

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 eficace ale reactiilor induse de deuteroni pe 95,96,97,98,100Mo, si analizei emisiei alfa indusa de neutroni pe izotopi de interes cu A~90 (Zr, Nb, Mo) si stabiliti si aprobati prin EUROfusion IDM.
3. Perioada de executie: Ianuarie-Decembrie 2022
4. Obiectivele fazei de executie:

Aceste obiective au fost in fapt cele ale *'deliverabilelor'* BB-S.05.02-T001-D004/D005/D017/D018, a caror responsabilitate a revenit autorilor raportului de fata, constand in **analiza si discutia rezultatelor de calcule de model** de reactii nucleare (Secs. 1-3 ale Refs. [1-5]) realizate **pe baza ipotezelor si parametrilor** de model formand in aceeasi perioada obiectul activitatii IFIN-HH (Secs. 4-6 ale Refs. [1-5]) precum si al componentei complementare a proiectului de fata in **cazuri particulare de ipoteze si parametri** de model [12,13], 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 eficace ale reactiilor induse de deuteroni pe 95,96,97,98,100Mo (BB-S.05.02-T001-D004/D017), si analizei emisiei alfa indusa de neutroni pe izotopii stabili de interes cu A~90 (ai elementelor Zr, Nb, si Mo) precum si in cazul particular al primei masuratori directe a sectiunii eficace a reactiei $^{59}\text{Cu}(p,\alpha)^{56}\text{Ni}$ la energia incidenta de 6 MeV (BB-S.05.02-T001-D005/D018).
5. Rezumatul fazei (maxim 1 pagina, atât în limba română cât și în limba engleză);

(RO) Extinderea codurilor de modele nucleare a fost considerata necesara in vederea evaluarii avansate a sectiunilor eficace ale reactiilor induse de deuteroni pe izotopii stabili 95,96,97,98,100Mo, avand obiectivul final al acestei activitati realizate in urmatoorii doi ani pentru Mo. Luarea in considerare a analizei tuturor datelor experimentale disponibile pentru izotopii stabili vizati, pentru energiile incidente de pana la 50 MeV, a fost realizata in acest sens dand atentie contributiilor tuturor mecanismelor de reactie implicate precum 'ruperea' deuteronului ('breakup', BU), reactiile directe (DR) de tip 'stripping' si 'pick-up', procesele de emisie la prechilibru si evaporare, cu rezultatele prezentate in formatul codului TALYS (ca, de exemple, pentru Mn in Phys. Rev. C **101**, 024605, 2020). 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). Diferitele reactii initiate de asemenea de neutronii si protonii proveniti din 'ruperea' deuteronului sunt de luat in considerare suplimentar reactiilor induse de deuteronii insisi. Analiza reactiilor (d,p) precum si a altor reactii directe care nu se regasesc in rezultatele codului TALYS a fost realizata utilizand codul FRESCO si datele disponibile pentru obtinerea factorilor spectroscopici necesari in acest scop, la fel ca si eventuale dezvoltari ale codului TALYS si/sau activitati de verificare si validare (V&V) ale sectiunilor eficace ale deuteronilor in cadrul proiectului 'ENS/EUROfusion'.

Pe de alta parte, validarea potentialului de model optic (OMP) pentru particule alfa relevant pentru evaluarea datelor de productie de gaze si defecte de iradiere a fost obtinuta prin analiza datelor de emisie alfa indusa de neutroni rapizi pe nuclelele tinta $^{90,91,92,94,96}\text{Zr}$, ^{93}Nb , si $^{92,95,98,100}\text{Mo}$. In acest scop au fost realizate calcule consistente de modele nucleare ale sectiunilor eficace de reactie, utilizand valori ale parametrilor de model stabiliti prin analiza unor date diferite independente precum si fara implicarea unor factori empirici de renormare pentru emisia de particule alfa si/sau nucleoni, pentru energii incidente de pana la ~21 MeV si toate datele disponibile pentru diferitele canale de reaction si izotopi ai unui element. Un acord satisfactor a fost astfel obtinut intre sectiunile eficace masurate ale reactiilor (n,a) induse pe

izotopii sus-mentionati, incluzand si toate canalele de reactie concurente, cu calcule consistente de modele nucleare folosind OMP dezvoltat anterior in IFIN-HH.

In acelasi timp, o supraestimare asumata recent cu un factor de 2 a primei masuratori directe a sectiunii eficace a reactiei $^{59}\text{Cu}(p,\alpha)^{56}\text{Ni}$ la energia incidenta de 6 MeV (Phys. Rev. C **104**, L042801, 2021) a facut necesara o analiza similara pentru a sustine potentialul de model optic (OMP) pentru particule alpha care este si optiunea standard a codului TALYS si, astfel, relevant pentru evaluarea datelor de productie de gaze si defecte de iradiere pentru neutronii de fuziune. In final am aratat (Phys. Rev. C **106**, 024615, 2022) ca noua masuratoare faciliteaza, in conditii unice, verificarea si pentru nuclee dincolo de linia de stabilitate a componentelor de potential atat real ('isoscalar' si 'isovector') cat si imaginar anomal, precum si a potentialului pentru particule alfa.

