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TITLE CALCULATION OF ^{239}Pu NEUTRON INELASTIC CROSS SECTIONS

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CALCULATION OF ^{239}Pu NEUTRON INELASTIC CROSS SECTIONS

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We have calculated cross sections for neutron-induced reactions on ^{239}Pu between 0.001 and 5 MeV, with particular emphasis on inelastic scattering. Coupled-channel and Hauser-Feshbach statistical models were used. Within the coupled-channel calculations we employed neutron optical parameters derived from simultaneous fits to total, elastic, inelastic, and resonance data. The resulting transmission coefficients were used in Hauser-Feshbach statistical calculations having a fission channel based on a double-humped barrier representation. Barrier parameters and transition state enhancements needed to reproduce well the (n,f) cross sections between 0.001 and 5 MeV were in general agreement with those from other published analyses. Calculated compound-nucleus and direct-reaction components for inelastic scattering were combined incoherently, and the resultant cross sections agreed well with the Bruyères-le-Châtel measurements for scattering from levels occupying the ground state rotational band. Our results are in substantial disagreement with ENDF/B-V values for these levels. We are presently performing DWBA calculations to determine direct-reaction components for states occupying higher-lying vibrational bands.

[^{239}Pu(n,n), ^{239}Pu(n,n'), ^{239}Pu(n,f), coupled channel optical and Hauser-Feshbach statistical model calculations, E_n = 0.001 to 5 MeV]

Introduction

As a step towards improvement of the ^{239}Pu evaluation appearing in the ENDF/B evaluated data library, we have performed neutron cross-section calculations in the incident energy range between 0.001 and 5 MeV. We placed particular emphasis on the realistic determination of inelastic scattering cross sections since relevant experimental data are sparse, and since such information is important for fast reactor applications. To accomplish this we used sophisticated nuclear models employing parameters constrained to reproduce concurrently a variety of available experimental data. This technique has proved successful in the extrapolation or prediction[1] of cross-section data where experimental measurements are not complete or do not exist.

Models and Parameters

Our ^{239}Pu calculations involved application of two main reaction models, the first being the coupled-channel optical model to describe direct-reaction contributions to inelastic scattering from collective states. The *ECIS*[2] program was used for this purpose as well as to provide neutron transmission coefficient. for the second portion of the calculation involving application of the Hauser-Feshbach statistical model code COMNUC.[3] This technique ensures consistency between the direct-reaction and compound-nucleus facets of the calculation. Cross-section contributions obtained separately from these two models were then combined incoherently to produce the final results.

ECIS calculations were made using the first six states of the ground state rotational band (1/2$^+$, 3/2$^+$, 5/2$^+$, 7/2$^+$, 9/2$^+$, and 11/2$^+$) as the coupling basis. The optical potential was represented in a standard manner (see Ref. 4 for details), while the coupling form factors needed in the expansion of the optical potential were assumed complex. We used neutron optical parameters based on the Bruyères-le-Châtel results[5] that were obtained primarily from fits to actinide total, elastic, and inelastic cross sections, as well as s- and p-wave strength functions. We did modify them slightly to produce better agreement to ^{239}Pu total cross sections measured by Poenitz,[6] particularly around 1 MeV. Our resulting optical and deformation parameters appear in Table I.

Table I Optical Model and Deformation Parameters Used in the Coupled-Channel Calculations (Depths in MeV, geometrical parameters in fm)

		r	a
V	$= 46.2 - 0.3E$	1.26	0.615
W_{SD}	$= 3.6 + 0.4E$	1.24	0.50
V_{SO}	$= 6.2$	1.12	0.47
β_2	$= 0.21$	$\beta_4 = 0.065$	

The Hauser-Feshbach ... Gilbert and Cameron[7] along with the parameters of Cook.[8] A maximum amount of discrete level information was included for each nucleus appearing in the calculation. Such data were used to adjust the constant temperature level density parameters so as to reproduce the cumulative number of levels while joining smoothly to the Fermi-gas form at higher excitation energies. Gamma-ray transmission coefficients were calculated using a Brink-Axel expression[9] that utilized two Lorentzian forms to represent the split giant dipole resonance. These gamma-ray transmission coefficients were normalized to reproduce measured $2\pi\langle\Gamma_\gamma\rangle/\langle D\rangle$ data[10] available for s-wave resonances near the neutron binding energy.

