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ADL-3

NUCLEAR DATA LIBRARY FOR ACTIVATION AND TRANSMUTATION CALCULATIONS

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Abstract

It is shown that the use of simplified approaches to calculate threshold neutron reaction cross-sections is not acceptable for the generation of cross-section libraries. Although rigorous models are complex and involve laborious calculations, they provide the only reliable means for evaluating cross-sections when no experimental data are available.

A brief description is given of the new version of the library ADL-3 generated by the authors. It contains 18 200 excitation functions of reactions induced by neutrons of up to 20 MeV. The threshold reaction cross-sections have been calculated in the Hauser-Feshbach-Moldauer formalism with allowance for the contribution of non-equilibrium processes. The cross-sections obtained have been tested by comparison with experimental data and evaluations from other libraries.

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Activation data libraries were developed to meet the requirements of calculations for structural material activation and radioactive waste transmutation at nuclear facilities with a high neutron flux. To meet these requirements, contemporary libraries have to include data on over ten thousand excitation functions for reactions induced by neutrons with energies of up to 20 MeV. This large volume of data is much greater than the files in general use (ENDF/B, BROND, JENDL) and is due to the need to know the cross-sections for both stable and unstable (including short-lived) target nuclei.

Need for improvement of the libraries

Analysis of the most recent versions of activation libraries (REAC, EAF) shows that the majority of cross-sections are obtained by calculation using simplified methods with subsequent normalization to the systematics or experimental data for E_n = 14.5 MeV. While this approach may be acceptable only at the first stage of generating a library, its further improvement requires the use of rigorous theoretical models for the most important reactions [1], and then for an increasingly wider range [2]. In addition, special studies [3, 4] have shown that there are fundamental reasons why it is necessary to use rigorous models. This relates primarily to reactions with isomeric targets and reactions leading to the formation of product nuclei in isomeric states.

Figure 1 shows a comparison of the excitation function of the ^{64}Zn(n,t) reaction from the EAF-3 library [5] (THRESH code) with the results of calculations using the statistical model of nuclear reactions in the Hauser-Feshbach-Moldauer formalism with allowance for the contribution of non-equilibrium processes (modified STAPRE code) [6, 7]. The energy dependences of cross-sections obtained by the rigorous and simple models differ considerably. This difference is probably due to the fact that no appropriate allowance was made of the Coulomb barrier in calculations using the THRESH code.

In the ADL-91 library [8], the threshold reaction cross-sections were calculated using the statistical model for nuclear reactions in the Weisskopf formalism, in which the competition of photons cannot be taken into account rigorously enough. This disadvantage does not generally have a significant influence on the calculation results. However, in some cases where the reaction energy and the threshold of emission of competing particles differ considerably, the Weisskopf approach is unacceptable. Figure 2 shows the calculation results for the cross-sections of reactions of (n,n'α) and (n,αn) with the ^{145}Pm target nucleus in the Hauser-Feshbach formalism (_____) and the Weisskopf formalism (- - -). The (n,n'α) reaction cross-sections differ considerably when different calculation approaches are used. The situation where the emission of a second neutron is energetically impossible and the photons cannot compete with α-particle emission is unfavourable for calculations using the Weisskopf approach.

In libraries, reaction cross-sections for isomeric target nuclei are generally taken as equal to cross-sections for nuclei in the ground state. However, the initial excitation and spin of the target nucleus have a considerable influence on the reaction cross-sections [3]. The reaction cross-section varies substantially (Fig. 3, curves 1 and 4) because of the high spin and initial excitation of the target nucleus.

There are fundamental disadvantages in the methods used for evaluating isomeric yields. Usually the excitation functions of the isomeric level are obtained by renormalization of the cross-section for the corresponding reaction from the isomer cross-section ratio. This approach, even without considering its inadequacies in the description of the energy dependence of the cross-section obtained, cannot be used owing to the absence of reliable systematics for isomeric ratios. At the same time, the development of the γ-cascade model for decay of the excited nucleus [4] made it possible to predict satisfactorily the isomeric

yield in different reactions. Figure 4 shows a comparison of calculation results for the $^{179}Hf(n,2n)^{178}Hf^{m2}$ reaction cross-section with experimental data [1]. The curves indicate the region of uncertainty of the model's predictions [4].