Fisierele incluzand rezultatele actuale ca si cele anterioare corespunzand reactiilor induse pe izotopii stabili ai elementelor Cr, Mn, Fe, Ni, and Cu, care pot fi considerate noi evaluari ale reactiilor induse de neutroni si protoni, precum si de deuteroni - prezentand un acord mai bun si consistent cu datele experimentale microscopice, fata de cele mai recente evaluari TENDL – urmeaza a fi transmise in functie de procesarea noilor biblioteci de date nucleare evaluate.

(EN) Improvements of the nuclear model code capabilities have been found necessary in order to extend the evaluated deuteron-induced reaction cross sections of the stable isotopes $^{95,96,97,98,100}\text{Mo}$, in view of a final work concerning natural Mo within next two years. Inclusion of the analysis of all available data for the related stable isotopes, up to 50 MeV has been carried out in this respect, taking properly into account the contributions of all involved reaction mechanisms as the breakup (BU), stripping and pick-up direct reactions (DR), pre-equilibrium and evaporation processes, with the results provided in TALYS code format (as, e.g., for Mn in Phys. Rev. C **101**, 024605, 2020). 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 data description validated the correctness of our theoretical procedure for deuteron activation cross section calculations. Various reactions initiated also by BU neutrons and protons, i.e. the inelastic BU component, should be taken into account in addition to those of deuterons themselves. The assessment of (d,p) and other direct-reactions not included within TALYS output has been carried on by using the code FRESKO and the available data for establishment of the needed spectroscopic factors, as well as eventually further development of related procedures required during the TALYS development and/or deuteron cross-section V&V activities within ENS/EUROfusion.

On the other hand, validation of the optical model potential (OMP) for alpha particles relevant for the evaluation of gas production and radiation damage data has been obtained by analysis of fast-neutron induced alpha emission data of the target nuclei $^{90,91,92,94,96}\text{Zr}$, ^{93}Nb , and $^{92,95,98,100}\text{Mo}$. Consistent nuclear model calculation of reaction cross sections have been concerned in this respect by using model parameters established through analysis of distinct independent data and with no empirical rescaling factors of the α -particle and/or nucleon widths, performed for incident energies up to ~ 21 MeV and all available data for various reaction channels and isotopes of an element. A suitable agreement has thus been obtained between measured cross sections of (n,alpha) reactions on the above-mentioned isotopes, including all competitive reaction channels, with consistent model calculations using the OMP previously developed at IFIN-HH.

At the same time, recently assumed overestimation of a first direct measurement for $^{59}\text{Cu}(p,\alpha)^{56}\text{Ni}$ reaction cross section by a factor of 2 at an energy of ~ 6 MeV (Phys. Rev. C **104**, L042801, 2021) made necessary the related analysis in order to fully support the alpha-particle optical-model potential being the default option in this respect of TALYS and, thus, currently involved within evaluation of gas production and radiation damage data of fusion neutrons. Finally it has been shown (Phys. Rev. C **106**, 024615, 2022) that the new measurement provides, under unique conditions, tests of proton both real-potential components (isoscalar and isovector) and the anomalous imaginary potential, as well as the above-mentioned alpha-particle OMP, also for nuclei off the line of stability.

