, as well as between 5 and MeV. The calculation is about as good as Rosfond 2010 and JENDL 4.0, and only ENDF VII.0 is slightly better.

- In Figure 4 the calculated compound-formation cross section for the selected parameterization is compared to the results using other deformation parameters. The difference between the (β_2=0.212, β_4=0.073) case and the (β_2=0.223, β_4=0.087) case helps to give an estimate of the uncertainty of the CN formation cross section. The difference between those two calculations is about 1% above 2 MeV, and around 4% below 1 MeV. Considering the uncertainties in the calculated total cross section, I estimate the overall uncertainty for the compound formation cross section to be about 5% above 1 MeV and 10% below 1 MeV.

- The cross section calculations show almost no sensitivity to the mass number of the nucleus, as can be seen in Figure 5 for the total and compound-formation cross sections, and in Figure 6 for the transmission coefficients. I expect to be able to use the n+^{241}Am formation cross section for the immediate neighbors without further increasing the uncertainty. I also expect that using the n+^{241}Am transmission coefficients in Hauser-Feshbach calculations involving neutrons on neighboring isotopes is a good approximation.

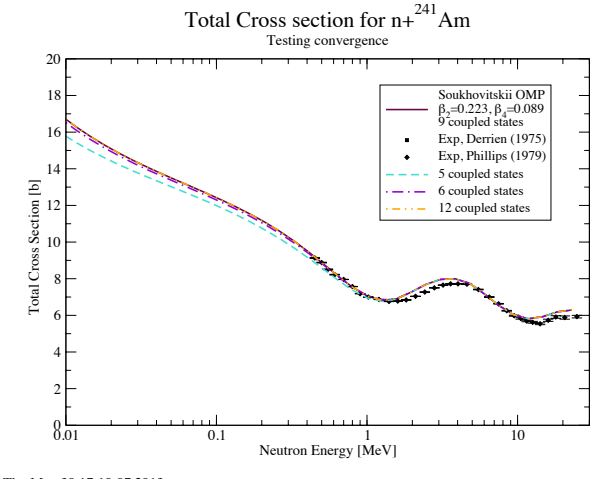

FIG. 1: Total cross section for n+^{241}Am calculated with 5, 6, 9, and 12 coupled states. The calculations for 9 and 12 states give identical results, illustrating that nine states are sufficient in this case to obtain converged cross sections.

The parametrization of choice is that using the Soukhovitskii potential, with deformation parameters β_2=0.212, β_4=0.073. It gives good agreement with available data and results that are similar to recent evaluations. The total cross section has an estimated uncertainty of less than 5% (less than 3% for some energies) and the compound-formation cross section is estimated to have a 10% uncertainty below 1 MeV and 5% between 1 MeV and 20 MeV.

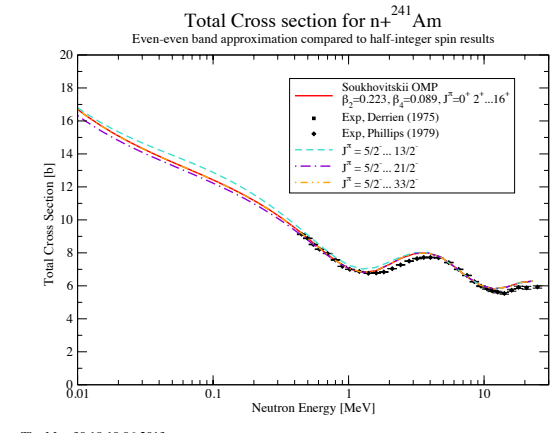

FIG. 2: Approximating the rotational band by a schematic $K = 0$ band with $J^\pi = 0^+, 2^+, 4^+ \ldots$. The CC calculations for n+^{241}Am show that both the schematic band and the band consisting of experimentally-observed levels give the same cross sections, as long as convergence is achieved (see also discussion in text).

