Deuteron breakup effects on activation cross sections at low and medium energies

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Abstract. An extended analysis of the reaction mechanisms involved in the deuterons interaction with light and medium nuclei, $^{27}$Al and $^{63,65}$Cu, at incident energies from 3 to 60 MeV starting with elastic scattering until the evaporation from fully equilibrated compound system is presented. An increased attention is devoted to the breakup mechanism, all its components, the elastic, inelastic (fusion), and total breakup, being carefully analysed. Moreover, the corresponding stripping mechanism contribution to the $(d, p)$ and $(d, n)$ reaction cross sections through population of the discrete levels of the residual nuclei, was calculated. Finally, following the decay path, the pre-equilibrium and evaporation cross sections, corrected for the breakup and stripping decrease of the total reaction cross section, have completed the deuteron activation cross sections analysis. The overall agreement between the measured data and model calculations proves the correctness of nuclear mechanism description taken into account for the deuteron-nucleus interaction.

1. Introduction

Recent evaluation of the deuteron-induced activation in the International Fusion Materials Irradiation Facility (IFMIF), e.g. [1], based on preliminary deuteron part of the EAF library [2], shows that the deuterons are much more important than the neutrons by a factor of about 70 for the ratio of the deuteron– and neutron–induced activity [3]. However, despite the high technologies like the fusion reactor projects request increased accuracy deuteron nuclear data, the corresponding evaluations are less extensive and mature than in the case of neutrons, e.g. Refs. [3, 4]. Therefore, the analysis of deuteron-induced reactions at low and medium incident energies needs improved model calculations and further measurements if the deuteron data libraries are to approach the standard of the established neutron-data bases.

The difficulties to interpret the deuteron-induced reaction data in terms of the usual reaction mechanism models are the result of the high enhancement of a variety of reactions, even at low bombarding energies, induced by the neutrons and protons coming from the deuteron breakup. Then, the weak binding of the deuteron (2.22 MeV) results in significant contributions of the breakup channel which hampered so far a comprehensive analysis of deuteron interactions with nuclei.

The accurate description of the deuteron interactions appears at low incident energies, below e.g. 20 MeV, is additionally difficult since there is no global optical model potential (OMP) which describes the scattering data sufficiently well over a wide range of nuclei and energies.
Because the OMP is a basic ingredient of almost all nuclear model analyses, there is a significant uncertainty of the calculated deuteron-induced reaction cross sections.

The present lecture, concerning the analysis of the nuclear reaction mechanisms involved in the deuteron interaction with nuclei, has paid larger attention to the deuteron breakup consideration as well as the OMP parameters which are able to describe the bulk of deuteron elastic scattering data. The ultimate results of the corresponding assumptions and forms on the calculated deuteron-induced reaction cross sections are also pointed out.

2. OMP analysis
In order to increase the accuracy of the optical potential parameterization, the OMP analysis may take the advantage of a two-steps approach [7, 8, 9, 10]. In the first step, a semi-microscopic optical potential analysis provides the imaginary and spin-orbit parameterization, while within a second step a full phenomenological OMP can be obtained.

2.1. Semi-microscopic optical potential analysis
A semi-microscopic OMP may consist of the real Double Folding (DF) part, \( U_{DF} \), and phenomenological imaginary volume and surface derivative Woods-Saxon potentials, as well as spin-orbit potential of the Thomas form [11]:

\[
U(r) = V_C(r) + U_{DF}(r) + iW_V f(r, R_V, a_V) + iW_D g(r, R_D, a_D) + V_{so}(r) \left( \frac{\hbar}{m_\pi c} \right) \frac{LS}{r} d/dr [f(r, R_{so}, a_{so})]
\] (1)

where \( V_C(r) \) is the Coulomb potential of a uniformly charged sphere of radius \( R_C = r_C A^{1/3} \), and \( r_C = 1.30 \) fm, \( f(r, r_i, a_i) = (1 + \exp[(r - r_i A^{1/3})/a_i])^{-1} \), \( g(r, r_i, a_i) = -4a_i d/dr [f(r, r_i, a_i)] \), and \( (\hbar/m_\pi c)^2 \) is the square of the pion Compton wavelength.

