

SECTIUNEA 1

RAPORTUL STIINTIFIC SI TEHNIC

FAZA DE EXECUTIE NR. 3

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 intermediař
3. Proces verbal de avizare internă

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 stabilite si aprobatate prin EUROfusion IDM, si a analizei emisiei alfa indusa de neutroni stabilite si aprobatate prin EUROfusion IDM.
3. Perioada de executie: Ianuarie-Septembrie 2024
4. Obiectivele fazei de execuție:
Aceste obiective au fost in fapt cele ale ‘*deliverabilelor*’ BB-S.05.02-T007-D004/D005, a caror responsabilitate a revenit autorilor raportului de fata, constand in **analiza si discutia rezultatelor de calcule de model** de reactii nucleare (Secs. 3-4 ale Refs. [1-3]) realizate **pe baza ipotezelor si parametrilor de model** formand in aceeasi perioada obiectul activitatii IFin-HH (Secs. 1-2 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 si deuteroni in cadrul noilor biblioteci de date nucleare evaluate. In particular, a fost realizata analiza emisiei de particule alfa indusa de neutroni incidenti pe izotopul 91Zr (BB-S.05.02-T007-D004), precum si evaluarea sectiunilor eficace ale reactiilor induse de deuteroni incidenti pe izotopul 93Zr (BB-S.05.02-T007-D005), formand si obiectul raportarilor de monitorizare EUROfusion semestriale [6,7].
5. Rezumatul fazei (maxim 1 pagina, atât în limba română cât și în limba engleză);
(RO) Validarea ulterioară a potențialului modelului optic (‘optical model potential’ - OMP) pentru particulele alfa dezvoltat în cadrul activitatilor F4E/EUROfusion, pentru o descriere rezonabilă a emisiei alfa în reacțiile induse de neutroni, a vizat cea mai recentă măsurare și analiză a secțiunilor eficace ale reacțiilor (n,α) [e.g. Phys. Rev. C **106**, 064602 (2022) pentru nucleul țintă 91Zr]. Datele măsurate mai mari cu ~100% decât evaluările reale (TENDL-2021/2023) au condus în primul rând la modificări ale OMP-ului menționat mai sus (de asemenea, opțiunea implicită efectivă a sistemului de coduri TALYS-2,0 folosit pentru a realiza TENDL), dar în contradicție cu alte măsurători recente realizate de colaborări largi (de exemplu, arXiv:2402.01534 [nucl-ex], 2 feb 2024). Astfel, s-a efectuat o analiză suplimentară a acestor date, precum și eventualul rol al deziexcitației cu emisia de particule alfa a nucleelor excitate la energiile de rezonanță cvadrupolară gigant izoscalara (‘Isoscalar Giant Quadrupole Resonance’ - ISGQR) în reacții (n,α) sub și în jurul energiei incidente de 14 MeV. Analize similare anterioare in cadrul EUROfusion/WPBB [EUR Phys. J. A **57**, 54 (2021), **58**, 189 (2022), Phys. Rev. C **107**, 034613 (2023)] au fost completate în acest sens și prin compararea datelor aferente regulii sumei ponderate energetic (‘Energy Weighted Sum Rule’ - EWSR) pentru cazurile disponibile. S-a demonstrat un „efect izotopic” suplimentar pentru fracțiunile EWSR ale rezonantelor ISGQR

care corespund reacțiilor (γ,α) și (n,α) , spre deosebire de sistematica rezultatelor anterioare pentru imprăstierea inelastica (α,α') . Această analiză suplimentară oferă o sustinere suplimentară a OMP menționat mai sus, dezvoltat în cadrul activitatilor F4E/EUROfusion.

