Phenomenological systematics of the (d,p) cross sections

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Abstract: The main shortcomings of the TENDL-2010 evaluations for deuteron induced reactions are discussed. A new phenomenological systematics of the (d,p) cross sections is developed and recommended as an alternative for the FENDL-3D corresponding data.

Introduction

In accordance with the recommendations of the last CRP Meetings [1, 2] new versions of the proton and deuteron data libraries FENDL-3P and FENDL-3D, based mainly on the recent TENDL-2010 evaluations, has been compiled. For the proton-induced reactions a reasonable agreement between these evaluations and the available experimental data was obtained in most cases. However, for the deuteron-induced reactions the TENDL-2010 evaluations essentially underestimate the (d,p) reaction cross sections. In the present report the main shortcomings of the previous evaluations are analyzed and a new phenomenological approach is proposed for a systematic description of the (d,p) cross sections.

Statistical codes and their modifications

A variety of codes based on the statistical theory of nuclear reactions are used nowadays for the calculation and evaluation of nuclear reaction cross-sections. Most of these codes include rather similar approximations for the description of nuclear processes and properties of excited nuclei, but the codes differ essentially in their input parameters and required computing time. One of the simplest is the ALICE code [3] based on the geometry-dependent hybrid (GDH) or the hybrid multi-step (HMS) pre-equilibrium models and the Weisskopf-Ewing evaporation description of equilibrium processes. The modified code ALICE-IPPE [4] was developed to include the pre-equilibrium cluster emission and the advanced systematics of the nuclear level densities.

Some shortcomings of the ALICE-family codes relate to a disregard of the angular momentum and parity conservation laws. More sophisticated codes taking into account these conservation rules require not only a larger computation time, but also much more input information on the nuclear level structure. The GNASH [5], EMPIRE [6] and TALYS [7] codes are widely used currently for practical evaluations of both the neutron and charged particle reaction cross sections. Main input parameters of these codes are usually estimated on the basis of the RIPL libraries [8] and that makes the obtained results quite similar. Essential discrepancies between calculations relate to the pre-equilibrium processes for which many various approaches are proposed. To reduce the dispersion of results, adjustment to experimental data could play a crucial role for an accurate evaluation of the corresponding cross sections.

During the last decade systematic measurements of the deuteron induced reactions have been performed for about 20 metal targets having mostly natural isotopic composition [9]. We will discuss only a part of the obtained data related to the (d,p) reaction.

The experimental data for the ^{181}Ta(d,p)^{182}Ta reaction are compared in Fig. 1 with the TENDL-2007 and TENDL-2010 evaluations, as well as with the calculations performed with the statistical codes [10]. The disagreement of the TENDL-2007 evaluation with the experiments is about a factor 20-100 for the whole energy region. It should be noted that the calculations with the previous versions of the ALICE-IPPE and EMPIRE-II codes demonstrated similar disagreements of the (d,p) cross sections for many nuclei [11-14].

It is well known that for the (d,p) reactions at low energies the direct stripping processes play a dominant role and such processes are not considered by the standard statistical models. To achieve a reasonable description of the available data the consistent direct reaction approaches should be used. The corresponding calculations are voluminous and very time-consuming. A more simple phenomenological approach was chosen to update the statistical codes. The general relations for direct transfer reactions in the continuum [15] were taken to simulate the (d,p) transitions and the energy dependent enhancement factor in these relations was adjusted empirically to describe the whole set of the observed (d,p) cross sections for medium and heavy nuclei [13]. The codes including such modifications were named ALICE-D and EMPIRE-D and their results for the ^{181}Ta(d,p)^{182}Ta reaction are compared with the experimental data in Fig. 1. Both codes were applied to describe the observed (d,p) cross sections for many other nuclei [13, 14], for which the disagreements with the TENDL-2007 evaluations were always similar to the shown one above.

The similar simulation of the (d,p) reaction was also included in the last version of the TALIS code used for the TENDL-2010 evaluations. The obtained cross section at the near-threshold energies is much higher than in the TENDL-2007 library, but it is still essentially lower than the experimental data (Fig. 1). The systematic underestimation of the (d,p) cross sections is observed in the TENDL-2010 files for all cases where the experimental data are available. Some additional examples will be considered below together with a phenomenological description shown in Fig. 1 by a red curve.