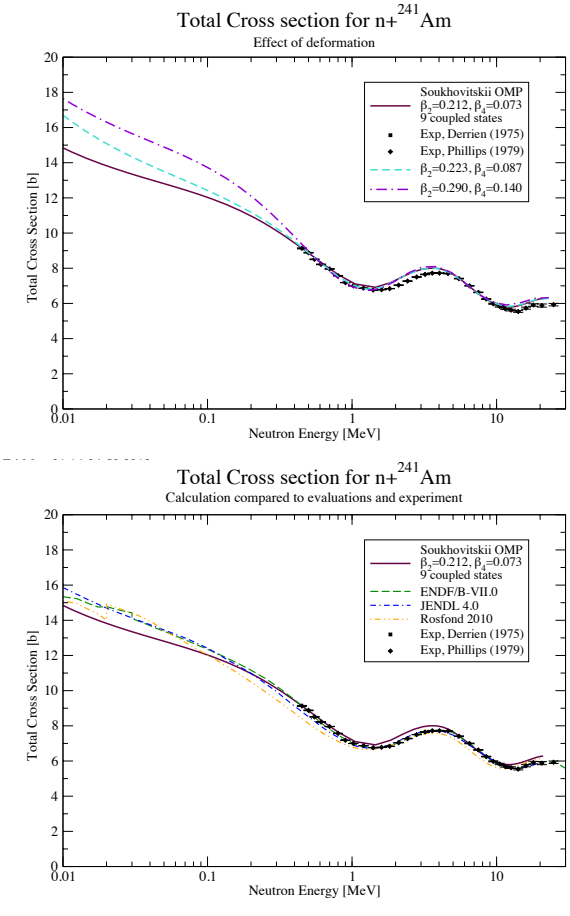

FIG. 3: Cross sections for n+^{241}Am. The top panel shows a comparison of several CC calculations to available experimental data. The bottom panel show the parametrization of choice compared to recent evaluations.

TABLE I: Energies of members of the $K = 5/2$ band in ^{241}Am. All levels have negative parity. The energies satisfy the relation $E_{ex} = c[J(J+1) - K(K+1)]$ with $c = 0.00568$. The data was taken from ENSDF at BNL. The horizontal lines are drawn after 5, 9, 12, 15 states.

Spin (Neg. Parity)	E_{ex} [MeV]
2.5	0.000
3.5	0.041
4.5	0.094
5.5	0.158
6.5	0.234
7.5	0.320
8.5	0.418
9.5	0.526
10.5	0.645
11.5	0.773
12.5	0.913
13.5	1.062
14.5	1.219
15.5	1.388
16.5	1.562
17.5	1.749
18.5	1.941
19.5	2.145
20.5	2.352
21.5	2.575

TABLE II: Calculated average resonance properties compared to experimental results (and a calculation by Capote *et al.* .)

Reference	Deformation Parameters	S_0 [10^{-4}]	S_1 [10^{-4}]	R' [fm]
myChoice	β_2=0.212, β_4=0.073	0.88	1.98	9.3
medDef	β_2=0.223, β_4=0.087	1.32	1.86	9.42
hiDef	β_2=0.290, β_4=0.140	1.07	2.10	10.20
Capote	β_2=0.209, β_4=0.070	0.89	2.15	9.47
RIPL-3	n/a	0.88 ± 0.06	–	–
Mugh	n/a	0.90 ± 0.09	–	–

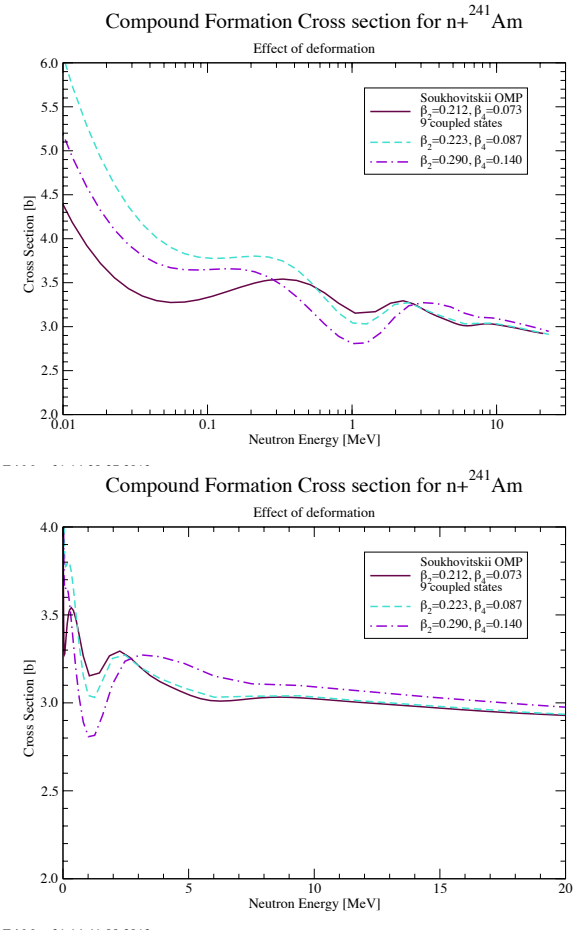

FIG. 4: Compound-formation cross sections for n+^{241}Am. The parameterization of choice (β_2=0.212, β_4=0.073) is compared to alternative parameterization from the literature. Two different energy scales are shown