Pe de alta parte, o analiză avansată a secțiunilor eficace izomerice ale reacțiilor induse de deuteron pe nuclee A=50-100 a fost inițiată alături de date cu descrierea corectă a contribuțiilor tuturor mecanismelor de reacție implicate, cum ar fi procesele de ‘*breakup*, *stripping*, *pick-up*’, emisie la preechilibru (PE) și nucleu compus CN. A fost urmărita descrierea corespunzătoare a funcțiilor de excitație măsurate pentru starea fundamentală și starea izomerică ale reacțiilor induse de deuteronii incidenti pe izotopii stabili ai elementelor Cr, Fe, Ni, Zr, Nb; și Mo în cadrul calculelor TALYS de ultimă generație prin modificarea parametrului de limitare a distribuției de spin a densității de nivele nucleare (‘nuclear-level density’ - NLD) cu un factor de 0,25 [Report EUROfusion WPBB-PR(24) 36171]. De fapt, aceste rezultate sunt în concordanță cu cea mai recentă analiza a rapoartelor izomerice ale reacțiilor induse nucleoni [At. Data Nucl. Data Tables **153**, 101583 (2023)], în timp ce autorii TALYS au subliniat cel mai recent că „*au existat destul de multe dezbateri cu privire la distribuțiile corecte de spin pentru reacțiile la preechilibru*”, în timp ce „*versiunile actualizate vor fi rezervate pentru viitoarele modele de pre-echilibru care iau în considerare în mod constant spin-ul de-a lungul întregului formalism*” [Eur. Phys. J. A (2023) **59**:131]. Rezultatele obținute, utilizând cele mai recente opțiuni ale codului TALYS-1.97, de exemplu „**preeqspin 4**”, au fost discutate în acest sens, în timp ce sunt în curs investigații suplimentare privind efectele opțiunii „**preeqspin Y**” asupra tranzițiilor izomerice. În același timp, se acordă atenție volumului mare de secțiuni izomerice măsurate ale reacțiilor induse de deuteroni pe Nb [Phys. C **88**, 014612 (2013)] precum și neutroni pe Mo [Phys. Rev. C **71**, 044617(2005)] care au fost deja bine descrise fară o ajustare a ‘spin cut-off’, ci cu o densitate avansată de stări ale găurilor și particule excitate [Comp. Phys. Comm. **112**, 191 (1998)].

(EN) Further validation of the alpha-particle optical model potential (OMP) developed within F4E/EUROfusion deliverables, for a sound description of the alpha-emission in neutron-induced reactions, has concerned the most recent measurement and analysis of (n,α) reaction cross sections [e.g., Phys. Rev. C **106**, 064602 (2022) for ^{91}Zr target nucleus]. Measured data larger by ~100% than actual evaluations (TENDL-2021/2023) led firstly to changes of the above-mentioned OMP (also the actual default option of the code-system TALYS-2.0 used to provide TENDL), however at variance with other recent measurements by wide collaborations (e.g., arXiv:2402.01534 [nucl-ex], 2 Feb 2024). Thus it has been carried out an additional analysis of these data as well as eventual role of the alpha-emission decay of nuclei excited just at the isoscalar Giant Quadrupole Resonance (ISGQR) energies within (n,α) reactions below and around the incident energy of 14 MeV. Former EUROfusion/WPBB similar analyses [Eur. Phys. J. A **57**, 54 (2021), **58**, 189 (2022), Phys. Rev. C **107**, 034613 (2023)] has been completed in this respect also by comparison of the corresponding Energy Weighted Sum Rule (EWSR) data with the available systematics. An additional ‘isotope effect’ has been proved for the ISGQR fractions of the EWSR, corresponding to the (γ,α) and (n,α) reactions, at variance to the systematics of the previous (α,α') results. This supplementary analysis is providing further support of the above-mentioned alpha-particle OMMP developed within F4E/EUROfusion deliverables.

On the other hand, an advanced analysis of isomeric cross sections of deuteron-induced reactions on A=50-100 nuclei has been initiated next to the proper account of the contributions of all involved reaction mechanisms as the breakup, stripping, pick-up, pre-equilibrium emission (PE) and compound-nucleus (CN) processes. It has been following the suitable account of the measured ground and isomeric state excitation functions of deuteron-induced reactions on Cr, Fe, Ni, Zr, Nb, and Mo stable isotopes within actual state-of-art TALYS calculations by amending the nuclear-level density (NLD) spin distribution cut-off parameter by a factor of 0.25 [EUROFUSION WPBB-PR(24) 36171]. Actually these results are in line with the most recent compilation of isomeric ratios of light particle induced reactions [At. Data Nucl. Data Tables **153**, 101583 (2023)], while most recently the TALYS authors underlined that “*there has been quite some debate about the correct spin distributions for preequilibrium reactions*” while “*updated versions will be reserved for future pre-equilibrium models which consistently take the spin into account throughout the entire formalism*” [Eur. Phys. J. A (2023) **59**:131]. The results obtained for the above-mentioned reactions using the latest options of TALYS-1.97, e.g. ‘**preeqspin 4**’ has been discussed in this respect while additional investigations are in progress concerning the ‘**preeqspin Y**’ option effects on the isomeric transitions. Attention is paid to the large amount of measured isomeric cross sections of reactions induced by deuterons on Nb [Phys. Rev. C **88**, 014612 (2013)] as well as neutrons on Mo [Phys. Rev. C **71**, 044617(2005)] being already well described using no spin cut-off adjustment but an advanced particle-hole state density [Comp. Phys. Comm. **112**, 191 (1998)] including a PE spin cut-off [Nucl. Sci. Eng. **92**, 440 (1986)].