It is necessary to note that a strong increase of the (d,p) cross sections is revealed in the TENDL-2010 data for many nuclei at the energies below the Coulomb barriers (Fig. 1). It is obvious, that such jumps are erroneous effects produced by the optical model calculations of the deuteron absorption cross sections at very low energies. The corresponding sections (MF=3, MT=5) of the TENDL-2010 files should be corrected for many nuclei.

Phenomenological systematics of the (d,p) cross sections

Taking into account uncertainties of theoretical models it was decided to construct a rather simple phenomenological description of the available experimental data. The analytical function used for this purpose should to have a shape similar to the results of theoretical models, but its parameters could be estimated from a fit to experimental data. The following function was selected

$$\sigma(E) = \frac{a_1}{1+\exp(\frac{b-E}{c})}[a_2 \exp(-E/d_1) + (1-a_2)\exp(-E/d_2)] \quad , \qquad (1)$$

where the factor before the square brackets defines the low-energy increasing part of the (d,p) cross section and the terms in the square brackets characterize the decreasing part. A need for two decreasing components corresponds to two different mechanisms of nuclear reaction: the direct processes connected with the low-energy excitation of single-particle degrees of freedom and the pre-equilibrium processes responsible for more complex excitations of nuclei.

To estimate all parameters of Eq. (1) we need the experimental data up to high enough energies. The available data for the ^{59}Co(d,p) reaction are compared in Fig. 2 with various model calculations and the phenomenological description (1) with the parameters fitted to the data. Similar results for the ^{197}Au(d,p) reaction are shown in Fig. 3. To better see the differences between the model descriptions of data the logarithmic ordinate scale is used for the last figure.

The obtained parameters of Eq. (1) for both targets are presented in Table 1. Because a rather small number of the experimental points are below the cross section maximum the parameter *c* was excluded from the fitting and its value *c*=0.75 MeV was fixed for the ^{59}Co target. Owing to the limited high-energy part of the ^{197}Au data the parameter d_2 was fixed to the value 35 MeV under the fitting.

Table 1. Parameters of the (d,p) cross section description estimated from the experimental data fitting

Parameter	^{59}Co(d,p)	^{197}Au(d,p)
a_1	751±87 mb	904±121 mb
b	5.13±0.22 MeV	9.86±0.11 MeV
c	0.75 MeV was fixed	0.716±.035 MeV
a_2	0.891±0.011	0.876±.015

d_1	7.21±0.61 MeV	7.05±0.84 MeV
d_2	37.34±2.76 MeV	35.0 MeV was fixed

Unfortunately, the amount of experimental data on the (d,p) reaction for other target is even smaller than for two above nuclei. So, it is difficult to estimate all the required parameters from an analysis of the available data. In the case of ^{181}Ta we were forced to fix beside the parameters c and d_2 also the parameter d_1 or a_2. The resulting description of experimental data with the fixed d_1=7.1 and d_2=35 MeV is shown for this nucleus in Fig. 1. The remaining fitted parameters are the following: a_1=832±68 mb, b=9.31±0.12 MeV, a_2=0.861±0.015.

Similar scattered experimental data are available for the target of ^{141}Pr. They are shown in Fig. 4 together with various calculations. Again one can note a strong underestimation of the (d,p) cross section in the TENDL-2007 and TENDL-2010 evaluations, as well as the false increase of the TENDL-2010 cross section at low energies. The phenomenological description is obtained in this case with the fixed parameters of c, d_1 and d_2 as above and the fitted parameters: a_1=742±70 mb, b=8.06±0.13 MeV, a_2=0.848±0.026.

The parameter b determines the effective threshold of the (d,p) reaction and it should be close to the height of the Coulomb barrier for the corresponding target. Using the relation for the barrier

$$b = \frac{e^2 Z}{r_{eff} A^{1/3}} \quad , \qquad (2)$$

where e^2=1.44 MeV·fm, Z is the charge and A is the mass numbers of the target, we can estimate the effective radius parameter r_{eff} corresponding to the obtained parameter b. The parameters a_1 and r_{eff} estimated from the performed analysis are shown in Fig. 5. The mean value of the radius parameter is r_{eff}=1.985±0.045 fm, while the dependence of the parameter a_1 on the mass number can be approximated as

$$a_1 = 672 + 0.871A \text{ mb}. \qquad (3)$$

An uncertainty of this estimation is about 10-15 %.

Eqs. (1-3) can be considered as a systematics of the (d,p) cross sections for the whole mass region with the remaining parameters taken as the fixed ones: c=.75 MeV, a_2=0.848, d_1=7.1 and d_2=35 MeV. Uncertainties of such a systematics are mainly determined by the uncertainties of the two parameters: a_1 and a_2. If we suppose that uncertainties of a_2 are about 7-10%, the uncertainty of the systematics with the recommended parameters should be about 25-30%.

