

Calculation of fission product yields for some nuclei with TALYS code

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Abstract. We have carried out a calculation of the transmission coefficients per fission mode and determined the fission product yields for some nuclei using the Talys-0.72 version of the code[1]. For fission, this code uses a statistical approach based on a revised version of the multi-modal random neck-rupture model (MM-RNRM). The fragment mass distribution is the sum of the three dominant fission modes: the superlong (SL), the standard I (ST I) and the standard II (ST II). The relative contribution of each mode is deduced from the calculation of the transmission coefficients according to the Hill-Wheeler expression taking into account the relevant transition states. The shell and pairing corrections are introduced in the level density parameter according to the Ignatyuk[2] formula. The calculated transmission coefficients values per fission mode are compared with the existing values. First, we reproduced the fragment mass distributions obtained using the Talys-0.64 version of the code for the fission of ²³⁸U induced by 1.6 and 5.5 MeV neutrons with the 'constant temperature model' of Gilbert and Cameron[3], then we extended the calculations to other actinides with other level density models[4][5]. Finally, these calculated values of fission yields are compared with the experimental data.

1 Introduction

The calculation of the fission products yields requires the knowledge of two determining factors: level density and transmission coefficient. The level density is described in different ways with excitation energy. Indeed, at low excitation energy, this is given by the experiments given discrete levels, whereas at high energy, it is given by the Fermi gas model. At intermediate energy, various phenomenological models can be utilised in TALYS code. The transmission coefficient is given by the Hill and Wheeler [6] expression with the assumptions of existence of the transition states.

2 Calculation of the transmission coefficients and fission modes SL, STI and STII probabilities

In the case of actinides, in their way towards fission, the nuclei meet a double (resp. triple) humped barriers. Several fission modes can be followed by these nuclei through the valleys of potential energy surface. Moreover, between the fission barriers, resonance states known as classes I or II (respectively, in the first and second well) can be built. These states increase the transmission through the barrier. The transmission coefficient per fission mode evaluated with the Hill-Wheeler[6] penetrability through parabolic barriers and using temperature-dependent barrier parameters is

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given by:

$$T_{f,FM}(Z_{FS}, A_{FS}, E_x) = \int \rho_{gs}(Z_{FS}, A_{FS}, \epsilon) d\epsilon \frac{1}{1 + \exp\left[\frac{2\pi(B_{f,FM}(Z_{FS}, A_{FS}, T(\epsilon)) + \epsilon - E_x)}{\hbar\omega_{f,FM}(Z_{FS}, A_{FS}, T(\epsilon))}\right]} \quad (1)$$

ρ_{gs} is the the ground state level density.

E_x is the excitation energy.

$B_{f,FM}$ is the fission mode barrier height.

ϵ is the excitation energy of the transition state.

The contribution of each fission mode is then given by:

$$W_{SL}(Z_{FS}, A_{FS}, E_x) = \frac{T_{f,SL}^B}{T_{f,SL}^B + T_{f,STI}^B + T_{f,STII}^B} \quad (2)$$

Figures 1, 2 and 3 show the fission mode probabilities of SL, STI and STII modes as function of the excitation energy (total energy of compound system) calculated using TALYS code respectively for the systems ²³²Th(*n, f*) and ²³⁸U(*n, f*) and ²⁴²Pu(*n, f*).

3 Fission fragment mass distribution

In order to determine the fission mode mass yield Y_{FM} , TALYS code uses a new version of the random neck-rupture model (RNRM) of Brosa[7] developed by Duijvestijn et al.[8], it includes the temperature in the calculation of the potential energy landscape of the nucleus. Finally the mass distribution is the result of the contribution of these three fission modes:

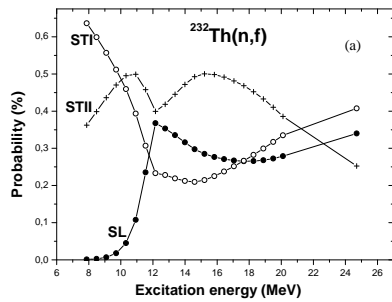


Fig. 1. Fission mode probability as a function of excitation energy, deduced from transmission coefficient for $^{232}\text{Th}(n, f)$.