The ability to fit measured (n,f) cross sections accurately (to within approximately 5%) over a wide energy range introduces important constraints on the Hauser-Feshbach calculation of cross sections for other competing channels. Thus, in order to reproduce (n,f) experimental data reasonably well using realistic fission channel parameters, we incorporated a double-humped fission model into the COMNUC Hauser-Feshbach code (Ref.11 provides a complete description). In this application, two uncoupled oscillators were used for the barrier representation, and penetrabilities through each barrier were calculated from a Hill-Wheeler expression.[12] The spectrum of transition states occurring at each barrier was constructed utilizing bandhead information[13] available for the ^{240}Pu compound system. At higher excitations, we assumed a continuum of transition states that we calculated using the Gilbert-Cameron level density expressions and parameters applicable for the ground state deformation case. To these calculated densities we applied enhancements directly to account for deviations from symmetry present at each barrier.

asymmetric and axially symmetric.[14] Theoretical enhancements[15] associated with these barrier shapes are $\sigma\sqrt{8\pi}$ (σ is the level density spin cutoff parameter) for the inner barrier and two for the outer one.

Our fission model also included corrections for Class II fluctuations based on the picket-fence approximation of Lynn et al.[16] These corrections are important primarily at low energies and were applied in addition to the width-fluctuation corrections[17] utilized throughout our Hauser-Feshbach calculations. Our ^{239}Pu(n,f) data fits yielded the barrier parameters and density enhancement factors shown in Table II. These are in general agreement with other published values[13,18] and in particular the density enhancements agree well with results[13] utilizing microscopic level-density expressions.

TABLE II Barrier Parameters and Density Enhancements Used to Calculate ^{239}Pu(n,f) Cross Sections

	Barrier Height (MeV)	$\hbar\omega$ (MeV)	Density Enhancement
Barrier A	5.80	0.8	16
Barrier B	5.45	0.6	2

Results

Calculated scattering cross sections for 0.7 MeV neutrons incident on ground band members of ^{239}Pu are compared in Fig. 1 to recent Bruyères-le-Châtel measurements.[5] At this energy, compound contributions can be significant so that direct and compound nucleus calculations can be tested in such a comparison. Figure 2 presents a comparison at 2.5 MeV to data of Smith et al[19] that includes elastic scattering as well as contributions from states having excitation energies up to 0.20 MeV.

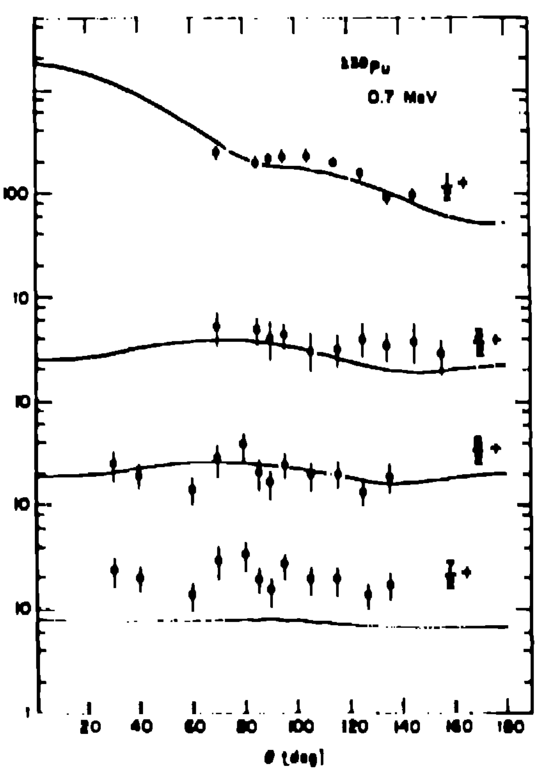

Fig. 1. Our calculated angular distributions are compared to recent measurements[5] of elastic and inelastic scattering on ^{239}Pu at a neutron energy of 0.7 MeV.