From the comparison with the experimental data considered above we can conclude that the proposed systematics is certainly much better than the available TENDL-2010 evaluations and for energies above 20 MeV it is even better than ALICE-D and EMPIRE-D calculations. The shortcomings of the latter calculations result from the selection of the pre-equilibrium model parameter. To improve the predictive power of the available statistical codes their parameters should be estimated more consistently for the channels with a significant contribution to the direct processes.

Conclusion

TENDL-2010 libraries for protons and deuterons were tested against the available experimental data for the most important materials related to the IFMIF project. Additional calculations with the ALICE-D and EMPIRE-D codes were performed to study effects of input model parameters on the analyzed data.

For the deuteron-induced reactions the TENDL-2010 evaluations essentially underestimate the (d,p) reaction cross sections for most of the nuclei. There are also unphysical jumps of the cross sections at low energies. So, the corresponding sections of the TENDL-2010 files should certainly be corrected in the process of the FENDL-3D library formation. The phenomeno-logical systematics of the (d,p) cross sections, proposed in the present report, can be recommended as an optimal evaluation of such data for all nuclei and the whole energy region.

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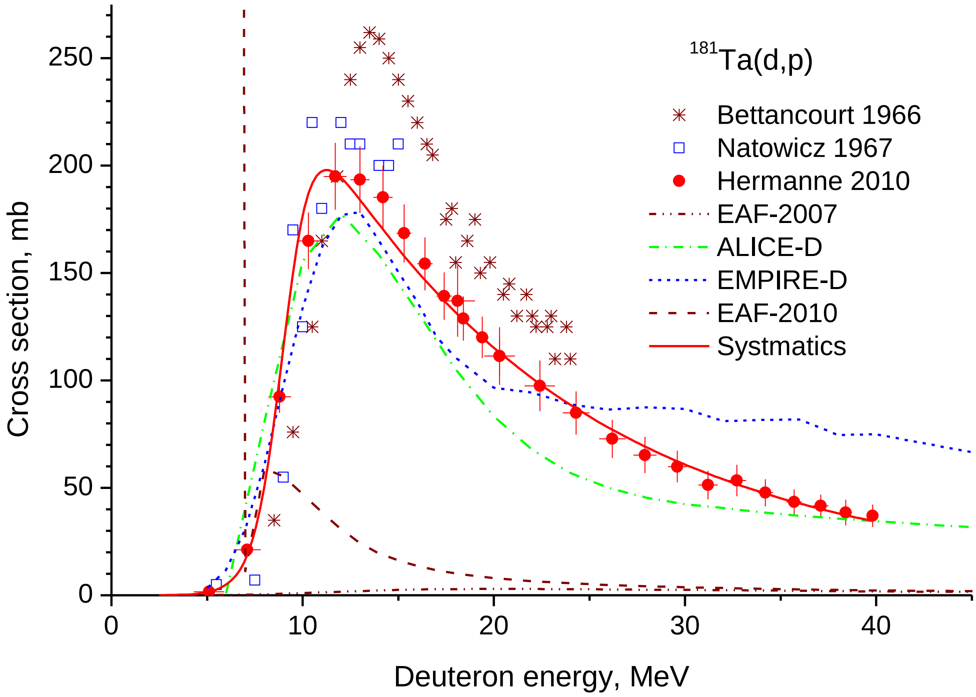

Fig. 1. Experimental data for the ^{181}Ta(d,p)^{182}Ta reaction cross section is compared with various calculations

