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Calculations of $(n,2n)$, (n,np) and
 (n,pn) cross sections taking into
account preequilibrium processes

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Abstract

The influence of preequilibrium processes as described by the exciton model, on the cross sections and particle spectra shape of $(n,2n)$, (n,np) and (n,pn) reactions is considered.

At first, the dependence of both equilibrium and preequilibrium cross sections on incident neutron energy is investigated in model nuclear systems for derivation of some systematic trends. After that, the above-mentioned cross sections at 14 MeV are calculated for 39 real nuclei in the mass region $60 \leq A \leq 209$. Comparison with experimental $(n,2n)$ cross sections at 14 MeV incident energy confirms the reduction of this cross section by up to 30 % due to preequilibrium emission. The influence on (n,np) and (n,pn) cross sections is even more pronounced - they are changed by up to more than two orders of magnitude, depending on binding energies, pairing effects and level densities.

1. Introduction

Preequilibrium processes play an important role in many nuclear reactions where the initial energy is between a few MeV and 100 MeV. Taking into account preequilibrium decay, it is in general possible to achieve a better understanding and description of these processes [1, 2].

The work described here is a study of the role of these processes in reactions, accompanied by multiple emission of nucleons. The main part of all calculations are carried-out for an initial neutron energy of 14 MeV, since most of (n,2n)-experiments have been performed at this energy. For the (n,pn) and (n,np) reactions only a very few experimental data are available even at 14 MeV. Some excitation functions in a wide energy range are examined also.

One aim of this work is to study the mechanism of these reactions. The other aim is to develop a new, more accurate method of calculating (n,2n), (n,pn) and (n,np) reaction cross sections, which are of practical importance, especially for fusion reactor design, but difficult to determine experimentally.

This paper represents a continuation of results described in ref. [3], in which this method was used first, and other recent publications [4, 5].

2. Description of the Model

After the bombardment of a nucleus by a neutron, the compound system, starting with a small number of degrees of freedom (two particles plus one hole correspond to $n = 3$ excitons), is gradually transformed into a more complex configuration (for each transition $\Delta n = 2$), until a state of statistical equilibrium is reached, i.e. the state of the compound nucleus. There is a specific probability of the emission of a nucleon from each preequilibrium state with n quasiparticles. This emission will lead to a unit decrease in A and n and to a decrease in the excitation energy. The nucleus (Z, N) will therefore give rise to a nucleus $(Z-1, N)$ in the case of emission of a proton or $(Z, N-1)$ in the case of emis-

sion of a neutron and so on.

Absolute spectra for both types of nucleons from all intermediate nuclei are calculated as long as the excitation energy does not become less than the nucleon binding energy. The calculations are performed on the basis of the hybrid model [6], according to which the probability $n_x^{P\pi}(E)$ of pre-equilibrium emission of a nucleon of type x from a state with n excitons is equal to

$$n_x^{P\pi}(E) = n_x^p \frac{\varrho_{n-1}(U)}{\varrho_n(E^*)} \frac{\lambda_{em}(E)}{\lambda_{em}(E) + \lambda_+(E)} \quad (1)$$

where n_x^p is the number of nucleons of type x in state n ; $\varrho_{n-1}(U)$, $\varrho_n(E^*)$ represent the densities of states with $n-1$ and n quasiparticles in the final and intermediate nucleus, respectively, as obtained by combination of equidistant, single-particle levels; λ_{em} is the probability of emission, obtained from σ_{inv} by means of the detailed balance principle; and λ_+ is the probability of an intranuclear transition with $\Delta n = 2$.

In accordance with Ref. [6], λ_+ is calculated on the basis of the probability of nucleon collision in the nuclear matter, which gives the expression:

$$\lambda_+(E) = \frac{1}{K} \left[1,4 \cdot 10^{21} (E + B) - 6,0 \cdot 10^{18} (E + B)^2 \right] s^{-1} \quad (2)$$

where K is a parameter which is independent of energy;

B is the nucleon binding energy.