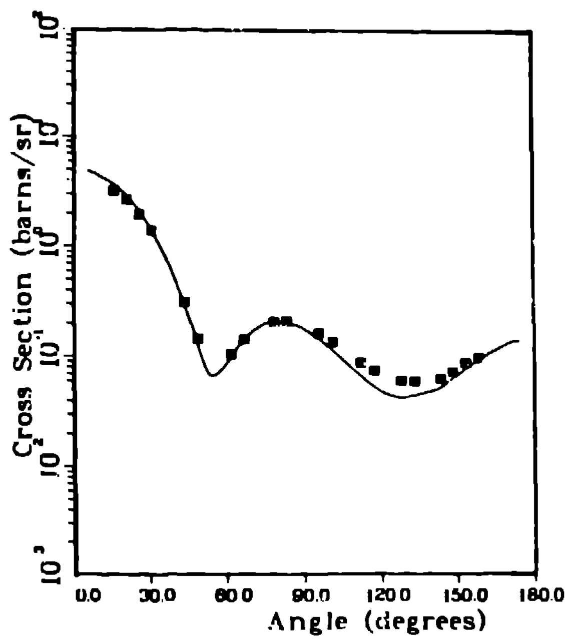

Fig. 2. Our calculations of cross sections for scattering reactions that excite ^{239}Pu states having energies $\leq$ 200 keV are compared to the data of Smith et al[19] for 2.5 MeV incident neutrons.

Figure 3 illustrates the large differences that exist between our calculated results and data appearing in the present ENDF/B-V evaluation. The comparison is made for excitation functions resulting from inelastic scattering on the 0.057 MeV ($5/2^+$) state and the 0.164 MeV ($9/2^+$) state. In the first example, the difference occurs because direct-reaction contributions were included in our calculations but not in ENDF/B. In the second example, our calculated excitation function shape occurs because of the state's relatively high spin (9/2) and because of direct-reaction components. The ENDF/B-V evaluation, on the other hand, probably employed a shape similar to those assumed for scattering from states with lower spin values.

Inelastic scattering reactions that leave the ^{239}Pu nucleus with 1 to 2 MeV of excitation are important for fast breeder reactor systems because of the energy transfers involved. This excitation energy region lies well above that encompassing the ground state rotational band so that experimental data are sparse and theoretical efforts are generally restricted to application (as in our present effort) of the Hauser-Feshbach statistical model. The experimental situation has been improved by recent measurements made by Smith et al[19] whereby the total inelastic cross section to levels lying above a given excitation energy can be inferred. Such thresholds range from 0.08 to 0.3 MeV for these measurements. The comparison of our calculations, as is done in Fig. 4, to these data provides indirect evidence regarding the behavior of inelastic scattering to higher levels for which we assumed only compound nucleus contributions. The solid core represents our results, which agree reasonably with the experimental data but which lie significantly lower than the dashed curve representing ENDF/B-V.

Recently we began calculations of direct-reaction contributions to scattering cross sections from states occupying higher-lying collective bands, particularly the K^{π} = 1/2- octupole vibrational band. These efforts were prompted by (n,n') cross sections inferred from (n,n'γ) measurements[20,21] on ^{232}Th and ^{238}U that indicate sizeable inelastic cross sections for similar states in the neutron energy range between 2 to 4 MeV. Initially we performed Distorted Wave Born Approximation (DWBA) calculations for scattering from the 0.555 MeV 7/2- state assuming an ℓ = 3 angular momentum transfer and using the spherical iteration of the