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

The scientific content of this project, including the results pointing out and suitable achievement of the concerned objectives, as well as the related outcome are showed within Refs. [1-5], related to the deliverables BB-S.05.02-T007-D004/D005 [6-7] and the web page <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*, Journal of Fusion Energy **43**, 15 (2024), <https://doi.org/10.1007/s10894-024-00407-w>; Report [arXiv:2405.15014](https://arxiv.org/abs/2405.15014) [nucl-ex] (May 23, 2024); EUROfusion Pinboard ID 752/2023, <https://users.euro-fusion.org/webapps/pinboard/EFDA-JET/journal/archived/2023/index.html>
- [2] E. Simeckova, M. Avrigeanu, J. Mrazek, J. Novak, M. Štefánik, C. Costache, and V. Avrigeanu, *Deuteron-induced reactions on molybdenum up to 40 MeV* (to be submitted for publication in Journal of Fusion Energy)
- [3] M. Avrigeanu and V. Avrigeanu, *Giant Quadrupole Resonances within neutron-induced alpha-particle emission?* (MS PLB-D-24-00871R2 under 2nd revision for publication in Phys. Lett. B; Report EUROfusion WPBB-PR(24) 38269); EUROfusion Pinboard ID 410/2024, <https://users.euro-fusion.org/webapps/pinboard/EFDA-JET/journal/index.html>

- [4] V. Avrigeanu and M. Avrigeanu, *Progress report on-neutron-induced alpha emission analysis*, Report EFFDOC-1538, OECD/NEA JEFF & EUROfusion WPBB-S.05.02-T005 Monitoring meeting, April 22, 2024, https://www.oecd-nea.org/dbdata/nds_effdoc/effdoc-1538.pdf
- [5] M. Avrigeanu and V. Avrigeanu, *Progress report on deuteron-induced reaction analysis*, Report EFFDOC-1539, OECD/NEA JEFF & EUROfusion WPBB-S.05.02-T005 Monitoring meeting, April 22, 2024, https://www.oecd-nea.org/dbdata/nds_effdoc/effdoc-1539.pdf
- [6] V. Avrigeanu and M. Avrigeanu, *Progress report on-neutron-induced alpha emission analysis*, Report EFFDOC-1538, OECD/NEA JEFF & EUROfusion WPBB-S.05.02-T005 Monitoring meeting, April 22, 2024, https://www.oecd-nea.org/dbdata/nds_effdoc/effdoc-1538.pdf
- [7] M. Avrigeanu and V. Avrigeanu, *Progress report on deuteron-induced reaction analysis*, Report EFFDOC-1539, OECD/NEA JEFF & EUROfusion WPBB-S.05.02-T005 Monitoring meeting, April 22, 2024, https://www.oecd-nea.org/dbdata/nds_effdoc/effdoc-1539.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 research / WPBB2-RO	
Deliverable title	Validation of the assessment of particular alpha-particle emission induced by fast-neutrons on structural materials around 10 MeV Deliverable BB-S-05.02-T007-D004 (Jan. 01 - Dec. 31, 2024)	
Reporting period	January 01 - September 30 2024	
Authors	Vlad Avrigeanu ¹ , Marilena 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 în limba romana si engleza se fac pe pagini separate.

(RO) Validarea ulterioară a potențialului modelului optic ('optical model potential' - OMP) pentru particulele alfa dezvoltat în cadrul activitatilor F4E/EUROfusion, pentru o descriere rezonabilă a emisiei alfa în reacțiile induse de neutroni, a vizat cea mai recentă măsurare și analiză a secțiunilor eficace ale reacțiilor (n,α) [e.g, Phys. Rev. C **106**, 064602 (2022) pentru nucleul țintă ^{91}Zr]. Datele măsurate mai mari cu ~100% decât evaluările reale (TENDL-2021/2023) au condus în primul rând la modificări ale OMP-ului menționat mai sus (de asemenea, opțiunea implicită efectivă a sistemului de coduri TALYS-2,0 folosit pentru a realiza TENDL), dar în contradicție cu alte măsurători recente realizate de colaborări largi (de exemplu, arXiv:2402.01534 [nucl-ex], 2 feb 2024). Astfel, s-a efectuat o analiză suplimentară a acestor date, precum și eventualul rol al deziexcitației cu emisia de particule alfa a nucleelor excitate la energiile de rezonanță cvadrupolară gigant izoscalară ('Isoscalar Giant Quadrupole Resonance' - ISGQR) în reacții (n,α) sub și în jurul energiei incidente de 14 MeV. Analize similare anterioare în cadrul EUROfusion/WPBB [EUR Phys. J. A **57**, 54 (2021), **58**, 189 (2022), Phys. Rev. C **107**, 034613 (2023)] au fost completate în acest sens și prin compararea datelor aferente regulii privind suma ponderată energetic ('Energy Weighted Sum Rule' - EWSR) pentru cazurile disponibile. S-a demonstrat un „efect izotopic” suplimentar pentru fracțiunile EWSR ale rezonantelor ISGQR care corespund reacțiilor (γ,α) și (n,α), spre deosebire de sistematica rezultatelor anterioare pentru imprăstierea inelastica (α,α'). Această analiză suplimentară oferă o sustinere suplimentară a potențialului optic al particulelor alfa menționat mai sus, dezvoltat în cadrul activitatilor F4E/EUROfusion, posibil numai prin corelația dintre barele de eroare ale datelor măsurate primare, utilizate pentru a stabili parametrii de intrare rezonabile și benzile de incertitudine finală ale rezultatelor calculate.