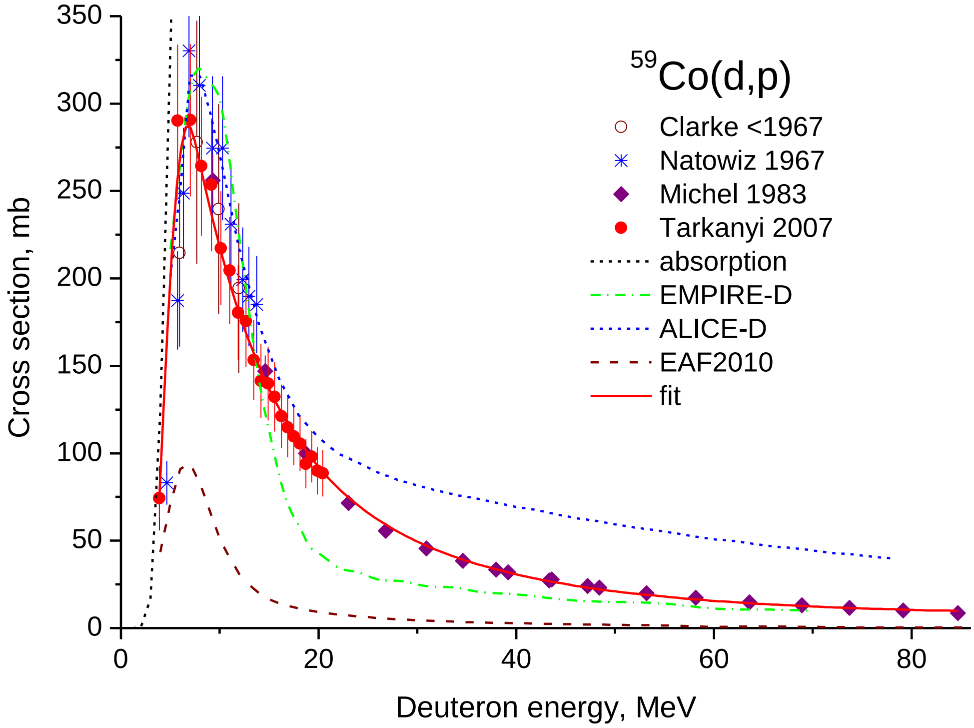

Fig. 2. The same as Fig. 1 for the ^{59}Co(d,p) reaction

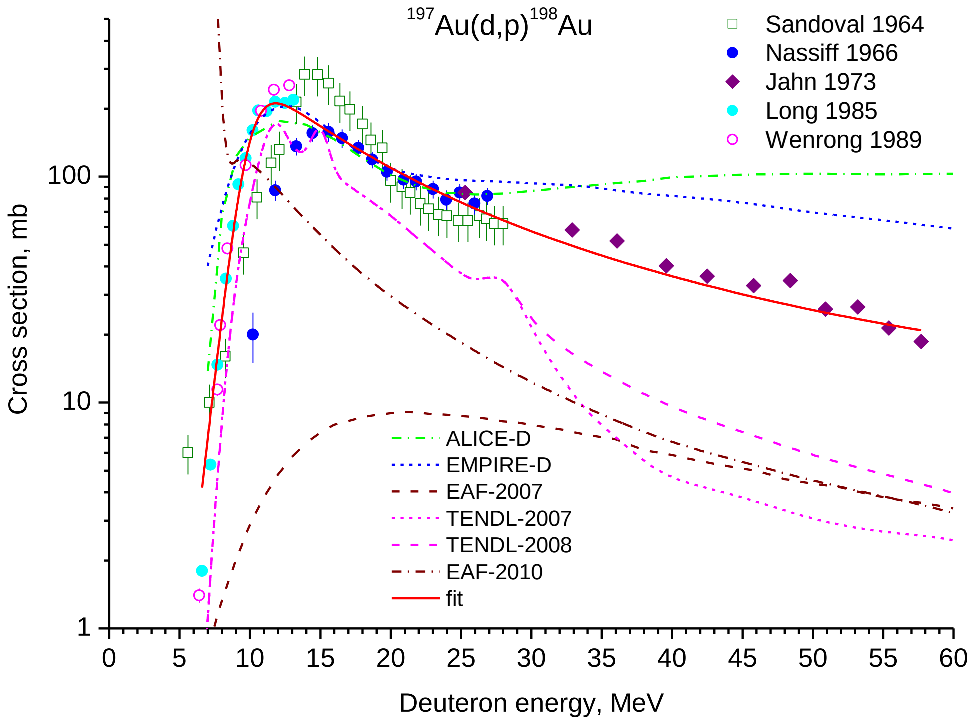

Fig. 3 . The same as Fig. 1 for the ^{197}Au(d,p) reaction

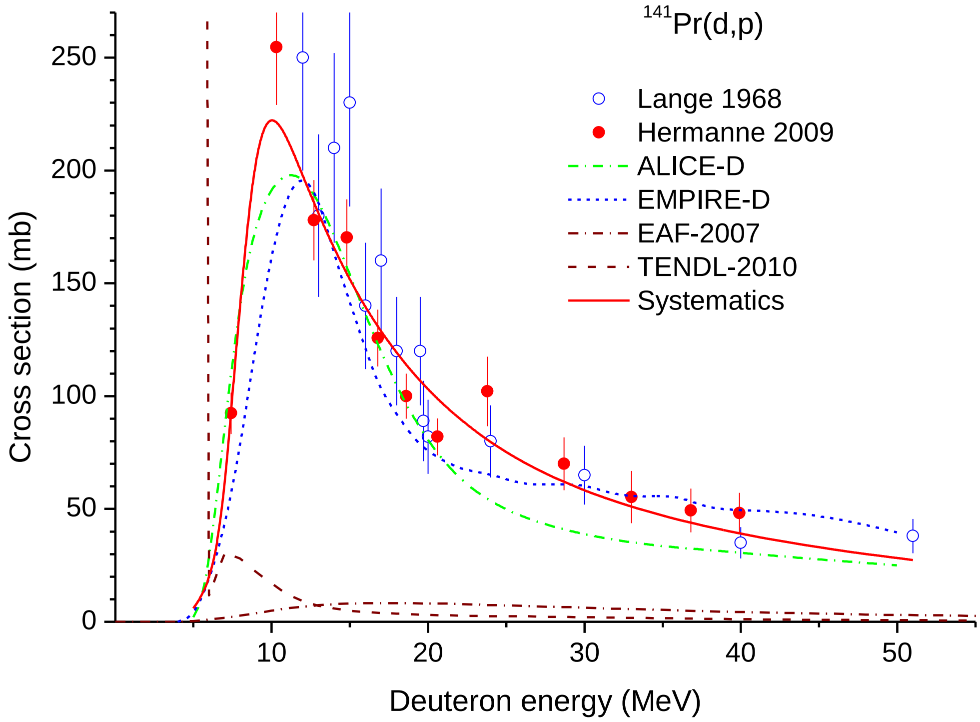