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

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 sunt prezentate în cele 5 lucrări [1-5] reprezentând deliverabilele BB-S.05.02-T001-D004/D005/D017/D018, 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] V. Avrigeanu and M. Avrigeanu, *Validation of an optical potential for incident and emitted low-energy alpha-particles in the A60 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), doi:10.1140/epja/198 s10050-020-00336-0; <https://link.springer.com/article/10.1140/epja/s10050-020-00336-0>
- [2] M. Avrigeanu, D. Rochman, A. J. Koning, U. Fischer, D. Leichtle, C. Costache, and V. Avrigeanu. *Advanced breakup nucleon enhancement of deuteron-induced reaction cross sections*. Eur. Phys. J. A **58**, 3 (2022), doi:10.1140/epja/s10050-021-00659-6; <https://link.springer.com/article/10.1140/epja/s10050-021-00659-6>
- [3] V. Avrigeanu and M. Avrigeanu, *Validation of an optical potential for incident and emitted low-energy alpha-particles in the A60 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), doi:10.1140/epja/s10050-022-00831-6; <https://link.springer.com/article/10.1140/epja/s10050-022-00831-6>
- [4] 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), doi:10.1103/PhysRevC.106.024615; <https://doi.org/10.1103/PhysRevC.106.024615>
- [5] 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*, Report EUROFUSION WPBB-PR(22) 33196, Oct. 11, 2022, <https://users.euro-fusion.org/webapps/pinboard/EFDA-JET/journal/index.html>, No. 499, Oct. 7 (2022); submitted for publication in Phys. Rev. C.
- [6] V. Avrigeanu and M. Avrigeanu, *Evaluation of fast-neutron induced alpha emission for A~90 nuclei*, Report EFFDOC-1472, OECD/NEA Data Bank, JEFF Meeting, April 26, 2022, https://www.oecd-nea.org/dbdata/nds_effdoc/effdoc-1472.pdf
- [7] M. Avrigeanu and V. Avrigeanu, *Progress report on analysis of deuteron-induced reactions on structural materials*, Report EFFDOC-1473, OECD/NEA JEFF Meeting, April 26, 2022, https://www.oecd-nea.org/dbdata/nds_effdoc/effdoc-1473.pdf
- [8] V. Avrigeanu and M. Avrigeanu, *Charged-particle optical potentials proved besides the stability line*, Report JEFDOC-2137, OECD/ NEA JEFF Meeting, April 26, 2022, https://www.oecd-nea.org/dbdata/nds_jefdoc/jefdoc-2137.pdf
- [9] M. Avrigeanu and V. Avrigeanu, *Analysis of the deuteron activation of neutron-rich Mo nuclei*, Report JEFDOC-2137, OECD/ NEA JEFF Meeting, April 26, 2022, https://www.oecd-nea.org/dbdata/nds_jefdoc/jefdoc-2138.pdf
- [10] M. Avrigeanu and V. Avrigeanu, *Progress report on analysis of deuteron-induced reactions on structural materials*, Report EFFDOC-1487, OECD/NEA JEFF Meeting, Nov. 24, 2022, https://www.oecd-nea.org/dbdata/nds_effdoc/effdoc-1487.pdf

- [11] 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, 2022, https://www.oecd-nea.org/dbdata/nds_effdoc/effdoc-1488.pdf
- [12] M. Avrigeanu and V. Avrigeanu, *Role of direct interactions in (d,p) and (d,2p) reactions*, submitted to EPJ Web of Conf. (14.10.2022); oral talk at [Int. Conf. on Nucl. Data for Sci. and Tech. \(ND2022\)](#), July 25-29, 2022, Sacramento, California, US.
- [13] V. Avrigeanu and M. Avrigeanu, *Additional reaction mechanisms to statistical alpha-emission and the related optical-potential validation*, submitted to EPJ Web of Conf. (15.10.2022) ; oral talk at [Int. Conf. on Nucl. Data for Sci. and Tech. \(ND2022\)](#), July 25-29, 2022, Sacramento, California, US

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, including eventually evaluated data files, on evaluation of deuteron-induced 98,100Mo cross sections 2021 Deliverable BB-S-05.02-T001-D004 (Dec. 31, 2021, moved to April 30, 2022) / BB-S-05.02-T004-D002 (May 30, 2022)	
Reporting period	January-May 2022	
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.

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

(RO) Extinderea codurilor de modele nucleare a fost considerata necesara in vederea evaluarii avansate a sectiunilor eficace ale reactiilor induse de deuteroni pe izotopii stabili 98,100Mo, avand obiectivul final al acestei activitati realizate in urmatoorii doi ani pentru Mo. Luarea in considerare a analizei tuturor datelor experimentale disponibile pentru izotopii stabili vizati, pentru energiile incidente de pana la 50 MeV, a fost realizata in acest sens dand atentie contributiilor tuturor mecanismelor de reactie implicate precum 'ruperea' deuteronului ('breakup', BU), reactiile directe (DR) de tip 'striping' si 'pick-up', procesele de emisie la prechilibru si evaporare, cu rezultatele prezentate in formatul codului TALYS (ca, de exemple, pentru Mn in Phys. Rev. C **101**, 024605, 2020). Descrierea datelor experimentale a confirmat corectitudinea metodei teoretice pentru calculul sectiunilor eficace de activare cu deuteroni. Diferitele reactii initiate de asemenea de neutronii si protonii proveniti din 'ruperea' deuteronului sunt de luat in considerare suplimentar reactiilor induse de deuteronii insisi. Analiza reactiilor (d,p) precum si a altor reactii directe care nu se regasesc in rezultatele codului TALYS a fost realizata utilizand codul FRESCO si datele disponibile pentru obtinerea factorilor spectroscopici necesari in acest scop, la fel ca si eventuale dezvoltari ale codului TALYS si/sau activitati de verificare si validare (V&V) ale sectiunilor eficace ale deuteronilor in cadrul proiectului 'ENS/EUROfusion'.