(EN) Further validation of the alpha-particle optical model potential (OMP) developed within F4E/EUROfusion deliverables, for a sound description of the alpha-emission in neutron-induced reactions, has concerned the most recent measurement and analysis of (n,α) reaction cross sections [e.g., Phys. Rev. C **106**, 064602 (2022) for ^{91}Zr target nucleus]. Measured data larger by $\sim 100\%$ than actual evaluations (TENDL-2021/2023) led firstly to changes of the above-mentioned OMP (also the actual default option of the code-system TALYS-2.0 used to provide TENDL), however at variance with other recent measurements by wide collaborations (e.g., arXiv:2402.01534 [nucl-ex], 2 Feb 2024). Thus it has been carried out an additional analysis of these data as well as eventual role of the alpha-emission decay of nuclei excited just at the isoscalar Giant Quadrupole Resonance (ISGQR) energies within (n,α) reactions below and around the incident energy of 14 MeV. Former EUROfusion/WPBB similar analyses [Eur. Phys. J. A **57**, 54 (2021), **58**, 189 (2022), Phys. Rev. C **107**, 034613 (2023)] has been completed in this respect also by comparison of the corresponding Energy Weighted Sum Rule (EWSR) data with the available systematics. An additional ‘isotope effect’ has been proved for the ISGQR fractions of the EWSR, corresponding to the (γ,α) and (n,α) reactions, at variance to the systematics of the previous (α,α') results. This supplementary analysis is providing further support of the above-mentioned alpha-particle optical potential developed within F4E/EUROfusion deliverables, made possible only by the correlation between the measured error bars of the primary data used to fix the consistent input parameters, and the final uncertainty bands of the calculated results.

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 research / WPBB2-RO	
Deliverable title	Advanced analysis of isomeric cross sections of deuteron-induced reactions on A=90-100 nuclei Deliverable BB-S-05.02-T007-D005 (Jan. 01 - Dec. 31, 2024)	
Reporting period	January 01 - September 30 2024	
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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Rezumatele in limba romana si engleza se fac pe pagini separate.

(RO) O analiză avansată a secțiunilor eficace izomerice ale reacțiilor induse de deuteron pe nucleee A=50-100 a fost inițiată alături de descrierea corectă a contribuțiilor tuturor mecanismelor de reacție implicate, cum ar fi procesele de ‘*breakup, stripping, pick-up*’, emisie la preechilibru (PE) și nucleu compus CN. A fost urmărită descrierea corespunzătoare a funcțiilor de excitație măsurate pentru starea fundamentală și starea izomerică ale reacțiilor induse de deuteronii incidenti pe izotopii stabili ai elementelor Cr, Fe, Ni, Zr, Nb; și Mo în cadrul calculelor TALYS de ultimă generație prin modificarea parametrului de limitare a distribuției de spin a densității de nivele nucleare (‘nuclear-level density’ - NLD) cu un factor de 0,25 [Report EUROfusion WPBB-PR(24) 36171]. De fapt, aceste rezultate sunt în concordanță cu cea mai recentă compilație a rapoartelor izomerice ale reacțiilor induse de particule ușoare [At. Data Nucl. Data Tables **153**, 101583 (2023)], în timp ce autorii TALYS au subliniat cel mai recent că „*au existat destul de multe dezbateri cu privire la distribuțiile corecte de spin pentru reacțiile la preechilibru*”, în timp ce „*versiunile actualizate vor fi rezervate pentru viitoarele modele de pre-echilibru care iau în considerare în mod constant spin-ul de-a lungul întregului formalism*” [Eur. Phys. J. A (2023) **59**:131]. Rezultatele obținute pentru reacțiile menționate mai sus, utilizând cele mai recente opțiuni ale codului TALYS-1.97, de exemplu „**preeqspin 4**”, au fost discutate în acest sens, în timp ce sunt în curs investigații suplimentare privind efectele opțiunii „**preeqspin Y**” asupra tranzițiilor izomerice. În același timp, se acordă atenție volumului mare de secțiuni izomerice măsurate ale reacțiilor induse de deuteroni pe Nb [Phys. C **88**, 014612 (2013)] precum și neutroni pe Mo [Phys. Rev. C **71**, 044617(2005)] care au fost deja bine descrise fară o ajustare a ‘spin cut-off’, ci o densitate avansată de stari ale găurilor și particule excitate [Comp. Phys. Comm. **112**, 191 (1998)] incluzând un ‘spin cut-off’ specific PE [Nucl. Sci. Eng. **92**, 440 (1986)], în acord cu concluzia anterioară potrivit căreia valorile reduse ale parametrului ‘spin cut-off’ obținute din analiza secțiunilor eficace izomerice, au fost artificiale și au rezultat din utilizarea unei distribuții de spin necorespunzătoare pentru procesele PE și anume distribuția de spin pentru CN [Phys. Rev. C **80**, 044612 (2009)].