Thus, the above arguments show that the reaction cross-sections contained in the most recent versions of activation libraries should be revised and that a higher quality can be achieved for new cross-sections only by using rigorous theoretical models.

Theoretical model

The main characteristics of the statistical model are the transmission coefficients for particles in the entrance and exit channels of the reaction and the density of excited levels of the corresponding residual nuclei. The calculations for individual cross-sections using this model can be performed without much difficulty but the calculations for over ten thousand excitation functions needed for generating activation data libraries were evidently not performed earlier. We used the SCAT2 code [9] to calculate the transmission coefficients and STAPRE [6] for statistical calculations of cross-sections. The latter code has been modified for a consistent description of non-equilibrium processes using the phenomenological approach suggested in Ref. [7]. The level density was calculated using the superfluid model of the nucleus with parameters from the systematics of Ref. [10]. The excitation functions of isomeric levels were determined by the method suggested in Ref. [4] and tested in the description of a lot of experimental data.

It is well known that the main difficulty in performing the calculations for a large number of threshold reaction excitation functions using rigorous models is preparation of the initial data. Each set of initial data should include the discrete level schemes and level density parameters of all nuclei in the entrance, exit and competing reaction channels. In addition, the neutron resonance characteristics and particle binding energies should be given

for all compound nuclei at each cascade of the reaction. All level schemes should be analysed in relation to the missing levels and individual level characteristics. The selection of level density parameters is of fundamental importance. Unknown experimental data on the neutron resonance density of nuclei are selected on the basis of local systematics. In this case, the selection of a level density model is not the deciding factor, since the physical inadequacy of the parameters can be compensated by fitting. A different situation arises in the case of a large volume of calculations, when the level density parameters can be selected only on the basis of a global systematics, as experimental data on neutron resonance density are available for a relatively small number of nuclei. Here the only model which can be used without the need to verify the parameters individually is the generalized superfluid model of the nucleus, which has physically adequate parameters and allows a good systematization of the level density parameter and an effective correction for the even-odd differences, independently of the availability of neutron resonance density data. It is thus possible to prepare sets of level density parameters with this model for nuclei for which an experimental discrete level scheme is available.

Contents of the library

The third version of the ADL library contains excitation functions for the following reactions: (n,γ), (n,n'), (n,p), (n,d), (n,t), (n,h), (n,α), (n,n'p), (n,n'α), (n,2n), (n,2p), (n,n'd), (n,n't) and (n,3n). The library contains a total of 18 200 reactions, including reactions for short-lived and isomeric target nuclei. The threshold reaction cross-sections were calculated from the Hauser-Feshbach-Moldauer relations with allowance for the contribution of non-equilibrium processes [6, 7]. The calculations made use of the libraries of model parameters, discrete level schemes and binding energies of nuclei prepared for this purpose [11].

Comparison of the results with experimental data and data from other libraries shows that the use of this approach is justified by the high quality of the cross-sections obtained. In some cases where the analysis demonstrated the advisability of doing so, the authors used evaluations from other libraries.

Conclusion

We have given a brief description of the third version of the activation data library, ADL-3. The library contains over eighteen thousand excitation functions of reactions induced by neutrons of up to 20 MeV. The cross-sections were evaluated with the use of calculations based on rigorous theoretical models. It is shown that simplified calculation methods are not acceptable for the generation of the latest versions of cross-section libraries. We have not compared the obtained cross-sections with evaluated data from other libraries and with experimental data, leaving this as a subject for a later article.