Fisierele incluzand rezultatele actuale ca si cele anterioare corespunzand reactiilor induse de deuteroni pe izotopii stabili ai elementelor Cr, Mn, Fe, Ni, si Cu, care pot fi considerate 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 – urmeaza a fi transmise in functie de procesarea noilor biblioteci de date nucleare evaluate.

(EN) Improvements of the nuclear model code capabilities have been found necessary in order to extend the evaluated deuteron-induced reaction cross sections of the stable isotopes $^{98,100}\text{Mo}$, in view of a final work concerning natural Mo within next two years. Inclusion of the analysis of all available data for the related stable isotopes, up to 50 MeV has been carried out in this respect, taking properly into account the contributions of all involved reaction mechanisms as the breakup (BU), stripping and pick-up direct reactions (DR), pre-equilibrium and evaporation processes, with the results provided in TALYS code format (as, e.g., for Mn in Phys. Rev. C **101**, 024605, 2020). The data description validated the correctness of our theoretical procedure for deuteron activation cross section calculations. Various reactions initiated also by BU neutrons and protons, i.e. the inelastic BU component, should be taken into account in addition to those of deuterons themselves. The assessment of (d,p) and other direct-reactions not included within TALYS output has been carried on by using the code FRESKO and the available data for establishment of the needed spectroscopic factors, as well as eventually further development of related procedures required during the TALYS development and/or deuteron cross-section V&V activities within ENS/EUROfusion.

Files including the present results as well the previous ones corresponding to reactions on the isotopes of Cr, Mn, Fe, Ni, and Cu, that 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 - are to be provided in relation to further processing of new evaluated-data libraries.

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, including eventually evaluated data files, on analysis of neutron-induced alpha-emission on isotopes of interest with $A \sim 90$ (Zr, Nb, Mo). Deliverable BB-S-05.02-T001-D005 (Dec. 31, 2021, moved to April 30, 2022) / BB-S-05.02-T004-D001 (May 30, 2022)	
Reporting period	January-May 2022	
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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Rezumatele in limba romana si engleza se fac pe pagini separate.

(RO) Validarea potentialului de model optic (OMP) pentru particule alpha relevant pentru evaluarea datelor de productie de gaze si defecte de iradiere a fost obtinuta prin analiza datelor de emisie alfa indusa de neutroni rapizi pe nucleele tinta $^{90,91,92,94,96}\text{Zr}$, ^{93}Nb , si $^{92,95,98,100}\text{Mo}$. In acest scop au fost realizate calcule consistente de modele nucleare ale sectiunilor eficace de reactie, utilizand valori ale parametrilor de model stabiliti prin analiza unor date diferite independente precum si fara implicarea unor factori empirici de renormare pentru emisia de particule α si/sau nucleoni, pentru energii incidente de pana la ~ 21 MeV si toate datele disponibile pentru diferitele canale de reaction si izotopi ai unui element. Un acord satisfacator a fost astfel obtinut intre sectiunile eficace masurate ale reactiilor (n,α) induse pe izotopii sus-mentionati, incluzand si toate canalele de reactie concurente, cu calcule consistente de modele nucleare folosind OMP dezvoltat anterior in IFIN-HH in cadrul EU/F4E 'Nuclear Data Consortium'. Luarea optima in considerare suplimentara s-a dovedit in final pentru (i) popularea starilor excitate joase ale nucleelor reziduale prin reactii directe (DR) de tip 'pick-up', si (ii) un process similar 'Giant Quadrupole Resonance' (GQR) care poate contribui la descrierea marimii sectiunilor eficace ale unor reactii (n,α) la energiile GQR ale nucleelor excitate respective.

Fisierele incluzand rezultatele actuale ca si cele anterioare corespunzand reactiilor induse pe izotopii stabili ai elementelor Fe, Co, Ni, Cu, si Zn, care pot fi considerate 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 – urmeaza a fi transmise in functie de procesarea noilor biblioteci de date nucleare evaluate.

(EN) Validation of the optical model potential (OMP) for alpha particles relevant for the evaluation of gas production and radiation damage data has been obtained by analysis of fast-neutron induced alpha emission data of the target nuclei $^{90,91,92,94,96}\text{Zr}$, ^{93}Nb , and $^{92,95,98,100}\text{Mo}$. Consistent nuclear model calculation of reaction cross sections have been concerned in this respect by using model parameters established through analysis of distinct independent data and with no empirical rescaling factors of the α -particle and/or nucleon widths, performed for incident energies up to ~ 21 MeV and all available data for various reaction channels and isotopes of an element. A suitable agreement has thus been obtained between measured cross sections of (n,α) reactions on the above-mentioned isotopes, including all competitive reaction channels, with consistent model calculations using the OMP previously developed at IFIN-HH within EU/F4E Nuclear Data Consortium. Additional assumptions proved successful have concerned (i) the pick-up direct-reaction (DR) population of the low-lying levels of residual nucle, and (ii) like Giant Quadrupole Resonance (GQR) processes that could make possible the account of some (n,a) reaction cross sections around the GQR energies of the related excited nuclei.

