

SECTIUNEA 1

RAPORTUL STIINTIFIC SI TEHNIC

FAZA DE EXECUTIE NR. 2

CU TITLUL

“Participarea Romaniei la EUROfusion WPbb si cercetari complementare”

Tipul proiectului: partea PRINCIPALA

Raportul stiintific intemediar va cuprinde urmatoarele documente:

1. Raportul de cercetare *in extenso*, conform modelului din Anexa 1.A, incluzand rezumatele in romana si engleza;
2. Indicatori de realizare intermediară
3. Proces verbal de avizare internă
4. Procese verbale de recepție a lucrărilor realizate de terți

Raport de cercetare in extenso

1. Titlul proiectului: Participarea Romaniei la EUROfusion WPBB si cercetari complementare / WPBB2-RO
2. Titlul fazei in executie: Raport, incluzand eventual fisiere de date evaluate, a evaluarii sectiunilor eficiente ale reactiilor induse de deuteroni pe $^{92,94}\text{natMo}$, si analizei emisiei alfa indusa de neutroni stabilite si aprobate prin EUROfusion IDM.
3. Perioada de executie: Ianuarie-Decembrie 2023
4. Obiectivele fazei de executie:

Aceste obiective au fost in fapt cele ale *'deliverabilelor'* BB-S.05.02-T005-D006/D007, a caror responsabilitate a revenit autorilor raportului de fata, constand in **analiza si discutia rezultatelor de calcule de model** de reactii nucleare (Secs. 4-6 ale Refs. [1-3]) realizate **pe baza ipotezelor si parametrilor de model** formand in aceeasi perioada obiectul activitatii IFIN-HH (Secs. 1-3 ale Refs. [1-3]) precum si al componentei complementare a proiectului de fata in **cazuri particulare de ipoteze si parametri** de model [4,5], in vederea evaluarii avansate a reactiilor induse de neutroni, protoni si deuteroni in cadrul noilor biblioteci de date nucleare evaluate. In particular, a fost realizata evaluarea sectiunilor eficiente ale reactiilor induse de deuteroni pe $^{92,94}\text{natMo}$ (BB-S.05.02-T005-D006), si analizei emisiei alfa indusa de neutroni pe izotopii stabili de interes cu $A \sim 90$ (BB-S.05.02-T005-D007), formand si obiectul raportarilor de monitorizare semestriale [6-9].
5. Rezumatul fazei (maxim 1 pagina, atât în limba română cât și în limba engleză);

(RO) Extinderea codurilor de modele nucleare, necesara in vederea evaluarii avansate a sectiunilor eficiente ale reactiilor induse de deuteroni pe izotopii stabili $^{92,94}\text{Mo}$ avand obiectivul final al acestei activitati realizate pentru natMo , a fost realizata prin luarea in considerare a analizei tuturor datelor experimentale disponibile pentru izotopii stabili vizati si natMo , pentru energiile incidente de pana la 50 MeV. Discrepanțele aparente dintre datele experimentale si cele evaluate corespunzatoare sunt dovedite ca fiind datorate unei abordari teoretice incomplete care ar necesita, suplimentar proceselor de emisie la prechilibru (PE) si dezexcitare a nucleelor compuse in intregime echilibrate (CN), includerea consistenta a contributiilor mecanismului de 'rupere' a deuteronului ('breakup', BU) precum si a reactiilor directe (DR) de tip 'stripping' si 'pick-up' in analiza activarii cu deuteroni. Luarea in considerare corespunzatoare a tuturor acestor contributii a fost realizata odata cu rezultatele prezentate in formatul codului TALYS, in mod similar analizelor anterioare pentru ^{93}Nb (Phys. Rev. C **88**, 014612, 2013) si $^{90,92,94,96}\text{Zr}$ (Phys. Rev. C **104**, 044615, 2021). Analiza reactiilor (d,p) precum si a altor reactii directe care nu sunt luate in considerare in codul TALYS a fost realizata utilizand codul FRESCO si datele disponibile pentru obtinerea factorilor spectroscopici necesari in acest scop.

Fisierele incluzand rezultatele actuale ca si cele anterioare corespunzand reactiilor induse de deuteroni pe izotopii stabili ai elementelor Cr, Mn, Fe, Ni, and Cu pot fi luate in considerare ca

noi evaluari ale reactiilor induse de deuteroni prezentand un acord mai bun si consistent cu datele experimentale microscopice, fata de cele mai recente evaluari TENDL.

In acelasi timp, o evaluare consistenta a tuturor functiilor de excitare masurate pentru reactiile induse de neutroni pe ^{93}Nb , considerata ca obiectiv de lucru pentru 2023, a fost realizata comparativ cu rezultatele evaluate cuprinse in baza de date TENDL-2021 pe baza parametrilor standard ai codului TALYS-1.96. Suplimentar, seturi consistente de parametri de model, care au fost obtinuti sau validati anterior pe baza analizei unor alte date experimentale independente, fara a mai fi ulterior ajustate folosind factori de scalare empirici ai largimilor de emisie gama sau de neutroni, au fost implicate in analiza sectiunilor eficiente ale reactiilor (α,γ) si (α,n) OMP induse pe nucleul tinta ^{144}Sm care au fost obtinute in ultimul cuplu de ani.. Aceasta analiza suplimentara a fost impusa imperativ in vederea unei validari actuale a potentialului de model optic (OMP) al particulelor alfa, dezvoltat in contextul activitatilor F4E/EUROfusion, de asemenea si in cazul descrierii corespunzatoare a emisiei alfa in reactii induse de neutroni. A fost evidentiata corelarea incertitudinilor datelor experimentale implicate in stabilirea parametrilor consistenti de modele nucleare, conducand la sectiunile eficiente de reactie calculate in final, cu incertitudinea acestora din urma. In acelasi timp, descrierea corespunzatoare a tuturor datelor experimentale pentru canalele de reactie aflate in competitie a evitat efectele compensatorii ale parametrilor de model avand o cunoastere insuficienta. Aspecte necesitand inca o atentie aparte au fost evidentiata in relatie cu imprastierea inelastica de natura directa colectiva a imprastierii inelastice a particulelor alfa, la energii inferioarea barierei Coulomb, sau proceselor similare rezonantelor gigantice cuadropolare (GQR) in cazul datelor masurate recent pentru reactia (n,α) pe nucleul tinta ^{91}Zr . A fost subliniata si disponibilitatea rezultatelor de fata in vederea unor evaluari viitoare de interes.

(EN) Improvements of the nuclear model analysis to extend the evaluated deuteron-induced reaction cross sections of the stable isotopes $^{92,94}\text{Mo}$ in view of a final work concerning natMo, have been considered including the analysis of all available data for these Mo stable isotopes and natMo up to 50 MeV. The apparent discrepancies between experimental data and the corresponding evaluated ones, are shown to follow the incomplete theoretical frame of the deuteron interaction process requesting, besides pre-equilibrium emission (PE) and fully equilibrated compound nucleus (CN) decay, the consistent inclusion of breakup mechanism (BU) as well as of stripping and pickup direct reactions (DR) contributions within deuteron activation analysis. Proper account of these contributions has been carried out with results that could be also provided in TALYS code format, within a similar way to previous analyses for ^{93}Nb (Phys. Rev. C **88**, 014612, 2013) and $^{90-92,94,96}\text{Zr}$ (Phys. Rev. C **104**, 044615, 2021). The assessment of (d,p) and other direct-reactions, otherwise not taken into account within TALYS, has made use of the code FRESCO and the available data for establishment of the needed spectroscopic factors.

Files including the present results as well the previous ones corresponding to reactions on the isotopes of Cr, Mn, Fe, Ni, and Cu, could be considered as new evaluations of deuteron-induced reactions showing a better and consistent agreement with microscopic experimental data than the most recent widely-used TENDL evaluations.

On the other hand, concurrent assessment of all measured excitation functions for various reactions induced by neutrons on ^{93}Nb , in addition to the results of TENDL-2021 and default parameters in TALYS-1.96, planned for 2023, was completed. Consistent parameter sets that are formerly obtained or validated by analysis of other independent data, with no further empirical rescaling factors of the gamma and/or neutron widths, have additionally been used also the account of the (α,γ) and (α,n) reaction cross sections newly available within last couple of years for the ^{144}Sm target nucleus. This supplementary analysis become imperative for a further support of the alpha-particle optical potential, developed within F4E/EUROfusion deliverables, also for a sound description of the alpha-emission in neutron-induced reactions. The correlation between the measured error bars of the primary data providing the consistent input parameters, and the final uncertainty bands of the calculated results has been pointed out. At the same time, a proper account in this work of all available data for competitive reaction channels prevented compensation effects of less accurate model parameters. Remaining questions are shown to correspond either to the direct collective alpha-particle inelastic scattering below the Coulomb barrier, for (α,γ) reaction on ^{144}Sm , or to a Giant Quadrupole Resonance like-process for most recently measured (n,α) reaction data for ^{91}Zr . The availability of these results for further evaluations of actual interest has been stressed.