(EN) An advanced analysis of isomeric cross sections of deuteron-induced reactions on A=50-100 nuclei has been initiated next to the proper account of the contributions of all involved reaction mechanisms as the breakup, stripping, pick-up, pre-equilibrium emission (PE) and compound-nucleus (CN) processes. It has been following the suitable account of the measured ground and isomeric state excitation functions of deuteron-induced reactions on Cr, Fe, Ni, Zr, Nb, and Mo stable isotopes within actual state-of-art TALYS calculations by amending the nuclear-level density (NLD) spin distribution cut-off parameter by a factor of 0.25 [EUROFUSION WPBB-PR(24) 36171]. Actually these results are in line with the most recent compilation of isomeric ratios of light particle induced reactions [At. Data Nucl. Data Tables **153**, 101583 (2023)], while most recently the TALYS authors underlined that “*there has been quite some debate about the correct spin distributions for preequilibrium reactions*” while “*updated versions will be reserved for future pre-equilibrium models which consistently take the spin into account throughout the entire formalism*” [Eur. Phys. J. A (2023) **59**:131]. The results obtained for the above-mentioned reactions using the latest options of TALYS-1.97, e.g. ‘**preeqspin 4**’ has been discussed in this respect while additional investigations are in progress concerning the ‘**preeqspin Y**’ option effects on the isomeric transitions. At the same time attention is paid to the large amount of measured isomeric cross sections of reactions induced by deuterons on Nb [Phys. Rev. C **88**, 014612 (2013)] as well as neutrons on Mo [Phys. Rev. C **71**, 044617(2005)] was already well described using no spin cut-off adjustment but an advanced particle-hole state density [Comp. Phys. Comm. **112**, 191 (1998)] including a PE spin cut-off [Nucl. Sci. Eng. **92**, 440 (1986)], in agreement with the previous conclusion that reduced values of the spin cut-off parameter, obtained from isomeric cross-section analysis, were artificial and resulted from the use of an improper PE spin distribution, namely the CN spin distribution [Phys. Rev. C **80**, 044612 (2009)].

ANEXA 1.A

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-T007-D004: Validation of the assessment of particular alpha-particle emission induced by fast-neutrons on structural materials around 10 MeV

BB-S.05.02-T007-D005: Advanced analysis of isomeric cross sections of deuteron-induced reactions on A=90-100 nuclei

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,alpha), is modest in opposition to the case of neutrons. At the same time, even the newest evaluation predictions, e.g. TENDL-2023 [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 [4].

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 [5]. However, in spite of becoming the default option of the widely-used code TALYS [6], there remained still open questions concerning its suitability to account of the alpha-emission [7].

Description of Results

Methods. 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 [2], 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 $A=50\text{-}100$ 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 [3,4].

At the same time, while the previous alpha-emission analysis [8] took the advantage of quite useful recent data of low-lying states feeding in neutron-induced reactions on Fe, Co, Ni, Cu, and Zn nuclei, similar ones for the stable Zr, Nb, and Mo isotopes are additionally quite useful [9-11]. 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. 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. [7-9]).

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 concerning the new measured data for $^{91}\text{Zr}(n,\alpha)^{88}\text{Sr}$ reaction [12]. 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 [13]. 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 [14]. 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 [7-11], the recent (n,α) data remain truly under-predicted for incident energies <9-12 MeV.