Files including the present results as well the previous ones corresponding to reactions on the isotopes of Fe, Co, Ni, Cu, and Zn, that 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 - are to be provided in relation to further processing of new evaluated-data libraries.

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 95,96,97Mo cross sections Deliverable BB-S-05.02-T001-D017 (Feb. 23 - Dec. 31, 2022)	
Reporting period	February 23 - December 31, 2022	
Authors	Marilena Avrigeanu ¹ , Vlad Avrigeanu ¹	
Affiliation	<i>Horia Hulubei National Institute for Physics and Nuclear Engineering, IFIN-HH</i>	

Summary

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(RO) Extinderea codurilor de modele nucleare, necesara in vederea evaluarii avansate a sectiunilor eficiente ale reactiilor induse de deuteroni pe izotopii stabili 95,96,97Mo avand obiectivul final al acestei activitati realizate pentru Mo, a fost realizata prin luarea in considerare a analizei tuturor datelor experimentale disponibile pentru izotopii stabili vizati, 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 '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 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, si 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 $^{95,96,97}\text{Mo}$ in view of a final work concerning natural Mo, have been considered including the analysis of all available data for these Mo stable isotopes 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.

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-T001-D018 (Feb. 23 - Dec. 31, 2022)	
Reporting period	February 23 - December 31, 2022	
Authors	Vlad Avrigeanu ¹ , Marilena Avrigeanu ¹	
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Summary

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

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

(RO) O supraestimare asumata recent cu un factor de 2 a primei masuratori directe a sectiunii eficace a reactiei $^{59}\text{Cu}(p,\alpha)^{56}\text{Ni}$ la energia incidenta de 6 MeV (Phys. Rev. C **104**, L042801, 2021) a facut necesara o analiza similara pentru a sustine potentialul de model optic (OMP) pentru particule alpha care este si optiunea standard a codului TALYS si, astfel, relevant pentru evaluarea datelor de productie de gaze si defecte de iradiere pentru neutronii de fuziune. In final am aratat (Phys. Rev. C **106**, 024615, 2022) ca noua masuratoare faciliteaza, in conditii unice, verificarea si pentru nuclee dincolo de linia de stabilitate a componentelor de potential atat real ('isoscalar' si 'isovector') cat si imaginar anomal, precum si a potentialului pentru particule alfa. A fost astfel demonstrata in plus corectitudinea acestui OMP al particulelor alfa, ulterior descrierea corespunzatoare a sectiunilor eficace ale reactiilor (n,alpha) si (p,alpha) pe izotopii stabili $^{63,65}\text{Cu}$ ai aceluiasi element, care au format obiectul unei lucrari anterioare in cadrul proiectului de fata (Eur. Phys. J A **57**, 54, 2021; **58**, 189, 2022). In final, validarea unui OMP al particulelor alfa in cazul descrierii corespunzatoare a emisiei alfa in reactii induse de neutroni ca si de protoni a completat cazul datelor similare pentru izotopii stabili ai Fe, Ni, Cu, Zn, Zr, Nb, si Mo. 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) A recently assumed overestimation of a first direct measurement for $^{59}\text{Cu}(p,\alpha)^{56}\text{Ni}$ reaction cross section by a factor of 2 at an energy of ~ 6 MeV (Phys. Rev. C **104**, L042801, 2021) made necessary the related analysis in order to fully support the alpha-particle optical-model potential being the default option in this respect of TALYS and, thus, currently involved within evaluation of gas production and radiation damage data of fusion neutrons. Finally it has been shown (Phys. Rev. C **106**, 024615, 2022) that the new measurement provides, under unique conditions, tests of proton both real-potential components (isoscalar and isovector) and the anomalous imaginary potential, as well as the above-mentioned alpha-particle OMP, also for nuclei off the line of stability. This has been proved additionally to the correctness of this alpha-particle OMP for the suitable account of the (n,alpha) and (p,alpha) reaction cross sections on the stable isotopes $^{63,65}\text{Cu}$ of the same element making the object of a previous work within present task (Eur. Phys. J A **57**, 54, 2021; **58**, 189, 2022). Finally, validation of an alpha-particle OMP for neutron- as well as proton-induced alpha-emission has completed similar data account for Fe, Ni, Cu, Zn, Zr, Nb, and Mo stable isotopes. 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

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

Short Introduction and Objectives of Work

The IAP/IFIN-HH contribution to the PPPT nuclear data development - evaluation of neutron cross sections, radiation damage data and benchmarking, has had to include (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. 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 (e.g. Paper [1]). On the other hand, the evaluation of deuteron-induced reaction cross sections of ^{nat}Mo up to 50 MeV on the basis of the proper account of contributions of all involved reaction mechanisms as the breakup, stripping, pick-up, pre-equilibrium 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] 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 [5] 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 (Paper [2]).