Files including the present results as well the previous ones corresponding to reactions on the isotopes of Fe, Co, Ni, Cu, and Zn, could be considered as new evaluations of neutron- as well as proton-induced reactions showing a better and consistent agreement with microscopic experimental data than the most recent widely-used TENDL evaluations.

6. Descrierea științifică și tehnică, cu punerea în evidență a rezultatelor fazei și gradul de realizare a obiectivelor, concluzii; (în limba engleză)
Gradul integral de realizare a obiectivelor și concluziile este prezentat în cele 5 lucrări [1-5] reprezentând deliverabilele BB-S.05.02-T005-D006/D007 [6-9], atasate ca anexe, precum și în pagina <https://www.nipne.ro/proiecte/pn3/57-proiecte.html>.
7. Lista de publicații, participări la conferințe, *meeting*-uri.
 - [1] M. Avrigeanu, E. Simeckova, J. Mrazek, C. Costache, and V. Avrigeanu, *Modeling of deuteron-induced reactions on molybdenum at low energies* (submitted for publication in Phys. Rev. C, Nov. 1st, 2023)
 - [2] V. Avrigeanu and M. Avrigeanu, *Consistent assessment of neutron-induced activation of ^{93}Nb* , Front. Phys. **11**, 1142436 (2023), <https://doi.org/10.3389/fphy.2023.1142436> (part of the *Research Topic on Nuclear Data for Fusion Technology from Basic Research to Full-Scale Applications*, <https://www.frontiersin.org/research-topics/39045/nuclear-data-for-fusion-technology-from-basic-research-to-full-scale-application>)
 - [3] V. Avrigeanu and M. Avrigeanu, *Constrained model assumptions using recent data of α -particle reactions on ^{144}Sm* , Front. Phys. **12**, 1247311 (2023), <https://doi.org/10.3389/fphy.2023.1247311> (part of the *Research Topic on Cross Section Data of Interest for Nuclear Astrophysics: Experimental and Theoretical Status, and Perspectives*. <https://www.frontiersin.org/research-topics/51270/cross-section-data-of-interest-for-nuclear-astrophysics-experimental-and-theoretical-status-and-perspectives#overview>)

- [4] M. Avrigeanu and V. Avrigeanu, *Structural material nuclear data basic research*, Front. Phys. 11, 1172697 (2023), <https://doi.org/10.3389/fphy.2023.1172697> (part of the *Research Topic on Nuclear Data for Fusion Technology from Basic Research to Full-Scale Applications*, <https://www.frontiersin.org/research-topics/39045/nuclear-data-for-fusion-technology-from-basic-research-to-full-scale-application>)
- [5] M. Avrigeanu and V. Avrigeanu, *Due consideration of the breakup and direct reaction mechanisms within (d,p), (d,2p), (d,xn2p), and (d,xn) reactions*, in *Proc. 16th Varenna Conference on Nuclear Reaction Mechanisms (NRM2023)*, Varenna, Italy, June 11-16, 2023, F. Cerutti and T. Kawano (Eds.), <https://indico.cern.ch/event/1132769/>; EPJ Web of Conf. (accepted, Oct. 2023)
- [6] V. Avrigeanu and M. Avrigeanu, *Evaluation of fast-neutron induced alpha emission*, Report EFFDOC-1503, OECD/NEA Data Bank, JEFF Meeting, April 24, 2023, https://www.oecd-nea.org/dbdata/nds_effdoc/effdoc-1503.pdf
- [7] M. Avrigeanu and V. Avrigeanu, *Progress report on analysis of deuteron-induced reactions on structural materials*, Report EFFDOC-1504, OECD/NEA JEFF Meeting, April 24, 2023, https://www.oecd-nea.org/dbdata/nds_effdoc/effdoc-1504.pdf
- [8] V. Avrigeanu and M. Avrigeanu, *Progress report on evaluation of fast-neutron induced alpha emission*, Report EFFDOC-1488, OECD/NEA Data Bank, JEFF Meeting, Nov. 24, 2023, https://www.oecd-nea.org/dbdata/nds_effdoc/effdoc-1518.pdf
- [9] M. Avrigeanu and V. Avrigeanu, *Progress report on analysis of deuteron-induced reactions on structural materials*, Report EFFDOC-1519, OECD/NEA JEFF Meeting, Nov. 27, 2023, https://www.oecd-nea.org/dbdata/nds_effdoc/effdoc-1519.pdf

ANEXA 1.A

Programme / Sub-programme / Module	5/5.2/EURATOM-RO FUSION	
EUROfusion Work Package	WPBB	Principal <input checked="" type="checkbox"/> Complementary <input type="checkbox"/>
Project title / Acronym	Romanian participation at EUROfusion WPBB and complementary reserach / WPBB2-RO	
Deliverable title	Report on evaluation of deuteron-induced 92,94,natMo cross sections Deliverable BB-S-05.02-T005-D006 (Jan. 01 - Dec. 31, 2023)	
Reporting period	January 01 - December 31, 2023	
Authors	Marilena Avrigeanu ¹ , Vlad Avrigeanu ¹	
Affiliation	<i>Horia Hulubei National Institute for Physics and Nuclear Engineering, IFIN-HH</i>	

Summary

Calibri 11, la 1,15 randuri. Pagina A4, cu margini de 1" pe toate laturile. Dimensiuni: ½ - 1 pag.

Rezumatetele in limba romana si engleza se fac pe pagini separate.

(RO) Extinderea codurilor de modele nucleare, necesara in vederea evaluarii avansate a sectiunilor eficiente ale reactiilor induse de deuteroni pe izotopii stabili 92,94Mo avand obiectivul final al acestei activitati realizate pentru natMo, a fost realizata prin luarea in considerare a analizei tuturor datelor experimentale disponibile pentru izotopii stabili vizati si natMo, pentru energiile incidente de pana la 50 MeV. Discrepantele aparente dintre datele experimentale si cele evaluate corespunzatoare sunt dovedite ca fiind datorate unei abordari teoretice incomplete care ar necesita, suplimentar proceselor de emisie la prechilibru (PE) si dezexcitare a nucleelor compuse in intregime echilibrate (CN), includerea consistenta a contributiilor mecanismului de 'rupere' a deuteronului ('breakup', BU) precum si a reactiilor directe (DR) de tip 'striping' si 'pick-up' in analiza activarii cu deuteroni. Luarea in considerare corespunzatoare a tuturor acestor contributii a fost realizata odata cu rezultatele prezentate in formatul codului TALYS, in mod similar analizelor anterioare pentru 93Nb (Phys. Rev. C **88**, 014612, 2013) si 90-92,94,96Zr (Phys. Rev. C **104**, 044615, 2021). Analiza reactiilor (d,p) precum si a altor reactii directe care nu sunt luate in considerare in codul TALYS a fost realizata utilizand codul FRESCO si datele disponibile pentru obtinerea factorilor spectroscopici necesari in acest scop.

Fisierele incluzand rezultatele actuale ca si cele anterioare corespunzand reactiilor induse de deuteroni pe izotopii stabili ai elementelor Cr, Mn, Fe, Ni, and Cu pot fi luate in considerare ca noi evaluari ale reactiilor induse de deuteroni prezentand un acord mai bun si consistent cu datele experimentale microscopice, fata de cele mai recente evaluari TENDL.

(EN) Improvements of the nuclear model analysis to extend the evaluated deuteron-induced reaction cross sections of the stable isotopes $^{92,94}\text{Mo}$ in view of a final work concerning natMo , have been considered including the analysis of all available data for these Mo stable isotopes and natMo up to 50 MeV. The apparent discrepancies between experimental data and the corresponding evaluated ones, are shown to follow the incomplete theoretical frame of the deuteron interaction process requesting, besides pre-equilibrium emission (PE) and fully equilibrated compound nucleus (CN) decay, the consistent inclusion of breakup mechanism (BU) as well as of stripping and pickup direct reactions (DR) contributions within deuteron activation analysis. Proper account of these contributions has been carried out with results that could be also provided in TALYS code format, within a similar way to previous analyses for ^{93}Nb (Phys. Rev. C **88**, 014612, 2013) and $^{90-92,94,96}\text{Zr}$ (Phys. Rev. C **104**, 044615, 2021). The assessment of (d,p) and other direct-reactions, otherwise not taken into account within TALYS, has made use of the code FRESKO and the available data for establishment of the needed spectroscopic factors.

Files including the present results as well the previous ones corresponding to reactions on the isotopes of Cr, Mn, Fe, Ni, and Cu, could be considered as new evaluations of deuteron-induced reactions showing a better and consistent agreement with microscopic experimental data than the most recent widely-used TENDL evaluations.