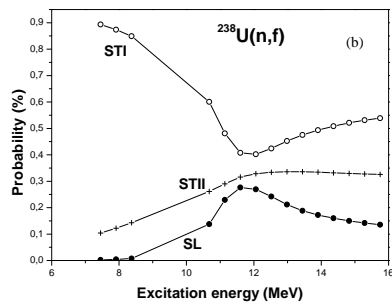


Fig. 2. Fission mode probability as a function of excitation energy, deduced from transmission coefficient for $^{238}\text{U}(n, f)$.

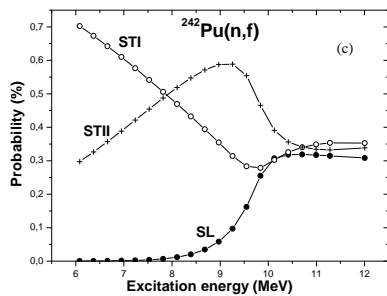


Fig. 3. Fission mode probability as a function of excitation energy, deduced from transmission coefficient for $^{242}\text{Pu}(n, f)$.

$$Y(A_{FF}; Z_{FS}, A_{FS}; E_x) =$$

$$\sum_{FM=SL, STI, STII} W_{FM}(Z_{FS}, Z_{FS}, Z_x) Y_{FM}(A_{FF}; Z_{FS}, A_{FS}; E_x) \quad (3)$$

TALYS code enables us to calculate fission product yields in (mb). The yields normalized to 100 fission obtained for monoenergetic neutrons induced fission of ^{238}U and ^{232}Th are given respectively on figures 4, 5. Three phenomenological level density models, namely the Constant Temperature Model (CTM)[3], the Back-shifted Fermi gas Model (BFM)[4] and Generalized Super fluid Model (GSM)[5] are carried out. CTM and BFM models seem to give very

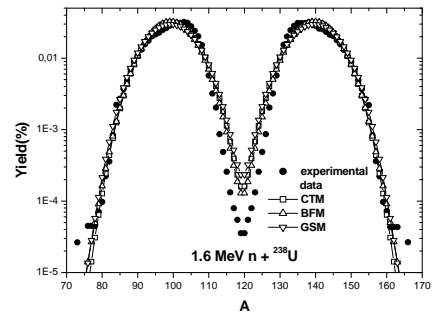


Fig. 4. Preneutron emission mass yields distribution in neutrons-induced fission of ^{238}U . The experimental data taken from [8] indicated by points are compared with the calculations by TALYS code using CTM[3], BFM[4] and GSM[5] level density models.

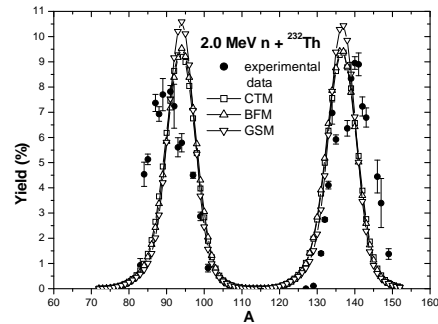


Fig. 5. Post-neutron emission mass yields in neutrons-induced fission of ^{232}Th . The experimental data taken from [8] indicated by points are compared with the calculations of TALYS code using CTM[3], BFM[4] and GSM[5] level density models.

close results for these nuclei and neutrons energy whereas GSM model overestimates the mass yields. Further, we used the CTM model for all the other calculations.

