Available online at www.sciencedirect.com

ScienceDirect

Journal of Nuclear Materials 367–370 (2007) 1531–1536

journal of nuclear materials

www.elsevier.com/locate/jnucmat

Evaluation and validation of d–Li cross section data for the IFMIF neutron source term simulation

U. Fischer [a,*], M. Avrigeanu [b], P. Pereslavtsev [a], S.P. Simakov [a], I. Schmuck [a]

[a] *Association FZK-EURATOM, Forschungszentrum Karlsruhe, Institut fuer Reaktorsicherheit, Hermann-von-Helmholtz-Platz 1, D-76344 Eggenstein-Leopoldshafen, Germany*

[b] *EURATOM-MEC Fusion Association, 'Horia Hulubei' National Institute for Physics and Nuclear Engineering, P.O. Box MG-6, Bucharest, Romania*

Abstract

A completely new evaluation of the d + ^{6,7}Li interaction cross sections up to 50 MeV has been performed applying a new methodology which takes into account compound nucleus reactions, pre-equilibrium processes, stripping and direct interactions. The evaluated d + ^{6,7}Li cross section data were prepared in the laboratory frame, stored in standard ENDF-6 data format and processed by the NJOY code system. A series of benchmark calculations was performed with the McDeLicious code to test the new data evaluations against experimental thick and thin lithium target neutron yield data up to 40 MeV deuteron energy. It was shown that the new d + ^{6,7}Li cross section data can well reproduce both the thick target neutron yields and differential neutron emission cross sections. Thus there is a clear improvement of the prediction accuracy for the IFMIF neutron source term simulation with the new d + ^{6,7}Li cross section data evaluations.

1. Introduction

The International Fusion Material Irradiation Facility (IFMIF) [1] will provide an accelerator based d–Li neutron source for high fluence test irradiations of fusion reactor candidate materials. In the IFMIF lithium target neutrons are generated through the d–Li stripping reaction and various other reaction mechanisms. The neutron source generation must be represented accordingly in the neutron transport calculation. The McDeLicious Monte Carlo code [2] was developed along this guideline to simulate in the transport calculation the neutron generation on the basis of evaluated d + ^{6,7}Li cross sections. A first set of d + ^{6,7}Li cross section data was evaluated previously in a collaboration of Forschungszentrum Karlsruhe and INPE Obninsk [3].

Tests against thick lithium target experiments showed good agreement for the total and forward neutron yields [4]. Recent measurements of double-differential d + ^{6,7}Li cross sections [5,6] revealed, however, severe deficiencies of the neutron angular distributions and the inability to properly represent the population of residual nucleus excited levels. These results initiated an effort to re-evaluate the d + ^{6,7}Li cross section data applying a new methodology which takes into account compound nucleus

* Corresponding author. Tel.: +49 7247 82 3407; fax: +49 7247 82 3718.
E-mail address: ulrich.fischer@irs.fzk.de (U. Fischer).

0022-3115/$ - see front matter © 2007 Elsevier B.V. All rights reserved.
doi:10.1016/j.jnucmat.2007.04.038

reactions, pre-equilibrium processes, stripping and direct interactions. The new evaluation methodology is described in the following and detailed results are given for benchmark calculations performed with McDeLicious to test the new data evaluations against experimental thick and thin lithium target neutron yield data up to 40 MeV deuteron energy.

2. Data evaluation for the d + Li reaction system up to 50 MeV

Much effort was spent during the last decade to find and adjust appropriate nuclear models for the description of d + Li interactions in the energy range from a few to 50 MeV. The available d + Li data evaluation of Konobeyev et al. [3] e.g. is based on the use of the intra-nuclear cascade model for non-elastic reactions, the Serber model [7] for stripping processes and the diffraction approximation [8] for elastic deuteron scattering.

In the evaluation approach of this work, the following nuclear processes are assumed to take place when a deuteron collides with a lithium nucleus: elastic scattering, evaporation (i.e. compound nucleus formation), pre-equilibrium processes, neutron/proton stripping and direct processes resulting in the excitation of specific residual nucleus levels.