The equilibrium spectrum $P_x^P(E)$ of particles of type x is calculated from the comprehensive statistical theory of nuclear reactions:

$$P_x^P(E) = \frac{(2s+1) m E \sigma_{inv}(E) \varrho_R(U)}{\sum_v m_v E_v \int_0^{E_{max}} E_v \sigma_{inv,v}(E_v) \varrho_v(U_v) dE_v} \quad (3)$$

where $\rho_R(U)$ is the level density of the residual nucleus, given in terms of the Fermi-gas model by:

$$\rho_R(U) \sim \frac{1}{(U_{\text{eff}} + t)^2} \exp \left[2 (a U_{\text{eff}})^{1/2} \right] \quad (4)$$

The influence of shell effects on the density $\rho_R(U)$ can be taken into account by using experimentally determined density parameters (a). As well known, allowance for the pairing effect is made by introducing an effective excitation energy $U_{\text{eff}} = U - \Delta$.

Given the known cross-section of formation of an initial system with $n = 3$, we thus obtain absolute spectra of the emitted nucleons and after summation with respect to energy we get the cross-sections of the (n, n') , (n, p) , $(n, 2n)$, (n, np) , (n, pn) etc. reactions.

All parameters, except K in formula (2) can be regarded as well-known. The value of K , employed in all the following calculations, is obtained comparing the predictions of the hybrid model with the high energy part of experimental (nn') spectra at 14 MeV incident energy. It was shown [7], that in a wide mass number range the constant parameter $K = 10$ can be regarded as a suitable parameter.

3. Systematic studies with Model Nuclei

3.1. Branching Ratios and absolute Cross Sections

The cross sections for equilibrium and preequilibrium decay of a compound system depend in a complex manner on such quantities as binding energy B_x , level density parameter a , the shell structure of single particle states, pairing energy etc. In order to appreciate both the importance of taking into account preequilibrium decay and the influence of nuclear structure effects on the investigated cross sections, calculations have been performed for a simple model compound system with well-defined parameters. The parameters of that system are the following:

- Initial energy of incident neutron $\epsilon_0 = 14$ MeV;

- binding energy of all occurring nuclei is constant $B_n = B_p = 7 \text{ MeV}$;
- level density parameter of all occurring nuclei is also taken as a constant value $a = 13,3 \text{ MeV}^{-1}$, which corresponds to a mass number $A = 100$ (since for the Fermi-gas model the mean mass-dependence of a is given by $a = \frac{A}{7,5} \text{ MeV}^{-1}$);
- the pairing energies of all occurring nuclei is supposed to be zero, i.e. $\Delta = 0$;
- cross sections of the inverse reactions σ_{inv} are calculated using the optical model for $A = 100$, following refs. [8] and [9].

The cross section values indicated on fig. 1 give a quantitative impression on the change of (n,p) , (n,n') , (n,pn) , (n,np) and $(n,2n)$ cross sections due-to preequilibrium emission of particles from the compound system. The compound system formation cross section, calculated as the absorption cross section with the optical model, in this case is equal to 1720 mb. The transitions strengths, indicated at the arrows, are given in mb as a sum of preequilibrium plus equilibrium emission components. The corresponding values without accounting for preequilibrium emission are quoted in parenthesis for comparison.

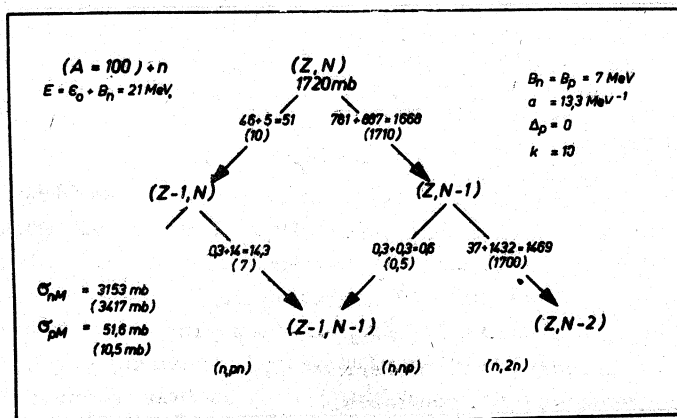


Fig. 1 Branching scheme for the first and second nucleon emission

From this example one can extract the following conclusion: The process of preequilibrium emission of primary nucleons has an marked effect on the integrated cross sections of all processes involved, in particular on processes with emission of two nucleons. The (n,pn) and (n,np) cross sections become 2,1 and 1,3 times greater, respectively. The $(n,2n)$ cross section is decreased by about 15 %. The total neutron and proton emission cross sections σ_{nM} and σ_{pM} are changed, favouring proton emission. The probability of preequilibrium emission of both neutrons in the $(n,2n)$ reaction amounts 2 % only, so that the spectra shape of secondary neutrons is expected to correspond to an almost pure evaporation case.