4 Comparison with the experimental results :

We obtained using TALYS code the mass yield distributions in (mb) and in (%) for some nuclei. The calculations were undertaken with the assumption of CTM level density model. All the experimental data are extracted from those used by M.C.Duijvestijn *et al* [8] for comparison with the calculations they carried out using the ALICE code. In figure 6, we present in logarithm scale the preneutron emission mass distribution for the fission of ^{232}Th by 1.21 MeV neutrons obtained with TALYS code and compared with experimental data[9]. The agreement is rather good both for the position of the most probable heavy mass and the width of the distribution. For the calculations of the post-neutron mass distributions, we took account of phenomenological correction for evaporated neutrons. The mass yield distributions for the fission of ^{232}Th by 1-10 MeV neutrons obtained with TALYS code are compared with those obtained by Glendenin *et al.*[10] (fig.7). The

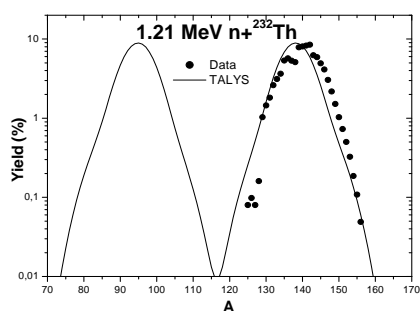


Fig. 6. Preneutron mass yields for the fission of ^{232}Th by 1.21 MeV neutrons. The lines correspond to the calculations with TALYS code and the experimental data are taken from [9].

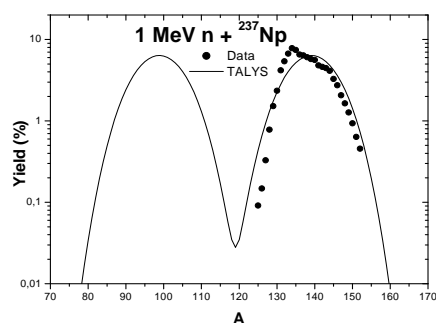


Fig. 8. Preneutron mass yields for the fission of ^{237}Np by 1.0 MeV energy neutrons. The lines correspond to the calculations with TALYS code and the experimental data are taken from [11].

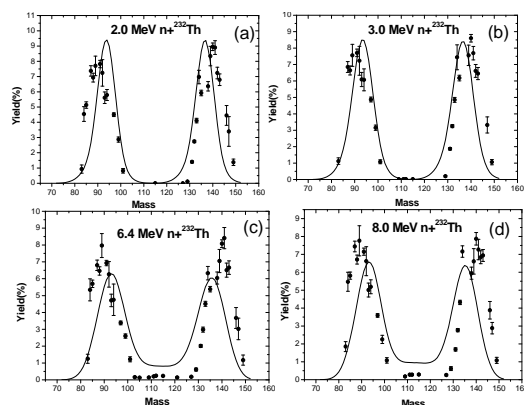


Fig. 7. Post-neutron emission mass yields in neutrons induced fission of ^{232}Th . The lines correspond to the calculations with TALYS code. The experimental data for 2, 3, 6.4 and 8 MeV energy neutrons are taken from [10].

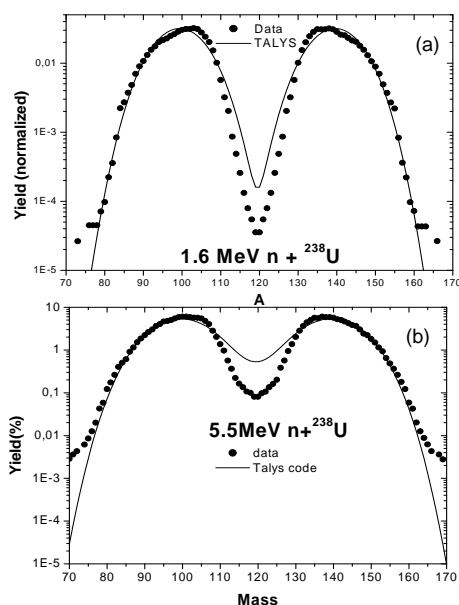


Fig. 9. Preneutron mass yields for the fission of ^{238}U by (a) 1.6 MeV energy neutrons (b) 5.5 MeV energy neutrons. The lines correspond to the calculations with TALYS code and the experimental data are taken from [12].