ANEXA 1.A

Programme / Sub-programme / Module	5/5.2/EURATOM-RO FUSION	
EUROfusion Work Package	WPBB	Principal <input checked="" type="checkbox"/> Complementary <input type="checkbox"/>
Project title / Acronym	Romanian participation at EUROfusion WPBB and complementary reserach / WPBB2-RO	
Deliverable title	Report on analysis of neutron-induced alpha-emission on medium-mass nuclei along and off the stability line Deliverable BB-S-05.02-T005-D007 (Jan. 01 - Dec. 31, 2023)	
Reporting period	January 01 - December 31, 2023	
Authors	Vlad Avrigeanu ¹ , Marilena Avrigeanu ¹	
Affiliation	<i>Horia Hulubei National Institute for Physics and Nuclear Engineering, IFIN-HH</i>	

Summary

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Rezumatetele in limba romana si engleza se fac pe pagini separate.

(RO) O evaluare consistenta a tuturor functiilor de excitare masurate pentru reactiile induse de neutroni pe ^{93}Nb , considerata ca obiectiv de lucru pentru 2023, a fost realizata comparativ cu rezultatele evaluate cuprinse in baza de date TENDL-2021 pe baza parametrilor standard ai codului TALYS-1.96. Suplimentar, seturi consistente de parametri de model, care au fost obtinuti sau validati anterior pe baza analizei unor alte date experimentale independente, fara a mai fi ulterior ajustate folosind factori de scalare empirici ai largimilor de emisie gama sau de neutroni, au fost implicate in analiza sectiunilor eficiente ale reactiilor (α,γ) si (α,n) OMP induse pe nucleul tinta ^{144}Sm care au fost obtinute in ultimul cuplu de ani.. Aceasta analiza suplimentara a fost impusa imperativ in vederea unei validari actuale a potentialului de model optic (OMP) al particulelor alfa, dezvoltat in contextul activitatilor F4E/EUROfusion, de asemenea si in cazul descrierii corespunzatoare a emisiei alfa in reactii induse de neutroni. A fost evidentiata corelarea incertitudinilor datelor experimentale implicate in stabilirea parametrilor consistenti de modele nucleare, conducand la sectiunile eficiente de reactie calculate in final, cu incertitudinea acestora din urma. In acelasi timp, descrierea corespunzatoare a tuturor datelor experimentale pentru canalele de reactie aflate in competitie a evitat efectele compensatorii ale parametrilor de model avand o cunoastere insuficienta. Aspecte necesitand inca o atentie aparte au fost evidentiata in relatie cu imprastierea inelastica de natura directa colectiva a imprastierii inelastice a particulelor alfa, la energii inferioarea barierei Coulomb, sau proceselor similare rezonantelor gigantice cuadrupolare (GQR) in cazul datelor masurate recent pentru reactia (n,α) pe nucleul tinta ^{91}Zr . A fost subliniata si disponibilitatea rezultatelor de fata in vederea unor evaluari viitoare de interes.

Fisierele incluzand rezultatele actuale ca si cele anterioare corespunzand reactiilor induse pe izotopii stabili ai elementelor Fe, Co, Ni, Cu, si Zn, pot fi luate in considerare ca noi evaluari ale reactiilor induse de neutroni precum si de protoni prezentand un acord mai bun si consistent cu datele experimentale microscopice, fata de cele mai recente evaluari TENDL.

(EN) Concurrent assessment of all measured excitation functions for various reactions induced by neutrons on ^{93}Nb , in addition to the results of TENDL-2021 and default parameters in TALYS-1.96, planned for 2023, was completed. Consistent parameter sets that are formerly obtained or validated by analysis of other independent data, with no further empirical rescaling factors of the gamma and/or neutron widths, have additionally been used also the account of the (α,γ) and (α,n) reaction cross sections newly available within last couple of years for the ^{144}Sm target nucleus. This supplementary analysis become imperative for a further support of the alpha-particle optical potential, developed within F4E/EUROfusion deliverables, also for a sound description of the alpha-emission in neutron-induced reactions. The correlation between the measured error bars of the primary data providing the consistent input parameters, and the final uncertainty bands of the calculated results has been pointed out. At the same time, a proper account in this work of all available data for competitive reaction channels prevented compensation effects of less accurate model parameters. Remaining questions are shown to correspond either to the direct collective alpha-particle inelastic scattering below the Coulomb barrier, for (α,γ) reaction on ^{144}Sm , or to a Giant Quadrupole Resonance like-process for most recently measured (n,α) reaction data for ^{91}Zr . The availability of these results for further evaluations of actual interest has been stressed.

Files including the present results as well the previous ones corresponding to reactions on the isotopes of Fe, Co, Ni, Cu, and Zn, could be considered as new evaluations of neutron- as well as proton-induced reactions showing a better and consistent agreement with microscopic experimental data than the most recent widely-used TENDL evaluations.

Programme / Sub-programme / Module	5/5.2/EURATOM-RO FUSION		
Project type	RD	Continuing <input type="checkbox"/>	New <input checked="" type="checkbox"/>
EUROfusion Work Package	WPBB		Principal <input checked="" type="checkbox"/> Complementary <input type="checkbox"/>
Project title / Acronym	Romanian participation at EUROfusion WPBB and complementary research / WPBB2-RO		
Project duration	33 months		

Raport de cercetare in extenso

Detailed results

Calibri 11, la 1,15 randuri. Pagina A4, cu margini de 1" pe toate laturile.

Textul va fi impartit in sectiuni asa cum considera fiecare autor in parte. Font Calibri 11.

Deliverables

BB-S.05.02-T005-D006: Report on evaluation of deuteron-induced $92,94, \text{natMo}$ cross section – 2023

BB-S.05.02-T005-D007: Alpha-particle emission within consistent analysis of neutron-activation of 93Nb - 2023

Short Introduction and Objectives of Work

The PPPT nuclear data development - evaluation of neutron cross sections, radiation damage data and benchmarking, has had to include the IAP/IFIN-HH contribution concerning the (i) the evaluation of deuteron-induced reaction data of structural materials and update of the deuteron-induced TENDL data library as required for activation analyses of the IFMIF-DONES facility (PPPT project ENS), as well as (ii) the advanced evaluation of optical model potentials (OMPs) for alpha particles.

Thus, the evaluation of deuteron-induced reaction cross sections of $^{\text{nat}}\text{Mo}$ up to 50 MeV on the basis of the proper account of contributions of all involved reaction mechanisms as the breakup (BU), stripping, pick-up direct reactions (DR), pre-equilibrium (PE) and evaporation processes, including the assessment of the related procedures recently involved in TALYS nuclear model calculations, has also been concerned in this respect, while formerly [1,2] this aim regarded the stable isotopes of Al, Cr, Mn, Fe, Ni, Cu, Zr, and Nb. The enhanced BU formalism most recently included in TALYS-1.96 [3] consists in an alternate parametrization of BU cross sections [2], as well as the estimation of the enhancement of the deuteron-induced reaction cross sections due to the variety of reactions initiated by the BU neutrons and protons. The main issues of this BU alternate parametrization and corresponding enhancement of the deuteron-induced reaction cross sections have been reviewed and additionally supported [4].

Actually, the statistical Hauser-Feshbach model has so far been involved as the main tool to calculate the deuteron reaction cross sections at low incident energies, the compound nucleus (CN) mechanism being considered dominant in this energy range. However, specific non-compound processes, which were not yet taken systematically into account for the corresponding deuteron-

induced reactions, make these reactions different from those induced by other projectiles. The deuteron interaction at incident energies below and around the Coulomb barrier proceeds largely through DR mechanisms of stripping and pick-up, while PE and evaporation from fully equilibrated CN become important with the increase of the incident energy. Moreover, in addition to these well known reaction mechanisms, the specific BU plays an important role that increases the complexity of the deuteron interaction analysis in the whole incident energy range due to the large variety of reactions initiated by the BU nucleons.

On the other hand, evaluation of neutron-induced alpha emission data on the basis of consistent nuclear model calculation of reaction cross sections, namely by using model parameters established through analysis of distinct independent data and with no empirical rescaling factors of the gamma and/or nucleon widths, performed for incident energies up to ~21 MeV and all available data for various reaction channels and isotopes of structural materials including EUROFER and SS-316 has been concerned in this respect. The present work has followed the development within the F4E projects of the Nuclear Data Consortium of an optical potential providing a suitable description of the incident alpha-particle data within the mass range $45 < A < 209$ [5] and then proved to describe also the most recent similar data published in the meantime [6,7]. However, there remained still open questions concerning its suitability to account of the alpha-emission.

Thus, while a suitable agreement has been obtained between measured cross sections of (n,α) reactions of $^{90,91,92,94,96}\text{Zr}$, ^{93}Nb , and $^{92,95,98,100}\text{Mo}$ [8], including all competitive reaction channels, with consistent model calculations using the OMP [5] as well as the pick-up direct-reaction population of the low-lying levels of residual nuclei. Moreover, also these results were compared with results of the TALYS-1.96 code [3] obtained by using global input parameters, and the most recent evaluated-data library TENDL-2021 [9], for an overall excitation function survey from both points of view of standard model calculations and advanced evaluations. It was shown thus the better agreement of the present calculation results with the experimental data, with the additional and more important comment that all parameters have been not changed following their former setting by analysis of independent data that have been distinct by the ones finally analyzed.