3.2. Excitation Functions

For the same model nucleus the incident neutron energy has been varied from 8 MeV until 30 MeV. Resulting excitation functions for the investigated reactions are shown on fig. 2.

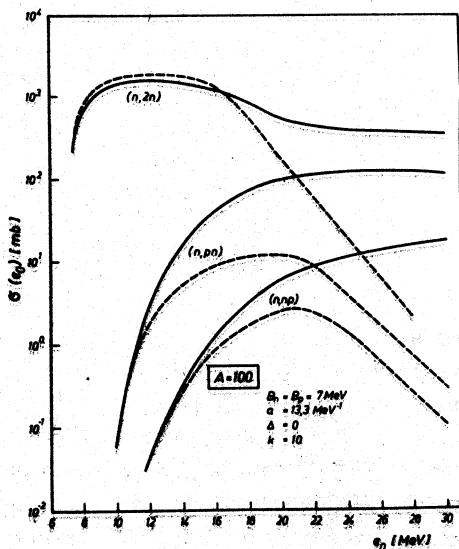


Fig. 2 Excitation functions of the reactions $(n,2n)$, (n,pn) , (n,np) for the $A=100$ model nucleus

The $(n,2n)$ cross section is decreased by preequilibrium emission of first particles, but that is true only in a limited low energy region near the maximum of the excitation function. At energies well above the $(n,3n)$ threshold, contrary to that, the $(n,2n)$ cross section is strongly increased. A similar behaviour of "high energy tails" in the excitation functions is well-known for (p,xn) and (α, xn) reactions [1, 2].

Due to the coulomb barrier, both the (n,pn) and (n,np) cross sections, in comparison with $(n,2n)$, rise slowly with increasing incident energy. These processes several MeV above threshold are strongly enhanced by preequilibrium emission. Again, the first preequilibrium emission of a charged particle followed by a neutron evaporation, i.e. the (n,pn) reaction; is favoured by about one order of magnitude in comparison with the first preequilibrium neutron emission followed by the evaporation of the charged proton, i.e. the (n,np) reaction.

3.3. Mass Number Dependence

For evaluation of the influence of preequilibrium decay on the mass number dependence of considered cross sections, the well-known mean mass number trends of nucleon binding energy, level density parameter and of the optical model absorption cross sections have been taken into account. In the upper part of fig. 3 three typical parameter sets for B_n , B_p , a , Δ and K are indicated. On the left side of fig. 4 the resulting cross sections for constant incident energy $\epsilon_0 = 14$ MeV are shown. At the right side results with constant excess energy $E_{ex} = \epsilon_0 - B_2 = 7$ MeV are presented, where B_2 is the binding energy of the second emitted proton or neutron.

The behaviour of $(n,2n)$ cross sections for $\epsilon_0 = 14$ MeV can be understood from the $(n,2n)$ excitation function as shown on fig. 3 and from the decreasing of binding energy with increasing mass number, which causes a shift of the maximum in the excitation function to lower energy. Therefore, at light and medium mass nuclei $(n,2n)$ cross section is decreased by preequilibrium emission, whereas in heavy nuclei, due-to the low $(n,3n)$ threshold,