predictions made for the postneutron emission mass distribution of ^{232}Th do not agree well with the experimental data particularly the light and heavy group positions. However, the width for light and heavy group seems to be in agreement with the experimental data. In figures 8,9(a),9(b) and 10, we show the preneutron emission mass yields for the fission of ^{237}Np , ^{238}U , and ^{242}Pu by neutrons and ^{226}Ra and ^{197}Au by protons. In the case of 5.5 MeV neutrons on ^{238}U , the symmetric fission portion is overestimated. The group of heavy fragments is described nicely for the ^{237}Np , except the structure in the heavy peak around mass 135. Examples of proton induced fission of ^{226}Ra and ^{197}Au are presented in the figures 11 and 12. The agreement with the calculations is very good for ^{197}Au . In fact, for these nuclei, the contribution of STI and STII modes is zero. In the case of ^{226}Ra , the calculations predict a triple humped distribution in accordance with experimental observations, but a dissension appears in the position of the asymmetric peaks and the estimation of the contributions of fission modes. Note that the calculations made with TALYS code does not predict any fine structure in masse distribution.

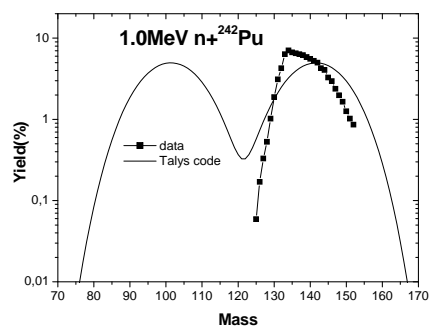


Fig. 10. Preneutron mass yields for the fission of ^{242}Pu by 1.0 MeV energy neutrons. The lines correspond to the calculations with TALYS code and the experimental data are taken from [13].

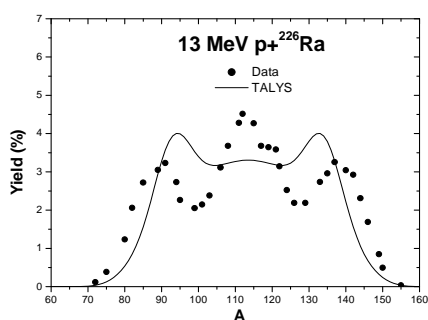


Fig. 11. Preneutron mass yields for the fission of ^{226}Ra by 1.0 MeV energy neutrons. The lines correspond to the calculations with TALYS code and the experimental data are taken from [14].

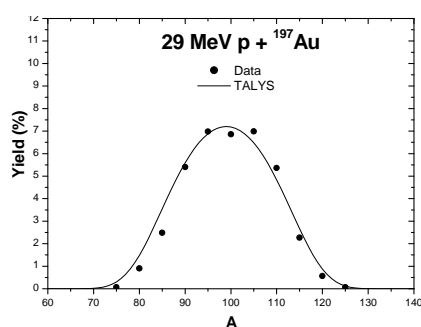


Fig. 12. Preneutron mass yields for the fission of ^{197}Au by 1.0 MeV energy neutrons. The lines correspond to the calculations with TALYS code and the experimental data are taken from [15].

5 Conclusion

The results obtained on the calculation of the transmission coefficient seem to be in agreement with the data of the literature and confirm the fact that the fission mode STI and STII have a more important contribution than SL modes for the studied nuclei, except in the case of ^{197}Au where the contribution of asymmetric modes STI and STII is null which is in quite agreement with the experimental data. The obtained results, although they find an asymmetrical distribution of the fission products whose amplitude is comparable with that of the experimental results, they show a dissension with regard to the position of the light and heavy mass groups. Moreover, TALYS code gave smooth curves for mass yield distribution and does not predict any fine structure which is essentially due to the shell effects. These effects such as introduced in level density parameter do not reproduce any fine structure. At the excitation around neutron separation energy, the competition between fission and neutron evaporation plays an important role in favor of the asymmetric fission. We propose to try to reproduce better the mass distribution by testing the microscopic level density from Hartree-Fock calculations based only on the nucleon-nucleon-interaction, without any parameter to be adjusted.

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