A suitable account of the measured alpha-emission cross sections is provided, on the other hand, by an additional contribution at the Giant Quadrupole Resonance (GQR) energy of excited nuclei. Because the Gaussian distributions added in this respect have widths which are much lower than the systematic 'best' values, we continue to call these components only like-GQR components. Nevertheless, they are even larger than the DR pickup for incident energies < 12 MeV. While further conclusions on the physics behind this empirical addition are not yet evident, it has been considered that more similar cases concerned in this respect may help.

Description of Results

Improvements of the nuclear model analysis to extend the evaluated deuteron-induced reaction cross sections of the stable isotopes $^{92,94}\text{Mo}$ in view of a final work concerning natMo, have been considered including the analysis of all available data for these Mo stable isotopes and natMo up to 50 MeV. The apparent discrepancies between experimental data and the corresponding evaluated ones, are shown to follow the incomplete theoretical frame of the deuteron interaction process requesting, besides pre-PE and fully equilibrated CN decay, the consistent inclusion of breakup mechanism as well

as of stripping and pickup DR contributions within deuteron activation analysis. Proper account of these contributions has been carried out with results that could be also provided in TALYS code format [10], within a similar way to previous analyses for ^{93}Nb and $^{90-92,94,96}\text{Zr}$ [1]. The assessment of (d,p) and other direct-reactions, otherwise not taken into account within TALYS, has made use of the code FRESCO and the available data for establishment of the needed spectroscopic factors.

The extended analysis in this work, on the basis of available data for deuteron interactions with natural Mo and its isotopes up to 50 MeV, includes every process from elastic scattering until pre-equilibrium and compound--nucleus decay. A particular attention has been paid to the breakup, stripping, and pick-up direct interactions which account overall for around half of the deuteron total-reaction cross section. The due account of most experimental data has thoroughly validated the present approach and highlighted some prevalent features.

On the other hand, concurrent assessment of all measured excitation functions for various reactions induced by neutrons on ^{93}Nb [11], in addition to the results of TENDL-2021 and default parameters in TALYS-1.96, planned for 2023, was completed. Consistent parameter sets that are formerly obtained or validated by analysis of other independent data, with no further empirical rescaling factors of the gamma and/or neutron widths, have additionally been used also the account of the (α,γ) and (α,n) reaction cross sections newly available within last couple of years for the ^{144}Sm target nucleus [12]. This supplementary analysis become imperative for a further support of the alpha-particle optical potential, developed within F4E/EUROfusion deliverables, also for a sound description of the alpha-emission in neutron-induced reactions. The correlation between the measured error bars of the primary data providing the consistent input parameters, and the final uncertainty bands of the calculated results has been pointed out. At the same time, a proper account in this work of all available data for competitive reaction channels prevented compensation effects of less accurate model parameters.

Increase of the alpha-particle direct collective inelastic scattering at lower energies is found responsible for this decrease of the (α,γ) reaction cross sections. The consequent lower nuclear effects may correspond to the Coulomb excitation effect assumed, although in a different manner, within the so-called 'alpha-potential mystery' for the same optical-potential account of alpha-particle absorption and emission as well.

Conclusions

This analysis has emphasized the weak points and consequently the need for modeling/evaluation upgrade. Most of them were related to overlooking the deuteron inelastic-breakup enhancement and appropriate treatment of stripping and pick-up processes. New data as well as complementary measurements of (d,px) and (n,x) as well as (d,nx) and (p,x) reaction cross sections, so scarce for the stable isotopes, are also essential for the improvement of the deuteron breakup account and feasible evaluation predictions so important for advanced engineering design projects.

Remaining questions are shown to correspond either to the direct collective alpha-particle inelastic scattering below the Coulomb barrier, for (α,γ) reaction on ^{144}Sm , or to a GQR-like-process for most recently measured (n, α) reaction data for ^{91}Zr . The availability of these results for further evaluations of actual interest has also been stressed. Files including the present results [10] as well the previous ones corresponding to reactions on the isotopes of Cr, Mn, Fe, Ni, and Cu [1-2], could be

considered as new evaluations of deuteron-induced reactions showing a better and consistent agreement with microscopic experimental data than the most recent widely-used TENDL evaluations.

On the other hand, files including the present results [11-12] as well the previous ones corresponding to reactions on the isotopes of Fe, Co, Ni, Cu, and Zn [6-8], could be considered as new evaluations of neutron- as well as proton-induced reactions showing a better and consistent agreement with microscopic experimental data than the most recent widely-used TENDL evaluations.

Acknowledgement

This work has been carried out within the framework of the EUROfusion Consortium, funded by the European Union via the Euratom Research and Training Programme (Grant Agreement No 101052200 — EUROfusion), and also from the Romanian Ministry of Research, Innovation and Digitalization under contract No. PN3/EURATOM-ROFuziune/EU-01/03.01.2022. Views and opinions expressed are however those of the author(s) only and do not necessarily reflect those of the European Union or the European Commission. Neither the European Union nor the European Commission can be held responsible for them. The reviews and opinion expressed herein do not necessarily reflect those of the European Commission.

References

- [1] M. Avrigeanu, E. Šimečková, U. Fischer, J. Mrázek, J. Novak, M. Štefánik, C. Costache, and V. Avrigeanu, Phys. Rev. C **101**, 024605 (2020); E. Šimečková, M. Avrigeanu, J. Mrázek, J. Novak, M. Štefánik, C. Costache, and V. Avrigeanu, Phys. Rev. C **104**, 044615 (2021).
- [2] M. Avrigeanu, W. von Oertzen, R.A. Forrest, A.C. Obreja, F.L. Roman, and V. Avrigeanu, Fusion Eng. Design **84**, 418 (2009); M. Avrigeanu and A. M. Moro, Phys. Rev. C **82**, 037601 (2010); M. Avrigeanu, V. Avrigeanu, and A.J. Koning, *ibid.* **85**, 034603 (2012); M. Avrigeanu and V. Avrigeanu, *ibid.* **92**, 021601(R) (2015); M. Avrigeanu and V. Avrigeanu, *ibid.* **95**, 024607 (2017).
- [3] A. J. Koning, S. Hilaire, and S. Goriely, *TALYS-1.96 - A nuclear reaction program*; <http://www.talys.eu/>
- [4] M. Avrigeanu, D. Rochman, A. J. Koning, U. Fischer, D. Leichtle, C. Costache, and V. Avrigeanu, Eur. Phys. J. A **58**, 3 (2022).
- [5] V. Avrigeanu, M. Avrigeanu, and C. Manaiescu, Phys. Rev. C **90**, 044612 (2014); V. Avrigeanu and M. Avrigeanu, *ibid.* **91**, 064611 (2015); *ibid.* **94**, 024621 (2016); *ibid.* **96**, 044610 (2017); *ibid.* **99**, 044613 (2019).
- [6] V Avrigeanu and M. Avrigeanu, *Validation of an optical potential for incident and emitted low-energy alpha-particles in the $A \sim 60$ mass range*. (Part of a collection: [Light Clusters in Nuclei and Nuclear Matter: Nuclear Structure and Decay, Heavy Ion Collisions, and Astrophysics](#)), Eur. Phys. J. A **57**, 54 (2021).
- [7] V Avrigeanu and M. Avrigeanu, *Validation of an optical potential for incident and emitted low-energy alpha-particles in the $A \sim 60$ mass range. II. Neutron-induced reactions on Ni isotopes* (Part of a collection: [Light Clusters in Nuclei and Nuclear Matter: Nuclear Structure and Decay, Heavy Ion Collisions, and Astrophysics](#)), Eur. Phys. J. A **58**, 189 (2022); V. Avrigeanu and M. Avrigeanu, *Charged-*

particle optical potentials tested by first direct measurement of the $59\text{Cu}(p,\alpha)56\text{Ni}$ reaction, Phys. Rev. C **106**, 024615 (2022)

- [8] M. Avrigeanu and V. Avrigeanu, *Optical potential for incident and emitted low-energy alpha particles. III. Non-statistical processes induced by neutrons on Zr, Nb, and Mo nuclei*, Phys. Rev. C **107**, 034613 (2023).
- [9] A. J. Koning and D. Rochman, TENDL-2021: TALYS-based evaluated nuclear data library, https://tendl.web.psi.ch/tendl_2021/tendl2021.html