For the deuteron elastic scattering, the diffraction approximation was proven to be inadequate, especially for back angle scattering. As a suitable alternative, the use of a phenomenological optical model potential (OMP) was elaborated for $d + {}^{6,7}Li$ interactions in the energy range up to 50 MeV [9]. The resulting agreement of calculated angular distributions of elastically scattered deuterons with experimental data is very good, thus suggesting the use of this OMP in the nuclear reaction cross section calculations.

Neutron emission is the most important reaction channel for applications to IFMIF. A proper neutron OMP must be available for the evaporation, pre-equilibrium and direct reaction models with neutrons in the entrance or exit channels. A combination of the Koning global neutron OMP [10] and a modified Chiba local potential [11] was shown to be suitable for neutron energies from 12 to 50 MeV and the energy range below 12 MeV, respectively. This choice was based on the observation that the global Koning OMP for the n + Be system shows good agreement with experimental data for total, reaction and elastic scattering cross sections above 12 MeV. The real part of the Chiba local potential had to be decreased to get agreement of calculated and measured $n + {}^9Be$ total, reaction, elastic scattering cross sections and elastic scattering angular distributions for neutron energies from 0.1 to 12 MeV.

The Bechetti and Greenlees [12] OMP was used for describing the emission of protons and tritons, and the Avrigeanu and Hodgson potential [13] for the α-particles.

The nuclear model calculations for the evaporation and pre-equilibrium reactions were performed with the GNASH code [14] in combination with ECIS95 [15]. Double-differential cross sections were produced using Kalbach systematics for angular distributions. The stripping processes were modelled on the basis of the Serber theory [7]. Direct reactions were described with the DWUCK4 code [16] which allows the calculation of angular distributions for Li(d,n) reactions leading to the formation of the nucleus either in ground or excited states. The level scheme for ^7Li isotope was represented by five excited levels, assuming that several levels with small width can be replaced by one 'wide' artificial level. The neutron energy distributions for the direct reactions were calculated by spreading the cross section for a particular level over its excitation energy with Gaussian distribution, accounting for the level width. For 16.6 MeV incident deuterons, Fig. 1 shows the calculated double-differential neutron emission cross section and its breakdown into the different reaction components. It is revealed that the inclusion of direct interaction processes is essential for representing the structures of the emission cross section at high neutron energies. This is due to the fact that the direct reaction mechanism is dominant for the emission of neutrons with energies above the deuteron incidence energy. It is noted that pre-equilibrium emission of neutrons do not significantly contribute at forward angles but become more important at backward scattering angles. Fig. 2 compares the results of the evaluated double-differential neutron emission cross sections and the measured data of Baba and co-workers [6] at 40 MeV deuteron incidence energy.

The deuteron cross sections evaluated for ^6Li and ^7Li were stored on ENDF-6 formatted data files and processed into the ACE format for the McDeLicious Monte Carlo code by using a modified version of the NJOY-99 code system [17]. The ENDF data files contain elastic scattering data and secondary particle emission spectra up to 50 MeV deuteron energy.