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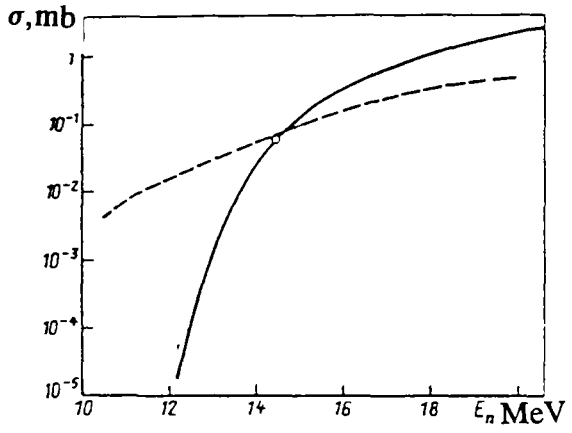

Fig. 1. Excitation function of the reaction $^{64}Zn(n,t)$: _____ and ------ denote data from the ADL-3 and EAF-3 libraries, respectively.

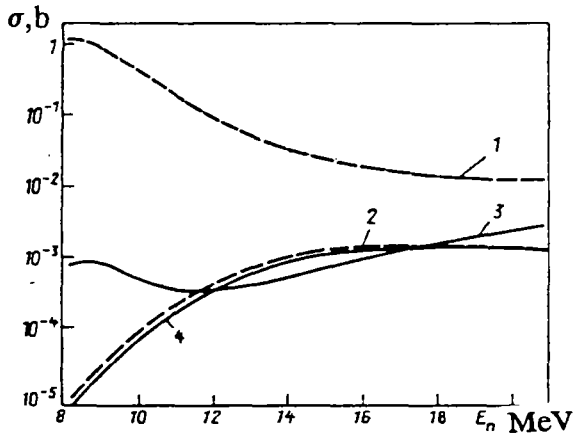

Fig. 2. Excitation function of the reaction $^{145}Pm(n,n'\alpha)$: (1, 3) $(n,n'\alpha)$ reaction cross-sections; (2, 4) $(n,\alpha n)$ reaction cross-sections; ------ denotes calculation without allowance for photon competition.

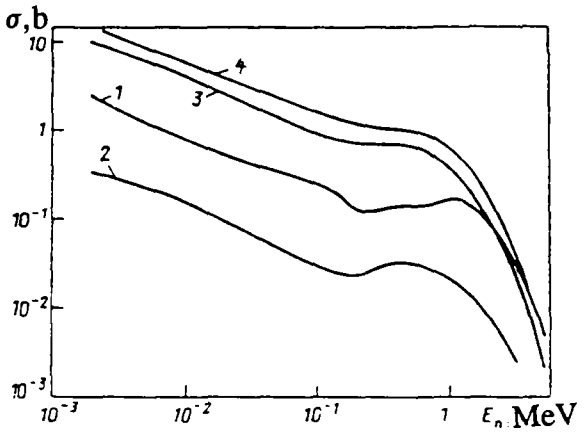

Fig. 3. Influence of initial excitation and spin of target nucleus on the $^{178}Hf(n,\gamma)$ reaction cross-section: (1, 2) cross-section of the reaction with the target nucleus in the ground state and in the excited state (E = 2.446 MeV) with spin $I_0 = 0$, respectively; (3) isomeric target (2.446 MeV, 16^+); (4) with allowance for changes in neutron resonance characteristics.

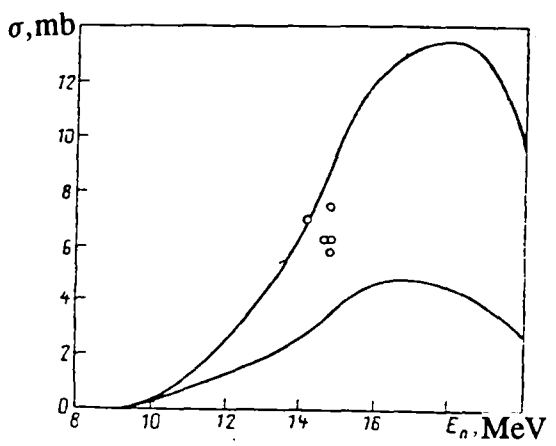

Fig. 4. Description of the yield of isomer $^{178}Hf^{m2}$ (2.446 MeV, 16^+) in the $^{179}Hf(n,2n)$ reaction: o - experiment.