Papers

- [10] M. Avrigeanu, E. Simeckova, J. Mrazek, C. Costache, and V. Avrigeanu, *Modeling of deuteron-induced reactions on molybdenum at low energies* (submitted for publication in Phys. Rev. C, Nov. 1st, 2023)
- [11] V. Avrigeanu and M. Avrigeanu, *Consistent assessment of neutron-induced activation of ^{93}Nb* , Front. Phys. **11**, 1142436 (2023), <https://doi.org/10.3389/fphy.2023.1142436> (part of the *Research Topic on Nuclear Data for Fusion Technology from Basic Research to Full-Scale Applications*, <https://www.frontiersin.org/research-topics/39045/nuclear-data-for-fusion-technology-from-basic-research-to-full-scale-application>)
- [12] V. Avrigeanu and M. Avrigeanu, *Constrained model assumptions using recent data of α -particle reactions on ^{144}Sm* , Front. Phys. **12**, 1247311 (2023), <https://doi.org/10.3389/fphy.2023.1247311> (part of the *Research Topic on Cross Section Data of Interest for Nuclear Astrophysics: Experimental and Theoretical Status, and Perspectives*. <https://www.frontiersin.org/research-topics/51270/cross-section-data-of-interest-for-nuclear-astrophysics-experimental-and-theoretical-status-and-perspectives#overview>)

Meetings

- [13] V. Avrigeanu and M. Avrigeanu, *Evaluation of fast-neutron induced alpha emission*, Report EFFDOC-1503, OECD/NEA Data Bank, JEFF Meeting, April 24, 2023, https://www.oecd-nea.org/dbdata/nds_effdoc/effdoc-1503.pdf
- [14] M. Avrigeanu and V. Avrigeanu, *Progress report on analysis of deuteron-induced reactions on structural materials*, Report EFFDOC-1504, OECD/NEA JEFF Meeting, April 24, 2023, https://www.oecd-nea.org/dbdata/nds_effdoc/effdoc-1504.pdf
- [15] V. Avrigeanu and M. Avrigeanu, *Progress report on evaluation of fast-neutron induced alpha emission*, Report EFFDOC-1488, OECD/NEA Data Bank, JEFF Meeting, Nov. 24, 2023, https://www.oecd-nea.org/dbdata/nds_effdoc/effdoc-1518.pdf
- [16] M. Avrigeanu and V. Avrigeanu, *Progress report on analysis of deuteron-induced reactions on structural materials*, Report EFFDOC-1519, OECD/NEA JEFF Meeting, Nov. 27, 2023, https://www.oecd-nea.org/dbdata/nds_effdoc/effdoc-1519.pdf

ANEXA 1.B Indicatori de realizare intermediara/finala

Tip indicator	Numar	Scurta descriere (daca este cazul)
Numar de articole stiintifice în reviste si volume indexate ISI	3	Phys. Rev. C 107 , 034613 (2023) Front. Phys. 11 , 1142436 (2023) Front. Phys. 12 , 1247311 (2023)
Numar de articole stiintifice în reviste indexate în alte baze de date internaționale recunoscute	4	Report EFFDOC-1503, NEA DB, Apr.2023 Report EFFDOC-1504, NEA DB, Apr.2023 Report EFFDOC-1518, NEA DB, Nov.2023 Report EFFDOC-1519, NEA DB, Nov.2023
Numar articole publicate in top 10% cele mai citate publicatii		
Numar de brevete obtinute la nivel national si international		
Numar de brevete in curs de obtinere la nivel national si international		
Numar de tehnologii elaborate/transferate in urma Colaborarii la EUROfusion		
Numar de modele experimentale/prototitpuri		
Numarul de posturi de cercetatori echivalent norma intreaga (ENI) sustinute *		
Numarul de cercetatori cu doctorat sustinuti *	2	
Numarul de ingineri sustinuti *		
Numarul de tehnicieni sustinuti *		
Numarul personalului economic/administrativ sustinut *		
Numarul de doctoranzi sustinuti *		
Numar de masteranzi sustinuti *		
Numarul de participari la experimente EUROfusion efectuate*		
Numar de conferinte organizate*		
Numar de participari la Conferinte Internationale*	1	
Numar de prezentari la Conferinte Internationale	1	
Numar de postere prezentate la Conferinte Internationale*		
Numar de participanti la Workshopuri*	2	
Numar de prezentari orale la Workshopuri	4	
Numar de postere prezentate la Workshopuri		
Numărul participanților la întruniri de proiect în cadrul contractelor EUROfusion	2	
Numarul de proiecte Orizont 2020 (inclusiv cele ale partenerilor daca este cazul)		
Numarul de evenimente de comunicare si popularizare a stiintei sustinute*		
Numar de cursuri de instruire sau perfectionare realizate		
Altele (specificati)		

*) din Fondurile Programului

Director de proiect,

Dr. Avrigeanu Vlad

**Institutul National de Cercetare-Dezvoltare pentru
Fizica si Inginerie Nucleara „Horia Hulubei”**

**PROCES VERBAL DE AVIZARE INTERNA A LUCRARILOR DE
CERCETARE-DEZVOLTARE SI INOVARE (PVAI)**

Comisia de avizare constituita prin Decizia nr. 266 din 01.04.2022 luand in examinare lucrarile efectuate de colectivul departamentului de Fizică Nucleară al IFIN-HH la **partea Principala a proiectului “Participarea Romaniei la EUROfusion WPBB si cercetari complementare”** (WPBB2-RO) in cadrul etapei nr. II, care fac obiectul contractului nr. EU-01/03.01.2022, act aditional nr. 1/2022 incheiat cu Institutul de Fizica Atomica, a constatat urmatoarele:

- a) Lucrarile executate corespund clauzelor contractuale;
- b) Toate documentele necesare efectuarii platii exista si sunt corect intocmite;
- c) Concluziile lucrarii, principalele rezultate obtinute si datele privind efectuarea cheltuielilor sunt prezentate in Raportul intermediar de activitate si in documentele sale insotitoare;
- d) Planificarea activitatilor si resurselor aferente realizarii etapei urmatoare de derulare a proiectului, prezentata in Raportul intermediar de activitate, este corespunzatoare realizarii obiectivului propus si in concordanta cu prevederile contractului;
- e) Cota de cofinantare realizata in faza de executie curenta este de.....lei.

Comisia avizeaza **FAVORABIL** lucrarile si documentele si considera ca pot fi prezentate pentru evaluare la Institutul de Fizica Atomica – IFA.

COMISIA DE AVIZARE

FUNCTIA IN COMISIE	NUME SI PRENUME	SEMNATURA
PRESEDINTE	Constantin Mihai	
MEMBRI (cel putin trei specialisti)	Adriana Rodica Raduta	
	Remus Amilcar Ionescu	
	Dorina Aranghel	
SECRETAR	Vlad Avrigeanu	

SECTIUNEA 1

RAPORTUL STIINTIFIC SI TEHNIC

FAZA DE EXECUTIE NR. 2

CU TITLUL

“Participarea Romaniei la EUROfusion WPbb si cercetari complementare”

Tipul proiectului: partea COMPLEMENTARA

Raportul stiintific intemediar va cuprinde urmatoarele documente:

1. Raportul de cercetare *in extenso*, conform modelului din Anexa 1.A, incluzand rezumatele in romana si engleza;
2. Indicatori de realizare intermediară
3. Proces verbal de avizare internă
4. Procese verbale de recepție a lucrărilor realizate de terți

Raport de cercetare in extenso

1. Titlul proiectului: Participarea Romaniei la EUROfusion WPBB si cercetari complementare / WPBB2-RO
2. Titlul fazei in executie: Raport al analizei si validarii ipotezelor si parametrilor de model pentru evaluarea reactiilor induse de deuteroni pe $^{92,94}\text{natMo}$, si a potentialului de model optic pentru particule alfa pentru evaluarea emisiei alfa indusa de neutroni stabilite si aprobate prin EUROfusion IDM.
- 3, Perioada de executie: Ianuarie-Decembrie 2023
4. Obiectivele fazei de executie:

Aceste obiective au fost corelate cu cele ale 'deliverabilelor' BB-S.05.02-T005-D006/D007, a caror responsabilitate a revenit autorilor raportului de fata, cu deosebirea ca ultimele au format obiectul componentei principale a proiectului WPBB2-RO, constand in **analiza si discutia rezultatelor de calcule de model** de reactii nucleare (Secs. 4-6 ale Refs. [1-3]) realizate **pe baza ipotezelor si parametrilor** de model formand in aceeaasi perioada obiectul activitatii IFIN-HH (Secs. 1-3 ale Refs. [1-3]), in timp ce aceasta componenta complementara a proiectului a vizat **cazuri particulare de ipoteze si parametri** de model (Refs. [4,5]), in vederea aceleiasi evaluari avansate a reactiilor induse de neutroni, protoni si deuteroni in cadrul noilor biblioteci de date nucleare evaluate. In particular, a fost realizata evaluarea sectiunilor eficiente ale producerii de H prin reactii induse de deuteroni inclusiv pe izotopii stabili ai Mo [4], si analiza importantei cunoasterii cat mai precise a parametrilor de modele nucleare in evaluarea emisiei alfa indusa de neutroni rapizi si protoni pe nuclee cu $A \sim 60$ [5].