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 $45 < A < 209$ and then proved to describe also the most recent similar data published in the meantime [3]. However, there remained still open questions concerning its suitability to account of the alpha-emission [4]. 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 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 (e.g., Paper [5]).

Description of Results

The consistent nuclear model analysis of deuteron-induced reactions on $^{95,96,97,98,100}\text{Mo}$ target nuclei proved the suitable account of all available experimental data provided that deuteron interactions involving BU, DR, PE and CN reaction mechanisms are considered. The corresponding results are shown and discussed (Meetings-Papers [2,4,5]).

Actually, the updated and completed code version TALYS-1.96 used in the present work can be used to provide more accurate deuteron-reaction data that are also eventually required during the deuteron cross-section V&V activities within ENS/EUROfusion, with addition of only the particular (d,p) reaction contribution to be obtained by using the code FRESCO.

On the whole, the enhancing effect of the BU mechanism is important mainly for describing the excitation functions for second and third chance emitted-particle channels. Particular comments concerned the inelastic BU contribution even larger than the PE+CN ones for the (d,2p) reaction for heavier nuclei at all incident energies, as well as (d,2n) reaction above 30 MeV, and even (d,3n) reaction just above the effective threshold. Moreover, the entire excitation functions of also (d,n), (d,p), and (d,t) would be not described without inelastic BU consideration despite of the dominant nature of the corresponding PE+CN components.

Comparisons of the theoretical results of the present work with measured excitation functions reported in the same references as well as previously have been discussed at the same time. Furthermore, the comparison of the experimental deuteron activation cross sections with our model calculations as well as the corresponding TENDL-2021 [6] evaluation supports the detailed theoretical treatment of deuteron interactions. The discrepancies between the measured data and that evaluation have been the result of overlooking the inelastic breakup enhancement and less appropriate treatment of stripping and pick-up processes.

At the same time, 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 $^{92,95,98,100}\text{Mo}$ (Paper [5]), including all competitive reaction channels, with consistent model calculations using the OMP [3] as well as the pick-up direct-reaction population of the low-lying levels of residual nuclei. Moreover, results of this work are compared with results of the TALYS-1.96 code [5] obtained by using global input parameters, and the most recent evaluated-data library TENDL-2021 [6], for an overall excitation function survey from both points of view of standard model calculations and advanced evaluations. It can be seen 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 (Meetings-Papers [1,3,6]).

A suitable account of the measured alpha-emission cross sections is provided, on the other hand, by an additional contribution at the GQR energy of $^{96,99}\text{Mo}$ 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, more similar cases to be concerned may help.

Conclusions

The overall agreement of the measured data and model calculations validates the description of nuclear mechanisms taken into account for deuteron-induced reactions on $^{95,96,97,98,100}\text{Mo}$, particularly the BU and DR that should be considered explicitly. The overall agreement between the measured data and model calculations supports the fact that major discrepancies shown by the current evaluations are due to missing the proper account of direct interactions. The consistent theoretical frame of the deuteron interactions supported by advanced codes associated to the nuclear reactions mechanisms provides predictability in addition to the use of various-order genuine approximations needed in applications.

Finally, it can be concluded that due consideration of all BU, DR, PE, and CN reaction mechanisms is indeed crucial for a consistent analysis of the deuteron-reaction measured data and even high production of proton-rich nuclei, while insufficient treatment and separation between different reaction mechanisms such as DR and BU components may be related to deviations between measurements and, e.g., advanced surrogate reaction studies. Completion of similar analysis for the rest of stable Mo isotopes will support better this conclusion as well as the further fusion technology needs.

Further account of additional reaction channels leading to increase of the alpha-emission cross sections, beyond the statistical predictions, has also concerned the DR pickup. The assessment of DR cross sections has been subject to available information on spectroscopic factors related to populated states, outgoing particle angular distributions, or at least differential cross-section maximum values.

On the other hand, recently assumed overestimation of a first direct measurement for $^{59}\text{Cu}(p,\alpha)^{56}\text{Ni}$ reaction cross section by a factor of 2 at an energy of ~ 6 MeV made necessary the related analysis in order to fully support the alpha-particle optical-model potential being the default option in this respect of TALYS and, thus, currently involved within evaluation of gas production and radiation damage data of fusion neutrons. Finally it has been shown (Paper [4]) that the new measurement provides, under unique conditions, tests of proton both real-potential components

(isoscalar and isovector) and the anomalous imaginary potential, as well as the above-mentioned alpha-particle OMP, also for nuclei off the line of stability.