Fig. 4 . The same as Fig. 1 for the ^{141}Pr(d,p) reaction

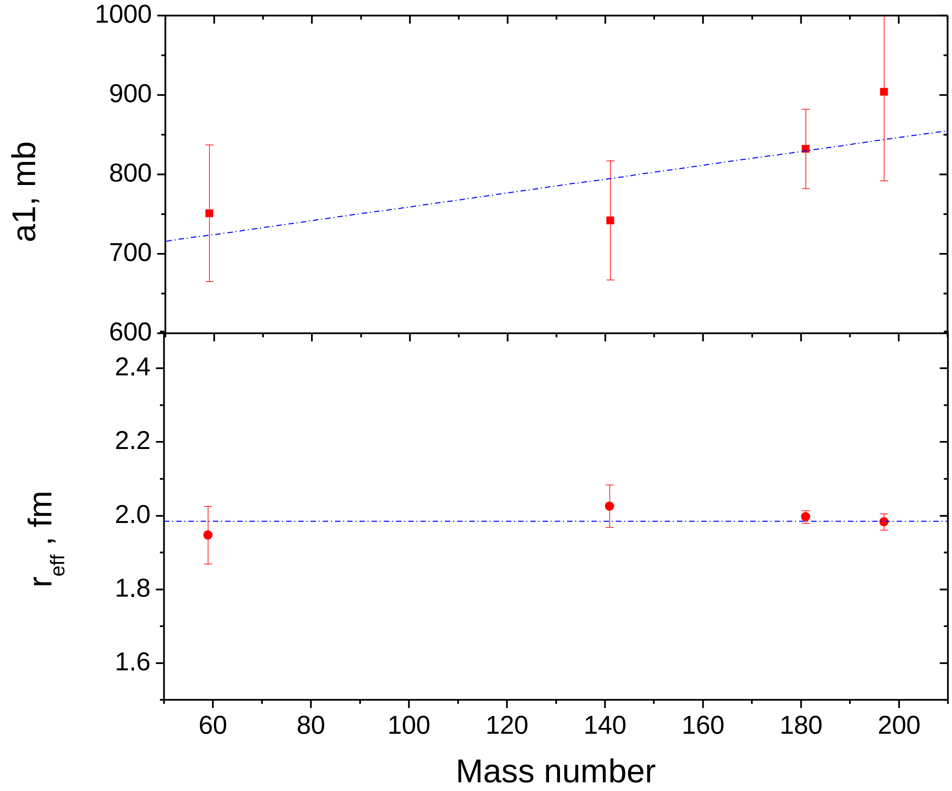

Fig. 5. Parameters of Eq. (1) and (2) estimated from the analysis of experimental data. Dash-dotted lines show the recommended parameters.