5. Rezumatul fazei (maxim 1 pagina, atat in limba romana cat si in limba engleza);

(RO) Evaluarea datelor nucleare ale reactiilor induse de deuteroni sau pentru emisia de particule α este unul din obiectele *Frontiers-in-Physics Research Topic "Nuclear data for fusion technology, from basic research to full-scale applications."* In consecinta, stadiul si aspectele de interes actual ale acestor subiecte din domeniul datelor nucleare pentru tehnologiile fuziunii nucleare sunt discutate cu referinta la proiectele ITER, DEMO, si IFMIF-DONES. Astel, fata de cercetarile corelate cu fisiunea nucleara, exista o necesitate majora pentru sectiuni eficiente precise ale reactiilor induse de neutroni si deuteroni intr-un domeniu extins de energii incidente de pana la 50 MeV. Cerintele actuale sunt indeplinite in cadrul "TALYS-base Evaluated Nuclear Data Library (TENDL)" realizata pe baza folosirii extinse a codului TALYS atat pentru cercetari fundamentale cat si pentru aplicatiile incluzand tehnologiile ale fuziunii nucleare. Cu toate acestea, dezvoltari ulterioare ale acestei biblioteci de date au fost conectate recent nu numai cu domeniul energetic mentionat mai sus dar si cu varietatea mai mare a datelor nucleare necesare pentru tehnologiile nucleare, fata de domeniul aplicatiilor fisiunii nucleare. In consecinta, progresul evaluarii de date nucleare corelate mai recent cu reactiile induse de deuteroni si emisia de particule α in reactiile induse de neutroni, in cadrul "European Fusion Program", in continuarea realizarii programelor F4E si EUROfusion, este discutat in particular pentru deuteroni incidenti pe ^{52}Cr , $^{54,56,58}\text{natFe}$, ^{59}Co , $^{96}\text{natZr}$, ^{93}Nb , si

94,100,natMo [4,5] precum și evaluarea emisie alfa indusă de neutroni rapizi și protoni pe nuclee cu $A \sim 60$ [4].

Rolul major al seturilor consistente de parametri de model pentru rezultatele analizelor de emisie a particulelor alfa, vizând posibilă diferență între potențialele de model optic (OMPs) ce descriu fie împrăștierea elastică și reacțiile induse de particulele alfa, fie emisia acestora din nucleele excitate în reacții nucleare, a fost de asemenea prezentat. Utilizarea acestora este opusă implicării oricărui factori empirici de scalare ale largimilor de stări nucleare pentru emisia gama și/sau de nucleoni, sau combinațiilor tuturor opțiunilor posibile pentru principalii parametri de model ale unui cod de calcul. Descrierea corespunzătoare a tuturor canalelor de reacție în competiție cu emisia alfa, confirmată printr-o analiză detaliată a incertitudinilor asociate, pentru a evita compensarea ambiguităților de model și/sau a erorilor diferitelor parametri, permite în final și luarea corectă în considerare a unor procese nucleare directe suplimentare.

(EN) The nuclear data evaluation for deuteron-induced reactions and α -particle emission by neutron interactions is addressed within *Frontiers-in-Physics Research Topic "Nuclear data for fusion technology, from basic research to full-scale applications."* The status and open questions related to these subjects in the area of nuclear data for fusion technology, specifically for the nuclear design of the ITER fusion device, the European DEMO fusion reactor, and the IFMIF-DONES Irradiation Facility, are briefly reviewed. A firm demand for accurate cross-sections of reactions induced by neutrons and deuterons exists, in this respect, within a more enlarged energy range up to 50 MeV than for fission applications. The current requirements are closely met by the TENDL Evaluated Nuclear Data Library, settled using the TALYS nuclear model code, which is one of the most widely used codes in basic research and applications including nuclear fusion technology. However, further improvement of this data library has recently been suggested, while, with respect to fission applications, not only the aforementioned energy range but also the diversity of nuclear data for fusion technologies is plainly stretched. Consequently, the progress of nuclear data activities conducted more recently on deuteron-induced reactions and α -emission by neutron interactions, throughout the European Fusion Program and subsequent to previous achievements within F4E and EUROfusion programs, is particularly discussed for deuterons incident on ^{52}Cr , $^{54,56,58}\text{natFe}$, ^{59}Co , $^{96}\text{natZr}$, ^{93}Nb , and $^{94,100}\text{natMo}$ [4,5] as well as alpha-particle emission in neutron- and proton-induced reactions on $A \sim 60$ nuclei [4].

The major role of consistent parameter sets within analysis of neutron-induced alpha-particle emission, for the assessment of a possible difference between the optical model potentials (OMPs) which describe either alpha-particle elastic scattering and induced reactions or alpha-emission from excited compound nuclei, is shown. They are involved at variance with use of either empirical rescaling factors of the gamma and/or neutron widths or even combinations of all options of a computer code for main input parameters. Suitable description of all competitive reaction channels, confirmed by a careful uncertainty analysis in order to avoid parameter ambiguities and/or error compensation, support further consideration of additional direct processes.

6. Descrierea științifică și tehnică, cu punerea în evidență a rezultatelor fazei și gradul de realizare a obiectivelor, concluzii; (în limba engleză)

Gradul integral de realizare a obiectivelor si concluziile sunt prezentate in cele 2 lucrari [12,13], atasate ca anexe, precum si in pagina <https://www.nipne.ro/proiecte/pn3/57-proiecte.html> .

7. Lista de publicatii, participari la conferinte, *meeting-uri*.

- [1] M. Avrigeanu, E. Simeckova, J. Mrazek, C. Costache, and V. Avrigeanu, *Modeling of deuteron-induced reactions on molybdenum at low energies* (submitted for publication in Phys. Rev. C, Nov. 1st, 2023)
- [2] V. Avrigeanu and M. Avrigeanu, *Consistent assessment of neutron-induced activation of ^{93}Nb* , Front. Phys. **11**, 1142436 (2023), <https://doi.org/10.3389/fphy.2023.1142436> (part of the *Research Topic on Nuclear Data for Fusion Technology from Basic Research to Full-Scale Applications*, <https://www.frontiersin.org/research-topics/39045/nuclear-data-for-fusion-technology-from-basic-research-to-full-scale-application>)
- [3] V. Avrigeanu and M. Avrigeanu, *Constrained model assumptions using recent data of α -particle reactions on ^{144}Sm* , Front. Phys. **12**, 1247311 (2023), <https://doi.org/10.3389/fphy.2023.1247311> (part of the *Research Topic on Cross Section Data of Interest for Nuclear Astrophysics: Experimental and Theoretical Status, and Perspectives*. <https://www.frontiersin.org/research-topics/51270/cross-section-data-of-interest-for-nuclear-astrophysics-experimental-and-theoretical-status-and-perspectives#overview>)
- [4] M. Avrigeanu and V. Avrigeanu, *Structural material nuclear data basic research*, Front. Phys. **11**, 1172697 (2023), <https://doi.org/10.3389/fphy.2023.1172697> (part of the *Research Topic on Nuclear Data for Fusion Technology from Basic Research to Full-Scale Applications*, <https://www.frontiersin.org/research-topics/39045/nuclear-data-for-fusion-technology-from-basic-research-to-full-scale-application>)
- [5] M. Avrigeanu and V. Avrigeanu, *Due consideration of the breakup and direct reaction mechanisms within (d,p) , $(d,2p)$, $(d,xn2p)$, and (d,xn) reactions*, in Proc. 16th Varenna Conference on Nuclear Reaction Mechanisms (NRM2023), Varenna, Italy, June 11-16, 2023, F. Cerutti and T. Kawano (Eds.), <https://indico.cern.ch/event/1132769/>; EPJ Web of Conf. (accepted, Oct. 2023)
- [6] V. Avrigeanu and M. Avrigeanu, *Evaluation of fast-neutron induced alpha emission*, Report EFFDOC-1503, OECD/NEA Data Bank, JEFF Meeting, April 24, 2023, https://www.oecd-nea.org/dbdata/nds_effdoc/effdoc-1503.pdf
- [7] M. Avrigeanu and V. Avrigeanu, *Progress report on analysis of deuteron-induced reactions on structural materials*, Report EFFDOC-1504, OECD/NEA JEFF Meeting, April 24, 2023, https://www.oecd-nea.org/dbdata/nds_effdoc/effdoc-1504.pdf
- [8] V. Avrigeanu and M. Avrigeanu, *Progress report on evaluation of fast-neutron induced alpha emission*, Report EFFDOC-1488, OECD/NEA Data Bank, JEFF Meeting, Nov. 24, 2023, https://www.oecd-nea.org/dbdata/nds_effdoc/effdoc-1518.pdf
- [9] M. Avrigeanu and V. Avrigeanu, *Progress report on analysis of deuteron-induced reactions on structural materials*, Report EFFDOC-1519, OECD/NEA JEFF Meeting, Nov. 27, 2023, https://www.oecd-nea.org/dbdata/nds_effdoc/effdoc-1519.pdf

Programme / Sub-programme / Module	5/5.2/EURATOM-RO FUSION		
Project type	RD	Continuing <input type="checkbox"/>	New <input checked="" type="checkbox"/>
EUROfusion Work Package	WPBB		Principal <input type="checkbox"/> Complementary <input checked="" type="checkbox"/>
Project title / Acronym	Romanian participation at EUROfusion WPBB and complementary research / WPBB2-RO		
Project duration	33 months		

Raport de cercetare *in extenso*

Detailed results

Calibri 11, la 1,15 randuri. Pagina A4, cu margini de 1" pe toate laturile.