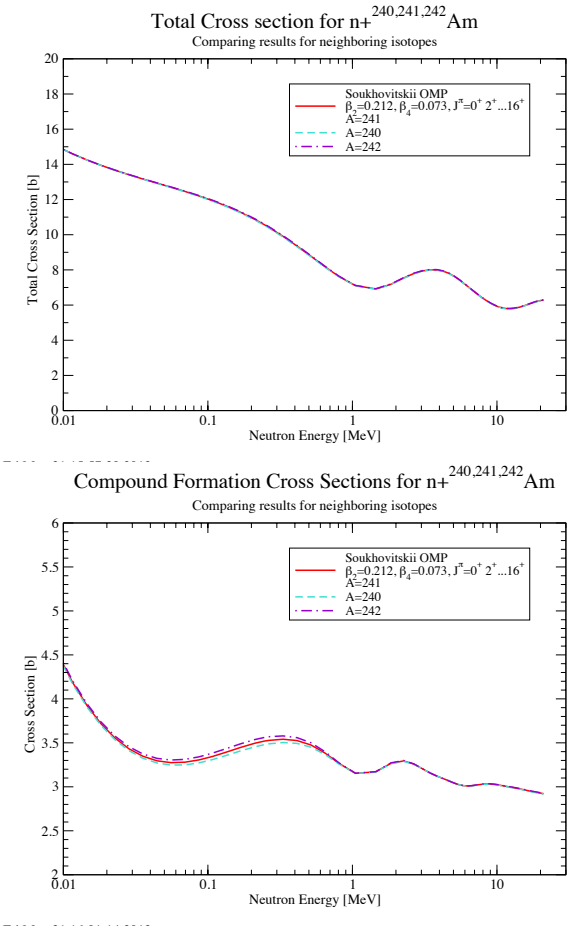

FIG. 5: Total (top) and compound-formation (bottom) cross sections for n+^{240,241,242}Am. The calculations give essentially the same results for all three neighboring nuclei.

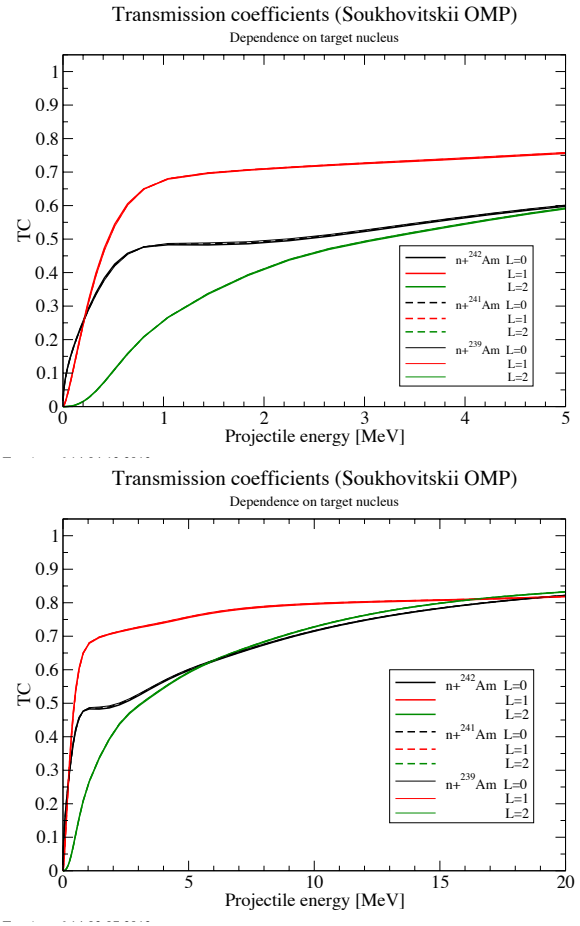

FIG. 6: Transmission coefficients for n+^{240,241,242}Am for the first three partial waves ($l = 0, 1, 2$), for neutron energies from 0 to 20 MeV (bottom) and enlarged for energies to 5 MeV (top). The calculations give essentially the same results for all three neighboring nuclei.

[1] F. S. Dietrich, I. J. Thompson, and T. Kawano, *Target-state dependence of cross sections for reactions on statically deformed nuclei*, Phys. Rev. C, **85** (2012), p. 044611.
[2] J. E. Escher and F. S. Dietrich, *Cross sections for neutron capture from surrogate measurements: An examination of Weisskopf-Ewing and ratio approximations*, Phys. Rev. C, **81** (2010), p. 024612.
[3] J. Raynal, *computer code ecis.* unpublished.
[4] E. S. Soukhovitskii, S. Chiba, J.-Y. Lee, O. Iwamoto, and T. Fukahori, *Global coupled-channel optical potential for nucleon–actinide interaction from 1 keV to 200 MeV*, Journal of Physics G: Nuclear and Particle Physics, **30** (2004), p. 905.
[5] E. S. Sukhovitskii, O. Iwamoto, S. Chiba, and T. Fukahori, *Nucleon optical potential of Uranium-238 up to 150 MeV*, Journal of Nuclear Science and Technology, **37** (2000), pp. 120–127.