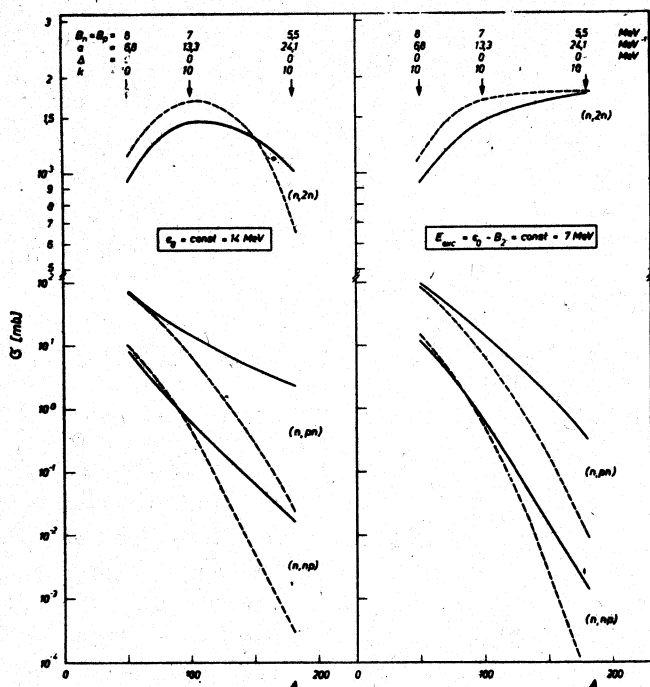


Fig. 3 Mass number dependence of considered cross sections

this cross reaction is increased. In the representation with constant excess energy, at the right hand side, this effect is excluded. In the later case $(n,2n)$ cross section in the whole mass number region is decreased, but the relative importance of preequilibrium emission becomes smaller with higher mass number. This is the result of different mass number dependences of equilibrium cross section, which is proportional to A , and preequilibrium cross section, which is proportional to $A^{1/3}$ [2, 7].

The importance of preequilibrium emission on (n,pn) and (n,np) is strongly increasing with mass number, due-to the higher coulomb barrier. At medium and light nuclei, where proton evaporation is a rather important mechanism, precompound emission dimi-

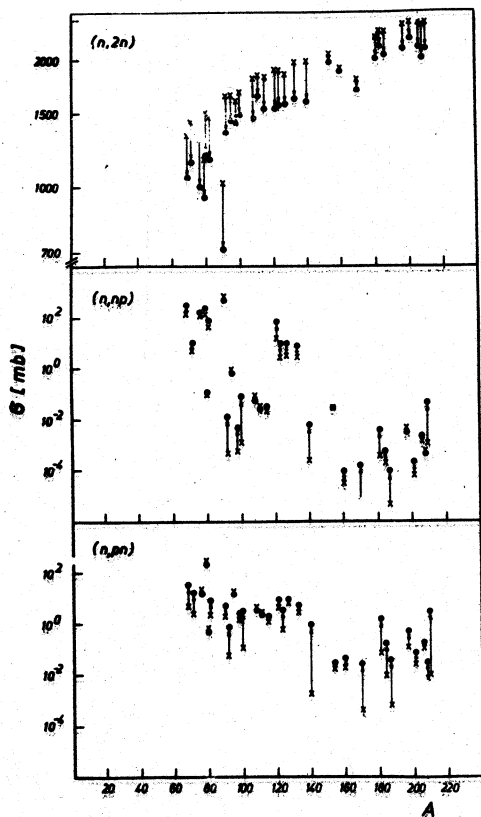


Fig. 4 Calculated cross sections for specific nuclei with (points) and without consideration of pre-equilibrium emission

nishes the (n,np) cross section in a similar manner as the $(n,2n)$ cross section

A more quantitative description and detailed discussion of this results is given elsewhere [5].

4. Calculations for specific Nuclei

As shown by refs. [4, 5] in real nuclei the effects of pre-equilibrium emission and nuclear structure are mixed and partly interconnected, for instance the filling of a shell is usually reflected both in the density and the binding energy. It is therefore generally not possible to predict the effect of pre-equilibrium emission on the cross-sections of the processes in which we are interested. For this reason we shall examine 39 isotopes in the range $60 \leq A \leq 209$, taking careful account of binding energy, density

parameters, and pairing energy in each nucleon-emission event.