Textul va fi impartit in sectiuni asa cum considera fiecare autor in parte. Font Calibri 11

Abstract

The nuclear data evaluation for deuteron-induced reactions and α -particle emission by neutron interactions is addressed within *Frontiers-in-Physics Research Topic "Nuclear data for fusion technology, from basic research to full-scale applications."* The status and open questions related to these subjects in the area of nuclear data for fusion technology, specifically for the nuclear design of the ITER fusion device, the European DEMO fusion reactor, and the IFMIF-DONES Irradiation Facility, are briefly reviewed. A firm demand for accurate cross-sections of reactions induced by neutrons and deuterons exists, in this respect, within a more enlarged energy range up to 50 MeV than for fission applications. The current requirements are closely met by the TENDL Evaluated Nuclear Data Library, settled using the TALYS nuclear model code, which is one of the most widely used codes in basic research and applications including nuclear fusion technology. However, further improvement of this data library has recently been suggested, while, with respect to fission applications, not only the aforementioned energy range but also the diversity of nuclear data for fusion technologies is plainly stretched. Consequently, the progress of nuclear data activities conducted more recently on deuteron-induced reactions and α -emission by neutron interactions, throughout the European Fusion Program and subsequent to previous achievements within F4E and EUROfusion programs, is particularly discussed for deuterons incident on ^{52}Cr , $^{54,56,58}\text{Fe}$, ^{59}Co , ^{96}Zr , ^{93}Nb , and $^{94,100}\text{Mo}$ as well as alpha-particle emission in neutron- and proton-induced reactions on $A \sim 60$ nuclei.

The major role of consistent parameter sets within analysis of neutron-induced alpha-particle emission, for the assessment of a possible difference between the optical model potentials (OMPs) which describe either alpha-particle elastic scattering and induced reactions or alpha-emission from excited compound nuclei, is shown. They are involved at variance with use of either empirical rescaling factors of the gamma and/or neutron widths or even combinations of all options of a computer code for main input

parameters. Suitable description of all competitive reaction channels, confirmed by a careful uncertainty analysis in order to avoid parameter ambiguities and/or error compensation, support further consideration of additional direct processes.

Deliverables

Report on nuclear-model assumption/parameter analysis and validation for evaluation of deuteron-induced reaction data of 95,96,97,98,100Mo target nuclei and alpha-particle optical model potential relevant for evaluation of neutron-induced alpha-emission on isotopes of interest with $A \sim 90$ (Zr, Nb, Mo) and to be issued and approved through EUROfusion IDM (part II)

Short Introduction and Objectives of Work

Following the design of the International Fusion Materials Irradiation Facility (IFMIF), accelerator-based D-Li neutron source, in order to produce an intense neutron field for testing ITER-fusion reactor candidate materials, the accurate deuteron nuclear data are critical for selecting and validating the best structural materials and a number of key technologies. Among the requested deuteron activation cross sections of great interest for shielding design as well as the radiation damage estimation, are those corresponding to hydrogen, tritium, and helium emission leading to "gas bubbles accumulation", which through the surface swelling affect finally deteriorate the material properties. However, the systematics of deuteron activation cross sections, including those leading to gas accumulation, e.g. (d,p), (d,2p), (d,t), and (d,α), is modest in opposition to the case of neutrons. At the same time, even the newest evaluation predictions, e.g. TENDL-2021 [1], still show evident discrepancies in respect with the existing data.

There have been thus stressed out neglected peculiarities of the deuteron interaction process, whose minimization requests the completion of the theoretical frame of the deuteron-nucleus interaction analysis with the non-compound processes, direct interactions (DI), namely breakup (BU) and direct reactions (DR), in addition to pre-equilibrium emission (PE) and evaporation from compound nucleus (CN). The BU complexity is given by the addition to the primary deuteron-target nucleus interaction of a variety of nuclear reactions initiated by the nucleons following the deuteron BU [2]. Additionally, the importance of the deuteron BU increases with the target-nucleus mass and charge, so that it becomes dominant for heavy target nuclei at deuteron incident energies particularly around the Coulomb barrier [3]. Otherwise, the deuteron interaction with medium-mass target nuclei below and around the Coulomb barrier proceeds largely through stripping and pick-up DR mechanisms, while PE and CN become important at higher energies.

On the other hand, evaluation of neutron-induced alpha emission data on the basis of consistent nuclear model calculation of reaction cross sections, and using an optical potential providing a suitable description of the incident alpha-particle data within the mass range $45 < A < 209$ and then proved to describe also the most recent similar data published in the meantime [4]. However, in spite of becoming the default option of the widely-used code TALYS [5], there remained still open questions concerning its suitability to account of the alpha-emission [6].

Description of Results

A comparative analysis of the experimental (d,p), (d,2p), (d,xn2p), and (d,xn) excitation functions, the model calculations, and the evaluations predictions has been carried on within this work

in order to emphasize the role of deuteron BU and stripping reactions for the hydrogen gas accumulation process. The physical picture of the deuteron BU in the Coulomb and nuclear fields of the target nucleus being recently emphasized [3], only particular points are mentioned here. They concern the two distinct BU processes, i.e. the elastic breakup (EB) in which the target nucleus remains in its ground state and none of the deuteron constituents interacts with it, and the inelastic breakup or breakup fusion (BF), where one of these deuteron constituents interacts nonelastically with this nucleus. Apart from the BU contributions to deuteron interaction, an increased attention has been devoted to the DR, stripping and pick-up processes, in spite of related very poor attention or being even not accounted so far in deuteron activation analysis.

The calculation of the (d,p) stripping mechanism contribution has been performed using the distorted-wave Born approximation (DWBA) method. The post form distorted-wave transition amplitudes and the finite-range interaction have been considered in this respect. The analysis excitation functions of the DR components, the total DR, BU, and their sum DI, for the deuteron interaction with $A=50-100$ target nuclei is stressing out the steep increase of the DI excitation functions at low incident energy, summing the DR and BU contributions, while above 20 MeV the BU remains the dominant contributor. It has to be pointed out the maximum of the (d,p) and (d,n) stripping excitation functions around 8-12 MeV, their contributions being essential for describing the measured activation functions corresponding to the first-chance emitted particles.

At the same time, while the previous alpha-emission analysis [4] took the advantage of quite useful recent data of low-lying states feeding in neutron-induced reactions on Fe, Co, Cu, and Zn nuclei, similar ones for the stable Ni isotopes are additionally quite useful. Thus, the issue of additional reaction channels able to increase the alpha-emission cross sections, beyond the statistical predictions, may prove similar to that pointed out formerly [7]. A suitable account of the measured alpha-emission cross sections at the Giant Quadrupole Resonance (GQR) energies of excited nuclei, in addition to the CN component, has also been attributed to a like-GQR component. However, before a definite consideration of additional mechanisms (DR, GQR), no empirical rescaling factors of the gamma and/or neutron widths should be used but consistent parameter sets already validated by analysis of other independent data (e.g. [4,6]).

Moreover, a careful uncertainty analysis should be concerned in order to avoid parameter ambiguities and/or error compensation effects due to less accurate model parameters. The consistent set of (i) nuclear level density (NLD) parameters, (ii) nucleon and (iii) gamma-ray transmission coefficients were established or validated using distinct measured data as low-lying levels and average s-wave nucleon-resonance spacings D_0 , neutron total cross sections, s- and p-wave neutron strength functions and potential scattering radius R' , (p,n) and (p,gamma) reaction cross sections, radiative strength functions (RSF), and average s-wave radiation widths, respectively. Fit of the error-bar limits of D_0 data has also been used to provide limits of the consequent level-density parameter a and g.s. shift Δ , corresponding to a spin cutoff factor with a variable moment of inertia [4,6]. For nuclei without resonance data, a -value average spread has been considered. Finally, the a and Δ limits have also been used within HF calculations to illustrate the NLD effects on the calculated cross-section uncertainty bands.

A comparison of these bands with calculated results obtained using the nucleon OMP, while energy-dependent real potential geometry of these OMPs is used in this work, is also included. Both neutron- and proton-OMP effects are larger than NLD effects, the latter obviously increasing with energy.

Altogether, the present work, devoted to the comparative analysis measurements, model calculations, and evaluation predictions corresponding to (d,p), and (d,2p) activation cross sections meets the high requests related to the estimation of the material damages and radioactivity risks raised by the design of the IFMIF accelerator structural components [8]. At the same time, requirements for new measurements for completion of the large gaps of (d,2p) data on specific nuclei along the priority list of candidate materials for ITER/IFMIF are obvious too. On the other hand, while no empirical rescaling factors of the gamma and/or neutron widths were used, and NLD, OMP, and PE effects have been shown to prove the alpha-particle OMP as the main CN parameter [9-12], the recent (n,alpha) data remain truly under-predicted for incident energies <9-12 MeV.