The basic formulas for calculations of the DF real part of the OMP [12] \( U_{DF} \) as well as the basic model assumptions have been discussed elsewhere [7]. The direct and exchange components of the real microscopic optical potential \( U_{DF} \) are given in terms of the projectile and target nuclear densities, which are folded with the Paris M3Y effective NN interaction [13]. The knock-on exchange term of the folded potential has been calculated by using the approximation of Campi and Bouyssy [14], which preserves the first term of the expansion given by Negele-Vautherin [15] for the realistic density-matrix while the average relative momenta of nucleons are obtained from the modified Thomas-Fermi approximation of Krivine and Treiner [16] for the kinetic-energy density.

The deuteron density distribution has been obtained from the experimental charge form factors measured by Abbott et al. [17], and the nuclear density distribution of the target nuclei has been described by means of a two-parameter Fermi-type function with Negele’s [18] parameters chosen to reproduce the electron scattering data.

Similarly to the previous studies [7, 8], within our two-step OMP approach the semi-microscopic analysis of the available experimental angular distributions of elastic-scattered deuterons provided the energy-dependent depths of the phenomenological imaginary surface \( W_D \) and volume \( W_V \) optical potential components. We have made use in this respect also of the corresponding dispersive correction \( \Delta U(r, E) \) [19], to the microscopic “parameter free” DF real potential. Concerning the spin-orbit potential we found the parameterization of Ref. [20] quite suitable and have preserved it within present analysis.

It should be emphasized that no adjustable parameter or normalization constant has been involved within this analysis for the real part of Eq. (1) in order to determine the phenomenological parameterization, so that the predictive power of this semi-microscopic potential is preserved. This can be seen from the comparison between the experimental [21]
and semi-microscopical angular distributions for the $^{27}$Al target nucleus and incident energies from 5 up to 15 MeV [21] shown in Fig. 1 (a). Angular distributions calculated with Daehnick et al. [20] and Lohr-Haeberli [22] global OMPs are also shown. The average energy dependence of the local imaginary volume and surface potential depths of the semi-microscopic OMP are shown in Fig. 1 (b), and the corresponding dispersive corrections to the real microscopic potential are shown in Fig. 1(c). The differential elastic scattering cross sections have been calculated by a modified version of the code SCAT2[23] which includes the DF model potential as an option for the OMP real part.

2.2. Phenomenological OMP
In the second step of our OMP analysis [5, 7, 8] the microscopic real potential is replaced by a phenomenological Woods-Saxon component. A full phenomenological OMP was then obtained from the analysis of the same experimental data, but keeping frozen the imaginary and spin-orbit potentials already determined. The advantage of having well settled already more than half of the usual OMP parameters, increases obviously the accuracy of fitting the data. The phenomenological elastic–scattering angular distributions for $^{27}$Al target nucleus, are shown in Fig. 1(d) and compared to predictions of the recent global OMP [24] and the default OMP of the computer code TALYS [25] based on Watanabe [26] folding approach. Neither the previous global OMPs nor the default OMP within the code TALYS are able to describe the experimental data.
angular distributions of the deuteron elastic scattering at the incident energies from 5 to 20 MeV, while a good agreement has been obtained with our energy–dependent phenomenological OMP parameter set, Table II of Ref. [10].

Moreover, the measured total reaction cross sections [21] of deuterons have also been compared with the predictions of the present OMP, the global OMPs [20, 24], the default OMP of TALYS code, as well as the evaluated data of the ACSELAM library [27]. The results shown in Fig. 1(e) for \(^{27}\)Al point out differences of at least 20%, up to the incident energies of 60 MeV, between the more recent OMPs and the former ones. Nevertheless, they support once more the present phenomenological OMP.

### 3. Direct Reactions (DR)

#### 3.1. Deuteron breakup

Following the deuteron elastic scattering analysis, an increased attention has been devoted to the direct interactions. They are dominant for deuteron energies below and around the Coulomb barrier, while other reaction mechanisms like pre–equilibrium emission (PE) or evaporation from the fully equilibrated compound nucleus (CN) become also important increasing the incident energy. The deuteron breakup mechanism responsible for the enhancement of a large variety of reactions is important along the whole incident energy range and its contribution to the reaction cross sections has to be taken explicitly into account [10].