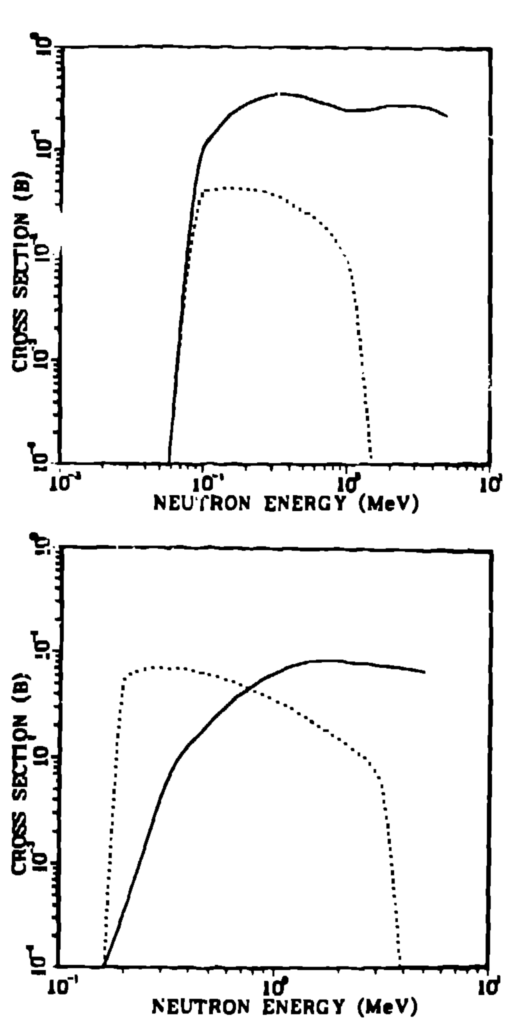

Fig. 3. Two calculated excitation functions (solid curves) for inelastic scattering from states in ^{239}Pu are compared to the ENDF/B-V evaluation (dashed curve). (a) 0.057 MeV $5/2^+$ state; (b) 0.164 MeV $9/2^+$ state.

Madland-Young neutron optical parameters.[22] To determine the β_3 deformation parameters necessary for normalization of the calculated DWBA results, we employed B(E3) values extracted from charged-particle reactions on similar octupole states in even plutonium nuclei[22] in the following expression

$$B(E\lambda) = (\frac{3}{4}\,\pi\, Ze\, R^{\lambda}\, A^{1/3\lambda})^2 \beta_{\lambda}^{\,2}\ . \qquad (1)$$

Here R_0 and B(E3) values of 1.24 fm and 0.4 e^2b^3 were used, respectively. The β_3 values determined in this manner yielded DWBA contributions on the order of 5-10 mb for neutron energies between 2 and 4 MeV. These results lie factors of 5-10 lower than values one would infer from the (n,n'γ) measurements mentioned previously.

As a further test we analyzed (p,p') measurements[23,24] for scattering from collective states in ^{238}U, with particular emphasis on data available for the 0.731 MeV 3- octupole state. Although such data are sparse, we were able to compare the relative strength for excitation of this state to reasonably known cross sections for ground-state rotational band members. This provided an independent normalization method applicable to our ℓ = 3 DWBA calculations, and and when inserted into Eq. (1) above produced a B(E3) value of 0.35 e^2b^3, which agrees with published values.[22,25] Figure 5 shows the results obtained when this normalization is applied to the calculated DWBA direct reaction contribution which is then added to the compound nucleus contribution (sum given by the solid line) for inelastic neutron scattering exciting the 0.731-MeV state in ^{238}U. The data are those of Olsen et al,[20] which were again inferred from (n,n'γ) cross sections In the energy range where direct reaction contributions dominate, our calculations are in disagreement with these measurements as well as theoretical analyses[26] performed for similar data[21] where the relative coupling between bands was treated as an adjustable parameter. We therefore see a possible discrepancy between cross sections extracted from such (n,n'γ) measurements and cross sections obtained using information inferred from charged-particle data.