Acknowledgement

This work has been carried out within the framework of the EUROfusion Consortium and has been received funding from the European Union's Horizon 2020 research innovation programme under grant agreement number 633053 and also from the Romanian National Education Minister under contract 2/23.02.2016. The reviews and opinion expressed herein do not necessarily reflect those of the European Commission.

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

Papers

- [1] V. Avrigeanu and M. Avrigeanu, *Validation of an optical potential for incident and emitted low-energy alpha-particles in the A60 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), doi:10.1140/epja/198_s10050-020-00336-0; <https://link.springer.com/article/10.1140/epja/s10050-020-00336-0>
- [2] M. Avrigeanu, D. Rochman, A. J. Koning, U. Fischer, D. Leichtle, C. Costache, and V. Avrigeanu. *Advanced breakup nucleon enhancement of deuteron-induced reaction cross sections*. Eur. Phys. J. A **58**, 3 (2022), doi:10.1140/epja/s10050-021-00659-6; <https://link.springer.com/article/10.1140/epja/s10050-021-00659-6>
- [3] V. Avrigeanu and M. Avrigeanu, *Validation of an optical potential for incident and emitted low-energy alpha-particles in the A60 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), doi:10.1140/epja/s10050-022-00831-6;
<https://link.springer.com/article/10.1140/epja/s10050-022-00831-6>

- [4] 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), doi:10.1103/PhysRevC.106.024615;
<https://doi.org/10.1103/PhysRevC.106.024615>
- [5] 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*, Report EUROFUSION WPBB-PR(22) 33196, Oct. 11, 2022, <https://users.euro-fusion.org/webapps/pinboard/EFDA-JET/journal/index.html>, No. 499, Oct. 7 (2022); submitted for publication in Phys. Rev. C.

Meetings

- [1] V. Avrigeanu and M. Avrigeanu, *Evaluation of fast-neutron induced alpha emission for $A\sim 90$ nuclei*, Report EFFDOC-1472, OECD/NEA Data Bank, JEFF Meeting, April 26, 2022, https://www.oecd-nea.org/dbdata/nds_effdoc/effdoc-1472.pdf
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- [3] V. Avrigeanu and M. Avrigeanu, *Charged-particle optical potentials proved besides the stability line*, Report JEFDOC-2137, OECD/NEA JEFF Meeting, April 26, 2022, https://www.oecd-nea.org/dbdata/nds_jefdoc/jefdoc-2137.pdf
- [4] M. Avrigeanu and V. Avrigeanu, *Analysis of the deuteron activation of neutron-rich Mo nuclei*, Report JEFDOC-2137, OECD/NEA JEFF Meeting, April 26, 2022, https://www.oecd-nea.org/dbdata/nds_jefdoc/jefdoc-2138.pdf
- [5] M. Avrigeanu and V. Avrigeanu, *Progress report on analysis of deuteron-induced reactions on structural materials*, Report EFFDOC-1487, OECD/NEA JEFF Meeting, Nov. 24, 2022, https://www.oecd-nea.org/dbdata/nds_effdoc/effdoc-1487.pdf
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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 95,96,97,98,100Mo, si a potentialului de model optic pentru particule alfa pentru evaluarea emisiei alfa indusa de neutroni pe izotopi de interes cu $A \sim 90$ (Zr, Nb, Mo) si stabiliti prin EUROfusion IDM
3. Perioada de executie: Ianuarie-December 2022
4. Obiectivele fazei de executie:

Aceste obiective au fost corelate cu cele ale 'deliverabilelor' BB-S.05.02-T001-D004/D005/D017/D018, 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. 1-3 ale Refs. [1-5]) realizate **pe baza ipotezelor si parametrilor** de model formand in aceeasi perioada obiectul activitatii IFIN-HH (Secs. 4-6 ale Refs. [1-5]), in timp ce aceasta componenta complementara a proiectului a vizat **cazuri particulare de ipoteze si parametri** de model (Refs. [12-13]), 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 eficace ale producerii de H prin reactii induse de deuteroni inclusiv pe izotopii 95,96,97,98,100Mo [12], si analiza importantei cunoasterii cat mai precise a parametrilor densitatii de nivele nucleare in evaluarea emisiei alfa indusa de neutroni rapizi [13].
5. Rezumatul fazei (maxim 1 pagina, atît în limba română cât și în limba engleză);