The physical picture of the deuteron breakup in the Coulomb and nuclear fields of the target nucleus considers two distinct chains, namely (i) the elastic breakup (EB) in which the target nucleus remains in its ground state and none of the deuteron constituents interacts with it, and (ii) the inelastic breakup or breakup fusion (BF) where one of these deuteron constituents interacts with the target nucleus while the remaining one is detected. An empirical parametrization of the total proton-emission breakup fraction, \(\sigma_B^p/\sigma_R\), and elastic breakup fraction, \(\sigma_{EB}/\sigma_R\), have been obtained [9] from the analysis of the experimental systematics [28, 29, 30, 31, 32] of the proton–emission spectra and angular distributions from deuteron–induced reactions on nuclei from Al to Pb at incident energies from 15 to 80 MeV. Their dependence of the charge (\(Z\)), the atomic number of the target nucleus (\(A\)), and the deuteron incident energy (\(E\)) is [9]:

\[
\begin{align*}
    f_B^{(p)} &= 0.087 - 0.0066Z + 0.00163ZA^{1/3} + 0.0017A^{1/3}E - 0.000002ZE^2, \\
    f_{EB} &= 0.031 - 0.0028Z + 0.00051ZA^{1/3} + 0.0005A^{1/3}E - 0.000001ZE^2.
\end{align*}
\]

Comparing with total proton- and neutron- emission breakup cross sections parametrization of Kalbach [33]:

\[
\sigma_B^{p(n)} = K_{d,p(n)} \frac{(A^{1/3} + 0.8)^2}{1 + \exp \left(\frac{13-E}{6}\right)}, \quad K_{d,p} = 21, \quad K_{d,n} = 18.
\]

the former parametrization [9] considers equal breakup fractions for proton and neutron emission, but supplementary gives all breakup total, elastic, and inelastic components.

In Fig. 2(a,b) it is shown that both parameterizations of Refs. [9, 33] are very close for \(^{63,65}\)Cu target nuclei, for deuteron incident energies above \(~7\) MeV, while at lowest incident energies the total breakup cross sections given by Kalbach parametrization [33] exceed even the deuteron total reaction cross sections.

On the whole, the deuteron total breakup reaction cross section reduces the amount of the total reaction cross section that would be shared among different outgoing channels. On the other hand, contributions to different reaction channels, enhancing the secondary chance emission of particles from the original deuteron-nucleus interaction are brought by the inelastic...
breakup process where one of deuteron constituents interacts with the target forming a secondary composite nucleus. Thus, the interactions of the neutron following the breakup proton emission contributes mainly to the enhancement of the \((d,2p)\) and \((d,p\alpha)\) reaction cross sections. In order to calculate this enhancement, the inelastic breakup proton-emission cross section \(\sigma_{BF}^{(p)}\) has been multiplied by the fraction of the neutron total cross section \(\sigma_{tot}\) leading to the above-mentioned reactions, i.e. \(\sigma_{(n,i)}/\sigma_{tot}\), where \(i\) stands for the \(\gamma\), \(p\), or \(\alpha\) outgoing channels [10]. The cross section \(\sigma_{BF}^{(p)}\) has been expressed as a function of the deuteron incident energy while the Kalbach [33] formula has been used for the centroid energy of the breakup neutron responsible for the specific reaction enhancements [10]. The quite large widths of the assumed Gaussian line shape of these peaks as showed in Fig.2 (c) emphasize however the broad approximation of this method. Therefore, the related contributions to the deuteron activation reaction cross sections have been additionally smoothed by using an average energy width of 3 MeV, with the results shown in Fig. 3 (d,e,f) by the dot-dashed curves.

A similar procedure has been followed in order to obtain the contribution to the \((d,2n)\) reaction cross section due to the protons which, following the breakup neutron emission, are absorbed in further interactions with the target nucleus. The inelastic breakup contributions \(\sigma_{BF}^{(n)}\sigma_{(p,i)}/\sigma_{R}\), where \(\sigma_{R}\) is the proton total reaction cross section, and \(i=n, p\) or \(\alpha\), have been considered in this respect.

The inelastic breakup component still remains difficult to be handled in the reaction calculations by using the available codes. Thus, Kalbach’s [33] absolute total neutron and proton breakup cross sections are considered in the TALYS-1.0 code for the first–chance neutron and respectively proton emission spectra while the consideration of a particular contribution following the absorption of one BF proton or neutron by the target remains an open question.
3.2. Single–nucleon stripping

The direct-reaction, stripping mechanism contributions to the \((d,p)\) and \((d,n)\) reaction cross sections through population of the low-lying discrete levels of the residual nuclei were calculated by means of the code FRESCO [34]. The post form distorted wave transition amplitude with finite-range interaction has been chosen in this respect. Apart from the incident channel, for which the OMP was subject of the unitary deuteron interaction analysis [9, 10, 35], for the neutron and proton outgoing channels the Koning and Delaroche [36] optical model potentials have been chosen. The neutron–proton interaction \(V_{np}\) was assumed to have a Gaussian shape

\[
V(r) = -V_0 e^{-\left(r/r_0\right)^2},
\]

where \(V_0=72.15\) MeV and \(r_0=1.484\) fm [37], determined from the fit of the deuteron binding energy. The nucleon bound states were generated in a Woods–Saxon real potential with global reduced radius of 1.25 fm and diffuseness of 0.65 fm, while its depth has been adjusted to the nucleon binding energies in the residual nuclei.