Conclusions

The overall agreement between the measured data and model calculations sustains the theoretical frame of reaction mechanisms taken into account for the deuteron-nucleus interaction, emphasizing the key role of direct interactions, i.e. the breakup and the stripping processes [13,14]. Neglecting these reaction-mechanism contributions to the deuteron activation cross-section estimation, discrepancies still shown by the current evaluation predictions are in order [8]. Finally, the strongest point of the consistent theoretical frame associated to the analysis of the deuteron-nucleus interactions, supported by advanced codes, is the improved predictability if no data exist.

Due consideration of the uncertainty bands for the CN+PE calculated cross sections has also been closely related to the error bars of the independent data fitted in order to establish the consistent parameter set. The need of additional reaction mechanisms to be taken into account is thus pointed out [13].

The involvement of early-stage researchers, making thus possible a transfer of knowledge from older to the new generation of Romanian scientists, was however not fulfilled because no appropriate application has been received until now following the corresponding advertisements posted at www.euraxess.ro/jobs/814405 and <https://jobs.research.gov.ro/anunt.php?id=5138>.

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References

- [1] A. J. Koning and D. Rochman, TENDL-2021: TALYS-based evaluated nuclear data library, https://tendl.web.psi.ch/tendl_2021/tendl2021.html

- [2] M. Avrigeanu, E. Šimečková, U. Fischer, J. Mrázek, J. Novak, M. Štefánik, C. Costache, and V. Avrigeanu, *Phys. Rev. C* **101**, 024605 (2020); E. Šimečková, M. Avrigeanu, J. Mrázek, J. Novak, M. Štefánik, C. Costache, and V. Avrigeanu, *Phys. Rev. C* **104**, 044615 (2021).
- [3] M. Avrigeanu, W. von Oertzen, R.A. Forrest, A.C. Obreja, F.L. Roman, and V. Avrigeanu, *Fusion Eng. Design* **84**, 418 (2009); M. Avrigeanu and A. M. Moro, *Phys. Rev. C* **82**, 037601 (2010); M. Avrigeanu, V. Avrigeanu, and A.J. Koning, *ibid.* **85**, 034603 (2012); M. Avrigeanu and V. Avrigeanu, *ibid.* **92**, 021601(R) (2015); M. Avrigeanu and V. Avrigeanu, *ibid.* **95**, 024607 (2017).
- [4] V. Avrigeanu, M. Avrigeanu, and C. Manulescu, *Phys. Rev. C* **90**, 044612 (2014); V. Avrigeanu and M. Avrigeanu, *Phys. Rev. C* **94**, 024621 (2016); *ibid.* **99**, 044613 (2019).
- [5] A. J. Koning, S. Hilaire, and S. Goriely, *TALYS-1.96 - A nuclear reaction program*; <http://www.talys.eu/>
- [6] V. Avrigeanu and M. Avrigeanu, *Phys. Rev. C* **91**, 064611 (2015); *ibid.* **96**, 044610 (2017).
- [7] V. Avrigeanu and M. Avrigeanu, *Eur. Phys. J. A* **57**, 54 (2021).
- [8] M. Avrigeanu, D. Rochman, A. J. Koning, U. Fischer, D. Leichtle, C. Costache, and V. Avrigeanu. *Eur. Phys. J. A* **58**, 3 (2022).
- [9] V. Avrigeanu and M. Avrigeanu, *Eur. Phys. J. A* **58**, 189 (2022).
- [10] M. Avrigeanu and V. Avrigeanu, *Phys. Rev. C* **107**, 034613 (2023).
- [11] V. Avrigeanu and M. Avrigeanu, *Front. Phys.* **11**, 1142436 (2023) (part of the *Research Topic on Nuclear Data for Fusion Technology from Basic Research to Full-Scale Applications*, <https://www.frontiersin.org/research-topics/39045/nuclear-data-for-fusion-technology-from-basic-research-to-full-scale-application>).
- [12] V. Avrigeanu and M. Avrigeanu, *Front. Phys.* **12**, 1247311 (2023) (part of the *Research Topic on Cross Section Data of Interest for Nuclear Astrophysics: Experimental and Theoretical Status, and Perspectives*. <https://www.frontiersin.org/research-topics/51270/cross-section-data-of-interest-for-nuclear-astrophysics-experimental-and-theoretical-status-and-perspectives#overview>).

Papers / Conferences

- [13] M. Avrigeanu and V. Avrigeanu, *Structural material nuclear data basic research*, *Front. Phys.* **11**, 1172697 (2023), <https://doi.org/10.3389/fphy.2023.1172697> (part of the *Research Topic on Nuclear Data for Fusion Technology from Basic Research to Full-Scale Applications*, <https://www.frontiersin.org/research-topics/39045/nuclear-data-for-fusion-technology-from-basic-research-to-full-scale-application>)
- [14] M. Avrigeanu and V. Avrigeanu, *Due consideration of the breakup and direct reaction mechanisms within (d,p) , $(d,2p)$, $(d,xn2p)$, and (d,xn) reactions*, in *Proc. 16th Varenna Conference on Nuclear Reaction Mechanisms (NRM2023)*, Varenna, Italy, June 11-16, 2023, F. Cerutti and T. Kawano (Eds.), <https://indico.cern.ch/event/1132769/>; EPJ Web of Conf. (accepted, Oct. 2023)

ANEXA 1.B Indicatori de realizare intermediara/finala

Tip indicator	Numar	Scurta descriere (daca este cazul)
Numar de articole stiintifice in reviste si volume indexate ISI	2	Front. Phys. 11 :1172697 (2023) EPJ Web of Conf. (accepted, Oct. 2023)
Numar de articole stiintifice în reviste indexate în alte baze de date internaționale recunoscute		
Numar articole publicate in top 10% cele mai citate publicatii		
Numar de brevete obtinute la nivel national si international		
Numar de brevete in curs de obtinere la nivel national si international		
Numar de tehnologii elaborate/transferate in urma Colaborarii la EUROfusion		
Numar de modele experimentale/prototitpuri		
Numarul de posturi de cercetatori echivalent norma intreaga (ENI) sustinute *		
Numarul de cercetatori cu doctorat sustinuti *	2	
Numarul de ingineri sustinuti *	1	
Numarul de tehnicieni sustinuti *		
Numarul personalului economic/administrativ sustinut *	1	
Numarul de doctoranzi sustinuti *		
Numar de masteranzi sustinuti *		
Numarul de participari la experimente EUROfusion efectuate*		
Numar de conferinte organizate*		
Numar de participari la Conferinte Internationale*	2	
Numar de prezentari la Conferinte Internationale		
Numar de postere prezentate la Conferinte Internationale*		
Numar de participanti la Workshopuri*		
Numar de prezentari orale la Workshopuri		
Numar de postere prezentate la Workshopuri		
Numărul participanților la întruniri de proiect în cadrul contractelor EUROfusion		
Numarul de proiecte Orizont 2020 (inclusiv cele ale partenerilor daca este cazul)		
Numarul de evenimente de comunicare si popularizare a stiintei sustinute*		
Numar de cursuri de instruire sau perfectionare realizate		
Altele (specificati)		

*) din Fondurile Programului

Director de proiect,

Dr. Avrigeanu Vlad

**Institutul National de Cercetare-Dezvoltare pentru
Fizica si Inginerie Nucleara „Horia Hulubei”**

**PROCES VERBAL DE AVIZARE INTERNA A LUCRARILOR DE
CERCETARE-DEZVOLTARE SI INOVARE (PVAI)**

Comisia de avizare constituita prin Decizia nr. 266 din 01.04.2022 luand in examinare lucrarile efectuate de colectivul departamentului de Fizică Nucleară al IFIN-HH la **partea Complementara a proiectul “Participarea Romaniei la EUROfusion WPBB si cercetari complementare”** (WPBB2-RO) in cadrul etapei nr. II, care fac obiectul contractului nr. EU-01/03.01.2022, act aditional nr. 1/2022 incheiat cu Institutul de Fizica Atomica, a constatat urmatoarele:

- a) Lucrarile executate corespund clauzelor contractuale;
- b) Toate documentele necesare efectuarii platii exista si sunt corect intocmite;
- c) Concluziile lucrarii, principalele rezultate obtinute si datele privind efectuarea cheltuielilor sunt prezentate in Raportul intermediar de activitate si in documentele sale insotitoare;
- d) Planificarea activitatilor si resurselor aferente realizarii etapei urmatoare de derulare a proiectului, prezentata in Raportul intermediar de activitate, este corespunzatoare realizarii obiectivului propus si in concordanta cu prevederile contractului;
- e) Cota de cofinantare realizata in faza de executie curenta este de.....lei.

Comisia avizeaza **FAVORABIL** lucrarile si documentele si considera ca pot fi prezentate pentru evaluare la Institutul de Fizica Atomica – IFA.

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