The cross-sections for compound-system formation and the inverse-process cross-sections are taken from the optical model [8, 9]. The emission of complex particles is taken into account by a slight reduction in the probability of the first compound system

being formed. In the second stage of the reaction the emission of complex particles is ignored. The binding energies are taken from the table of Q values in Ref. [10]. The density parameters are taken from the semi-empirical formula in Ref. [11] and from the experimental values obtained in the analysis of neutron resonances in Ref. [12]. The pairing energies for calculating the density from expression (4) were taken from Ref. [13]. In the preequilibrium decay models, account has so far not been taken of the effect of nucleon pair correlation on level density.

The results of the calculations are given in Fig. 4. The upper part of the figure shows the $(n,2n)$ cross-sections with and without consideration of preequilibrium decay models. In all cases, the expected reduction of 14-29 % is found in the $(n,2n)$ cross-section. For a constant incident neutron energy 14 MeV, the effect of considering the preequilibrium decay models decreases with increasing mass number. In a recent paper of Holub and Cindro [14] was shown, that actually the experimental cross-sections of the $(n,2n)$ process are somewhat lower than the values obtained from calculations based on the statistical theory of nuclear reactions. It must be emphasized that not very long ago this process was regarded as a "standard example" of a model of successive evaporation of two neutrons.

The (n,np) cross sections, with exception of only a few nuclei, are enhanced by preequilibrium emission, as expected. Especially at higher mass numbers the main contribution to the (n,np) process comes from events, when both neutron and proton are emitted during preequilibrium stage of reaction.

The (n,pn) cross sections are enhanced also with exception of a few nuclei. For heavy nuclei protons are emitted almost completely during the preequilibrium stage of the reaction, whereas neutrons are "evaporated". For medium nuclei proton "evaporation" is important and there is a competition between preequilibrium and equilibrium emission of the proton.

The following fig. 5 shows an example for the experimental excitation function of ^{197}Au $(n,2n)$ from [15-17], in comparison with

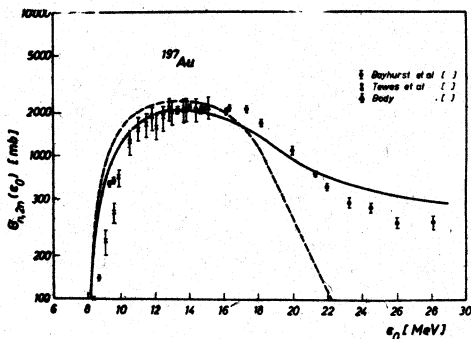


Fig. 5 Experimental and calculated $^{197}\text{Au}(n,2n)$ excitation function: data from [15-17]

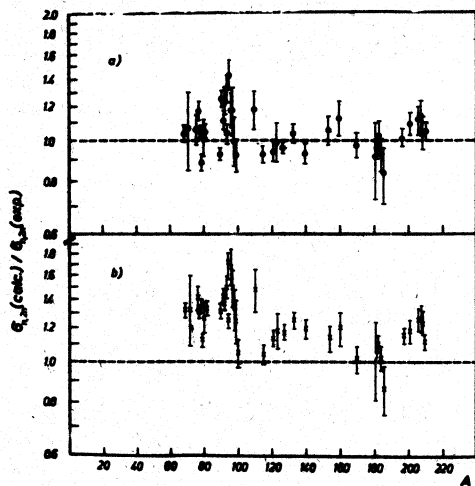


Fig. 6 Comparison between experimental and calculated $(n,2n)$ cross sections at 14 MeV; a) calculations include preequilibrium emission, b) calculations based on equilibrium statistical theory only.

calculated curves. It is obvious, that inclusion of preequilibrium emission gives better results. However, near the threshold of the $(n,2n)$ reaction there is still a remarkable difference between theory and experiment. Probably, this difference is caused by the competition between gamma and neutron emission [19], which was not taken into account here.

On fig. 6 experimental values of $(n,2n)$ cross sections at 14.7 MeV for 39 nuclei [17] are compared with our calculations. This comparison clearly favours the calculation including precompound processes (upper part of fig. 6). The deviation between experiment and the results from the equilibrium statistical theory (lower part) decreases with increasing mass number. Near $A = 180$ this theory gives satisfying results at 14.7 MeV - as expected from fig. 3. Increasing of $(n,2n)$ cross sections at $A > 200$ is due to the strong shell effect in this region.

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