For the \(^{27}\text{Al}(d,p)\) reaction cross section calculations a number of 35 final states of the odd-odd residual nucleus \(^{28}\text{Al}\) extending up to 5.135 MeV have been considered, using the corresponding spectroscopic factors obtained experimentally from proton angular distribution measurements [38]. Similarly, the \(^{27}\text{Al}(d,n)\) reaction cross section calculation has taken into account 24 final states of the even–even residual nucleus \(^{28}\text{Si}\), up to 11.4 MeV, with the spectroscopic factors given by analysis of neutron angular–distributions [39]. Finally the energy dependence of the stripping reaction cross section contributions to the activation cross sections \(^{27}\text{Al}(d,p)^{28}\text{Al}\) and \(^{27}\text{Al}(d,n)^{28}\text{Si}\) are shown by dot-dashed curves in Fig. 3(a,b).

The single neutron stripping, \(^{63,65}\text{Cu}(d,p)\), reaction cross section calculations involved transitions to 63 final states of the odd-odd residual nucleus \(^{64}\text{Cu}\) and 52 final states of the residual nucleus \(^{66}\text{Cu}\) extending up to \(\sim 3\) MeV for which spectroscopic factors exist [40].
4. Pre-equilibrium and statistical emission
Following the decay path, the pre-equilibrium (PE) and evaporation cross sections (CN), corrected for the breakup and stripping decrease of the total reaction cross section, completed the deuteron activation cross sections calculations by using the code STAPRE-H [41]. The main assumptions and parameters involved in Geometry Dependent Hybrid Model and Hauser-Feschbach formalism for PE and respectively CN calculations have recently been described elsewhere [42], while the specific parameters for the mass range A<30 are given in Ref. [10].

The comparison of the measured and calculated activation reaction cross sections corresponding to deuteron interaction with $^{27}$Al is presented in Fig. 3 (a-f), including the global (TALYS code [25]) and local analysis results described here, as well as the ACSELAM library [27] results. The common statement for all activation cross sections shown in Fig. 3 is that of the need to update the ACSELAM library.

The results of the local analysis of the final $(d, n)$ and $(d, p)$ activation cross sections of $^{27}$Al shown in Figs. 3(a) and 3(b) include all three mechanisms components i.e. the DR cross sections provided by the code FRESCO and the PE+CN contributions supplied by STAPRE-H. The latter is alone rather close to the TALYS predictions while the complete local approach has led to much better agreement with the most recent $(d, p)$ reaction data [10] especially due to the DR stripping contribution.

Concerning the complete description of the $(d, 2n)$, $(d, 2p)$, and $(d, p\alpha)$ reaction cross sections, the inelastic breakup mechanism may contribute up to 50% of the activation cross sections for deuteron incident energies of $\sim$25 MeV, as it is shown by the dot-dashed curves in Fig. 3(d), 3(e), and 3(f) respectively. A simpler analysis concerns the $(d, \alpha)$ reaction, Fig. 3(c) which has no other breakup corrections except the corresponding decrease of the total reaction cross section. The DR effects have also been overlooked, due to the symmetrical experimental $(d, \alpha)$ reaction angular distributions [21] which are already reproduced by the PE+CN contributions. Thus the PE+CN components provide alone the corresponding activation cross sections [10].

5. Conclusions
The main applied-oriented aim of this lecture has been to present an unitary analysis of the nuclear reaction mechanisms responsible for the deuteron interactions with nuclei. An extended analysis of elastic-scattering, breakup and direct-reaction of deuterons followed by the pre-equilibrium and statistical emissions has been considered.

The overall agreement between the measured data and model calculations proves the correctness of nuclear mechanism description taken into account for the deuteron-nucleus interaction. Also, the simultaneous analysis of the deuteron elastic scattering and induced activation appears essential for a consistent input into the nuclear reaction model studies. Finally the comparison of the present calculations with predictions of the TALYS code stress out the importance of the appropriate consideration of the deuteron breakup mechanism contribution to the activation cross-section calculations.

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