Results. Further validation of the alpha-particle optical model potential (OMP) developed within F4E/EUROfusion deliverables, for a sound description of the alpha-emission in neutron-induced reactions, has concerned the most recent measurement and analysis of (n,α) reaction cross sections (e.g. for ^{91}Zr target nucleus[12]). Measured data larger by ~100% than actual evaluations (TENDL-2021/2023) led firstly to changes of the above-mentioned OMP (also the actual default option of the code-system TALYS-2.0 used to provide TENDL), however at variance with other recent measurements by wide collaborations. Thus it has been carried out an additional analysis of these data as well as eventual role of the alpha-emission decay of nuclei excited just at the isoscalar Giant Quadrupole Resonance (ISGQR) energies within (n,α) reactions below and around the incident energy of 14 MeV. Former EUROfusion/WPBB similar analyses [8-9] has been completed in this respect also by comparison of the corresponding Energy Weighted Sum Rule (EWSR) data with the available systematics. An additional ‘isotope effect’ has been proved for the ISGQR fractions of the EWSR, corresponding to the (γ,α) and (n,α) reactions, at variance to the systematics of the previous (α,α') results. This supplementary analysis is providing further support of the above-mentioned alpha-particle optical potential developed within F4E/EUROfusion deliverables, made possible only by the correlation

between the measured error bars of the primary data used to fix the consistent input parameters, and the final uncertainty bands of the calculated results.

An advanced analysis of isomeric cross sections of deuteron-induced reactions on A=50-100 nuclei has been initiated next to the proper account of the contributions of all involved reaction mechanisms as the breakup, stripping, pick-up, pre-equilibrium emission (PE) and compound-nucleus (CN) processes. It has been following the suitable account of the measured ground and isomeric state excitation functions of deuteron-induced reactions on Cr, Fe, Ni, Zr, Nb, and Mo stable isotopes within actual state-of-art TALYS calculations by amending the nuclear-level density (NLD) spin distribution cut-off parameter by a factor of 0.25 [13]. Actually these results are in line with the most recent compilation of isomeric ratios of light particle induced reactions, while most recently the TALYS authors underlined that “*there has been quite some debate about the correct spin distributions for preequilibrium reactions*” while “*updated versions will be reserved for future pre-equilibrium models which consistently take the spin into account throughout the entire formalism*” [6]. The results obtained for the above-mentioned reactions using the latest options of TALYS-1.97, e.g. ‘**preeqspin 4**’ has been discussed in this respect while additional investigations are in progress concerning the ‘**preeqspin Y**’ option effects on the isomeric transitions. At the same time attention is paid to the large amount of measured isomeric cross sections of reactions induced by deuterons on Nb [4].

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. 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 alpha-emission CN+PE calculated cross sections has also been closely related to the error bars of the independent date fitted in order to establish the consistent parameter set. The need of additional reaction mechanisms to be taken into account is thus pointed out [15].

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>.

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.

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Papers

- [13] M. Avrigeanu, E. Simeckova, J. Mrazek, C. Costache, and V. Avrigeanu, *Modeling of deuteron-induced reactions on molybdenum at low energies*, Journal of Fusion Energy **43**, 15 (2024), <https://doi.org/10.1007/s10894-024-00407-w>; Report arXiv:2405.15014 [nucl-ex] (May 23, 2024); EUROfusion Pinboard ID 752/2023, <https://users.euro-fusion.org/webapps/pinboard/EFDA-JET/journal/archived/2023/index.html>
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[15]M. Avrigeanu and V. Avrigeanu, *Giant Quadrupole Resonances within neutron-induced alpha-particle emission?* (MS PLB-D-24-00871R2 under 2nd revision for publication in Phys. Lett. B; Report EUROfusion WPBB-PR(24) 38269); EUROfusion Pinboard ID 410/2024, <https://users.euro-fusion.org/webapps/pinboard/EFDA-JET/journal/index.html>

Meetings

[16]V. Avrigeanu and M. Avrigeanu, *Progress report on-neutron-induced alpha emission analysis*, Report EFFDOC-1538, OECD/NEA JEFF & EUROfusion WPBB-S.05.02-T005 Monitoring meeting, April 22, 2024, https://www.oecd-nea.org/dbdata/nds_effdoc/effdoc-1538.pdf

[17]M. Avrigeanu and V. Avrigeanu, *Progress report on deuteron-induced reaction analysis*, Report EFFDOC-1539, OECD/NEA JEFF & EUROfusion WPBB-S.05.02-T005 Monitoring meeting, April 22, 2024, https://www.oecd-nea.org/dbdata/nds_effdoc/effdoc-1539.pdf