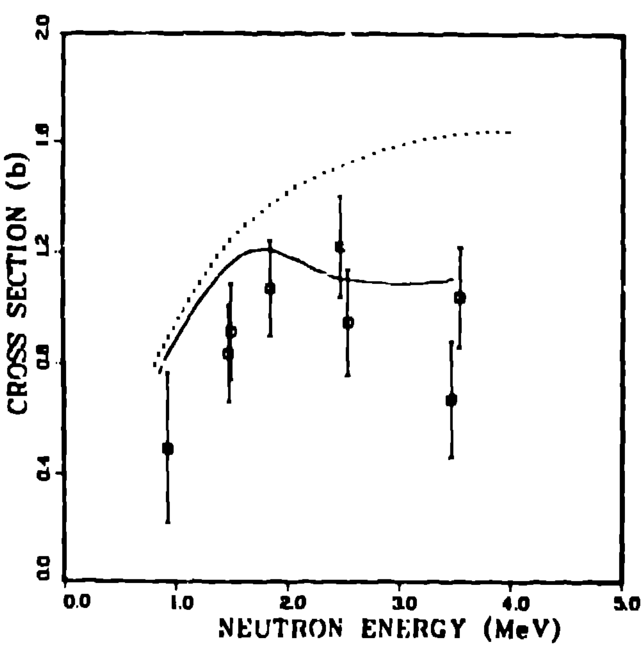

Fig. 4. Comparisons of our calculated inelastic cross sections (solid curve) for production of ^{239}Pu states above a given excitation energy (0.08-0.3 MeV over this neutron energy range) to cross sections inferred from measurements by Smith et al.[19] The dashed curve is ENDF/B-V.

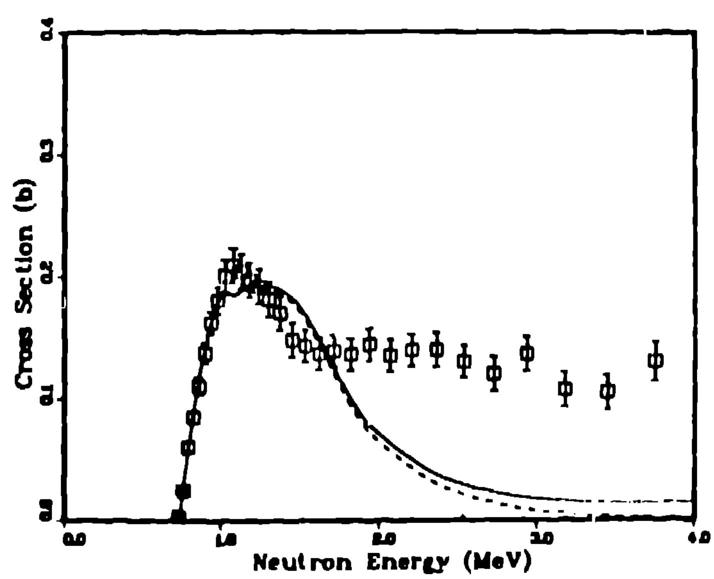

Fig. 5. Comparison of the calculated (n,n'γ) cross section for excitation of the 0.731 MeV 3- octupole state in ^{238}U to data of Olsen et al.[20] as deduced from (n,n'γ) measurements. The dashed curve is the compound-nucleus (CN) contribution; the solid curve contains both CN and direct-reaction (DWBA) components.

Conclusion

Using nuclear-model calculations that incorporate realistic parameter sets, we are able to reproduce neutron inelastic scattering data for the ground state rotational band members of ^{239}Pu at energies less than 5 MeV. Similarly, our calculations of integrated inelastic cross sections agree well with such information inferred from recent experimental measurements. There do appear to be discrepancies between cross sections extracted from (n,n'γ) measurements for levels occupying higher collective bands and results obtained from charged-particle measurements.

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