(RO) Necesitatile marite pentru date nucleare ale reactiilor induse de deuteroni sunt o consecinta directa a programelor strategice actuale de cercetare (ITER, IFMIF, SPIRAL2-NFS) care implica fascicule accelerate de deuteroni. In randul acestor solicitari de date ale reactiilor induse de deuteroni, foarte importante sunt sectiunile eficace ale reactiilor (d,p) si (d,2p) conducand la acumularea de bule de gaz (hidrogen) in materialele structurale. In opozitie cu situatia datelor nucleare pentru reactii induse de neutroni, sistematica sectiunilor eficace de activare a deuteronilor, incluzand pe cele corespunzand producerii si acumularii de gaze precum hidrogen, tritium, si heliu, este modesta in timp ce chiar si evaluarile cele mai recente prezinta discrepante evidente. In consecinta, aceasta lucrare este orientata spre completarea cadrului modelelor teoretice asociat analizei reactiilor (d,p) si (d,2p), in vederea imbunatatirii descrierii datelor experimentale existente si, astfel, a realizarii de previziuni teoretice pentru cazurile in care nu exista masuratori.

Pe de alta parte, a fost evidentiat rolul major al seturilor consistente de parametri de model pentru rezultatele analizelor de emisie a particulelor alfa. In particular a fost vizata posibila diferenta intre potentialele de model optic (OMPs) ce descriu fie imprastierea elastica si reactiile induse de particulele alfa, fie emisia acestora din nucleeele excitate in reactii nucleare. Analiza acestor cazuri a fost realizata in lucrarea de fata fara implicarea oricaror factori empirici de scalare ale largimilor de stari nucleare pentru emisia gama si/sau de nucleoni, precum si fara a apela la combinatii ale tuturor optiunilor posibile pentru principalii parametri de model ale unui cod de calcul. Descrierea corespunzatoare a tuturor canalelor de reactie in competitie cu emisia alfa, confirmata printr-o analiza detaliata a incertitudinilor asociate, pentru a evita compensarea ambiguitatilor de model si/sau a erorilor diferitilor parametri, permite in final si luarea corecta in considerare a unor procese nucleare directe suplimentare.

(EN) Enlarged deuteron-data needs follow the demands of on-going strategic research programs (ITER, IFMIF, SPIRAL2-NFS) using deuteron beams. Among these requested deuteron-data, the (d,p) and (d,2p) cross sections leading to hydrogen-gas bubble accumulation in the structural materials are very important

for radiation damage studies. In opposition to the case of neutrons, the systematics of deuteron activation cross sections, including those leading to hydrogen, triton, and helium--gas accumulation is modest, while even the newest evaluations show apparent discrepancies. Therefore, the present work is devoted to the completion of the theoretical frame associated to the analysis of (d,p) and (d,2p) reactions in order to improve the description of the existing data and thus to provide trustful predictions where the measurements are missing.

On the other hand, 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 și concluziile sunt prezentate în cele 2 lucrări [12,13], 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] V Avrigeanu and M. Avrigeanu, *Validation of an optical potential for incident and emitted low-energy alpha-particles in the A60 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), doi:10.1140/epja/198 s10050-020-00336-0; <https://link.springer.com/article/10.1140/epja/s10050-020-00336-0>
- [2] M. Avrigeanu, D. Rochman, A. J. Koning, U. Fischer, D. Leichtle, C. Costache, and V. Avrigeanu. *Advanced breakup nucleon enhancement of deuteron-induced reaction cross sections*. Eur. Phys. J. A **58**, 3 (2022), doi:10.1140/epja/s10050-021-00659-6; <https://link.springer.com/article/10.1140/epja/s10050-021-00659-6>
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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

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

Short Introduction and Objectives of Work

The International Fusion Materials Irradiation Facility (IFMIF), accelerator-based D-Li neutron source, was designed to produce an intense neutron field for testing ITER-fusion reactor candidate materials. In this respect, 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. In opposition to the case of neutrons, the systematics of deuteron activation cross sections, including those leading to gas accumulation, e.g. (d,p), (d,2p), (d,t), and (d,alpha), is modest, while even the newest evaluation predictions, e.g. TENDL-2021 [1], still show evident discrepancies in respect with the existing data. These discrepancies stress out neglected peculiarities of the deuteron interaction process, which 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]. Moreover, 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

In the present work a comparative analysis of the experimental (d,p) and (d,2p) excitation functions, the model calculations and the evaluations predictions is presented 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 (Paper [1]).

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 55,57,58Fe 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 (Paper [2]). 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.

Conclusions

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. On the other hand, 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. 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. 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 where no data exist.

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, the recent (n,alpha) data remain truly under-predicted for incident energies <9-12 MeV. Due consideration of the uncertainty bands for the CN+PE calculated cross sections has 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.

Acknowledgement

This work has been carried out within the framework of the EUROfusion Consortium and has been received funding from the European Union's Horizon 2020 research innovation programme under grant agreement number 633053 and also from the Romanian National Education Minister under contract 2/23.02.2016. The reviews and opinion expressed herein do not necessarily reflect those of the European Commission.

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