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	Journal of Fusion Energy 43, 15 (2024) Phys. Lett. B (MS PLB-D-24-00871R2, Report EUROfusion WPBB-PR(24) 38269)
Numar de articole stiintifice in reviste indexate in alte baze de date internationale recunoscute	2	Report EFFDOC-1538, NEA DB, Apr.2024 Report EFFDOC-1539, NEA DB, Apr.2024
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/prototipuri		
Numarul de posturi de cercetatori echivalent norma intreaga (ENI) sustinute *	0.66	
Numarul de cercetatori cu doctorat sustinuti *	2	
Numarul de ingineri sustinuti *		
Numarul de tehnicieni sustinuti *		
Nuamrul 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*	2	
Numar de prezentari la Conferinte Internationale	2	
Numar de postere prezentate la Conferinte Internationale*		
Numar de participantii la Workshopuri*	2	
Numar de prezentari orale la Workshopuri	2	
Numar de postere prezentate la Workshopuri		
Numarul participantilor la intruniri de proiect in 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 lucrările efectuate de colectivul departamentului de Fizică Nucelară al IFIN-HH la **partea Principala a** proiectului **“Participarea Romaniei la EUROfusion WPBB si cercetari complementare”** (WPBB2-RO) in cadrul etapei nr. III, 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) Lucrările executate corespund clauzelor contractuale;
- b) Toate documentele necesare efectuarii platii există și sunt corect întocmite;
- c) Concluziile lucrării, principalele rezultate obținute și datele privind efectuarea cheltuielilor sunt prezentate în Raportul intermediar de activitate și în documentele sale însoțitoare;
- d) Planificarea activităților și resurselor aferente realizării etapei următoare de derulare a proiectului, prezentată în Raportul intermediar de activitate, este corespunzătoare realizării obiectivului propus și în concordanță cu prevederile contractului;
- e) Cota de cofinanțare realizată în faza de execuție curentă este de.....lei.

Comisia avizează **FAVORABIL** lucrările și documentele și consideră că 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. 3

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 intermediař
3. Proces verbal de avizare internă

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 si a potentialului de model optic pentru particule alfa pentru evaluarea producerii de gaze stabilite prin EUROfusion IDM.

3. Perioada de executie: Ianuarie- Septembrie 2024

4. Obiectivele fazei de executie:

Aceste obiective au fost corelate cu cele ale ‘*deliverabilelor*’ BB-S.05.02-T007-D004/D005, 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 aceeasi 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 eficace ale producerii de H prin reactii induse de deuteroni inclusiv pe ^{93}Zr [4], si analiza importantei cunoasterii cat mai precise a parametrilor de modele nucleare pentru evaluarea emisiei alfa indusa de neutroni rapizi pe nucleee cu $54 \leq A \leq 99$ [5].

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

(RO) Evaluarea datelor nucleare ale reactiilor induse de deuteroni sau pentru emisia de particule α precum si 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. Astfel, fata de cercetarile corelate cu fisiunea nucleara, exista o necesitate majora pentru sectiuni eficace 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 nuceare, 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 realizarilor programelor F4E si EUROfusion, este discutat in particular pentru deuteroni incidenti pe ^{93}Zr and izotopii stabili ai Mo [1-2] precum si evaluarea emisiei alfa indusa de neutroni rapizi pe nucleee cu $54 \leq A \leq 99$ [3].

Rolul major al seturilor consistente de parametri de model pentru rezultatele analizelor de emisie a particulelor alfa, vizand posibila diferenta intre potentialele de model optic (OMPs) ce

descriu fie imprastierea elastica si reactiile induse de particulele alfa, fie emisia acestora din nucleele excitate in reactii nucleare, a fost de asemenea prezentat. Utilizarea acestora este opusa implicarii oricaror factori empirici de scalare ale largimilor de stari nucleare pentru emisia gama si/sau de nucleoni, sau combinatiilor 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 consideratie a unor procese nucleare directe suplimentare.

(EN) The nuclear data evaluation for deuteron-induced reactions and α -particle emission by neutron interactions as well as the status and open questions related to these subjects are of real interest 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 ^{93}Zr and Mo stable isotopes [1-2] as well as alpha-particle emission in neutron-induced reactions on $54 \leq A \leq 99$ nuclei [3].

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)

The scientific content of this project, including the results pointing out and suitable achievement of the concerned objectives, as well as the related outcome are showed within Refs. [4-5], and the web page <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*, Journal of Fusion Energy **43**, 15 (2024),

- <https://doi.org/10.1007/s10894-024-00407-w>; Report arXiv:2405.15014 [nucl-ex] (May 23, 2024); EUROfusion Pinboard ID 752/2023, <https://users.euro-fusion.org/webapps/pinboard/EFDA-JET/journal/archived/2023/index.html>
- [2] E. Simeckova, M. Avrigeanu, J. Mrazek, J. Novak, M. Štefánik, C. Costache, and V. Avrigeanu, *Deuteron-induced reactions on molybdenum up to 40 MeV* (to be submitted for publication in Journal of Fusion Energy)
- [3] M. Avrigeanu and V. Avrigeanu, *Giant Quadrupole Resonances within neutron-induced alpha-particle emission?* (MS PLB-D-24-00871R2 under 2nd revision for publication in Phys. Lett. B; Report EUROfusion WPBB-PR(24) 38269); EUROfusion Pinboard ID 410/2024, <https://users.euro-fusion.org/webapps/pinboard/EFDA-JET/journal/index.html>
- [4] M. Avrigeanu and V. Avrigeanu, *Deuteron-induced reaction cross sections for 93Zr up to 200 MeV*, <https://conferences.iaea.org/event/368/contributions/31731/>, in Proc. *The 7th international workshop on Compound-Nuclear Reactions and Related Topics (CNR*24), 8-12 July 2024, Vienna, Austria*, P. Dimitriou, R. Capote Noy, and G. Schnabel (Eds.), <https://conferences.iaea.org/event/368/>; EPJ Web of Conf. (submitted, Sept. 2024) ; EUROfusion Pinboard ID CNR*24/2/2024, https://users.euro-fusion.org/repository/pinboard/EFDA-JET/conference/114665_cnr2024_mavrigeanu.pdf
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ANEXA 1.A

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		

Abstract

The nuclear data evaluation for deuteron-induced reactions and α -particle emission by neutron interactions as well as the status and open questions related to these subjects are of real interest 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 ^{93}Zr and Mo stable isotopes as well as alpha-particle emission in neutron-induced reactions on $54 \leq A \leq 99$ 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 and alpha-particle optical model potential relevant for evaluation of gas production to be issued and approved through EUROfusion IDM.

Detailed results

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,alpha), is modest in opposition to the case of neutrons. At the same time, even the newest evaluation predictions, e.g. TENDL-2023 [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 [4].

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 [5]. However, in spite of becoming the default option of the widely-used code TALYS [6], there remained still open questions concerning its suitability to account of the alpha-emission [7].

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 [2], 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 [3,4].

At the same time, while the previous alpha-emission analysis [8] took the advantage of quite useful recent data of low-lying states feeding in neutron-induced reactions on Fe, Co, Ni, Cu, and Zn nuclei, similar ones for the stable Zr, Nb, and Mo isotopes are additionally quite useful [9-11]. 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. 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. [7-9]).

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 concerning the new measured data for $^{91}\text{Zr}(n,a)^{88}\text{Sr}$ reaction [12]. 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 [13]. 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 [14]. 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 [7-11], 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 work concerning the new measured data for $^{93}\text{Zr}(\text{d},\text{x})$ reactions [15]. 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 alpha-emission CN+PE calculated cross sections has also been closely related to the error bars of the independent date fitted in order to establish the consistent parameter set. The need of additional reaction mechanisms to be taken into account is thus pointed out [16].

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>.

Acknowledgement

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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	EPJ Web of Conf. (submitted, Sept. 2024) EPJ Web of Conf. (submitted, Sept. 2024)
Numar de articole stiintifice in reviste indexate in alte baze de date internationale 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/prototipuri		
Numarul de posturi de cercetatori echivalent norma intreaga (ENI) sustinute *	0.33	
Numarul de cercetatori cu doctorat sustinuti *	2	
Numarul de ingineri sustinuti *	1	
Numarul de tehnicieni sustinuti *		
Nuamrul 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	2	
Numar de postere prezentate la Conferinte Internationale*		
Numar de participantii la Workshopuri*		
Numar de prezentari orale la Workshopuri		
Numar de postere prezentate la Workshopuri		
Numarul participantilor la intruniri de proiect in 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 lucrările 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. III, 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) Lucrările executate corespund clauzelor contractuale;
- b) Toate documentele necesare efectuării platii există și sunt corect întocmite;
- c) Concluziile lucrării, principalele rezultate obținute și datele privind efectuarea cheltuielilor sunt prezentate în Raportul intermediar de activitate și în documentele sale însoțitoare;
- d) Planificarea activităților și resurselor aferente realizării etapei următoare de derulare a proiectului, prezentată în Raportul intermediar de activitate, este corespunzătoare realizării obiectivului propus și în concordanță cu prevederile contractului;
- e) Cota de cofinanțare realizată în faza de execuție curentă este de.....lei.

Comisia avizează **FAVORABIL** lucrările și documentele și consideră că pot fi prezentate pentru evaluare la Institutul de Fizica Atomica – IFA.

COMISIA DE AVIZARE

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	Dorina Aranghel	
SECRETAR	Vlad Avrigeanu	

Sectiunea 2 – Raport explicativ al cheltuielilor

SECTIUNEA 2

RAPORTUL EXPLICATIV AL CHELTUIELILOR

ETAPA DE EXECUTIE NR. 3

1. Devizul postcalcul al etapei (DP) – ANEXA 2.A
2. Fisa de evidenta a cheltuielilor (FEC) – ANEXA 2.B
3. Fisa de evidenta analitica postcalcul (FEAP) – ANEXA 2.C