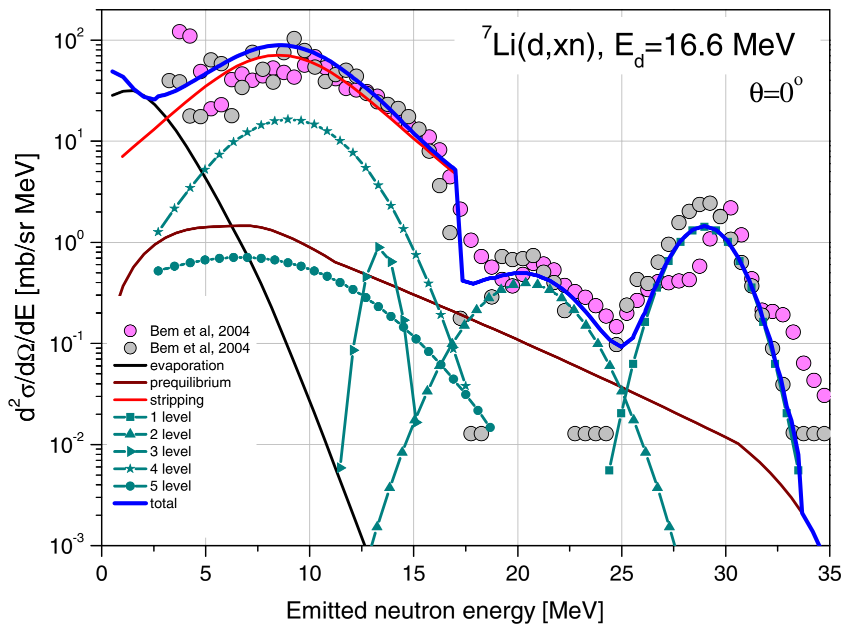

Fig. 1. Measured [5] and evaluated ^{7}Li(d,xn) double-differential neutron emission cross section and its decomposition into reaction components for 16.6 MeV deuterons.

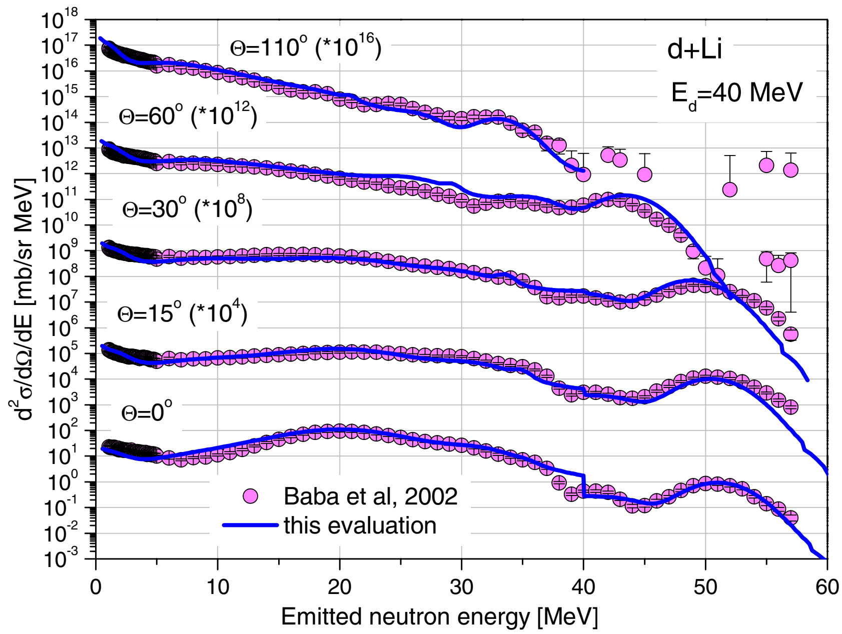

Fig. 2. Double-differential neutron emission cross sections for 40 MeV incident deuterons: comparison of evaluated and measured [6] data.

3. Validation against thick Li target neutron yields

A set of 11 independent experiments on thick lithium target yields is available for validation analyses including the recent measurements by Bém et al. [5] at 16.3 and 17 MeV and Baba and co-workers [6] at 25 and 40 MeV deuteron incidence energy. These experimental data sets cover the deuteron energy range from 5 to 40 MeV and thus are well suited for benchmarking the IFMIF d–Li source term.

The validation analyses were conducted on the basis of Monte Carlo calculations with the McDeLicious code which is capable of using the d–Li evaluated cross section data. For comparison, benchmark calculations were also performed with the semi-empirical d–Li reaction model of McDeLi [18], the predecessor to McDeLicious, and the ISABEL intra-nuclear cascade model of the high energy particle Monte Carlo code MCNPX [19].

The comparison of measured and calculated forward neutron yields, Fig. 3, shows that McDeLicious with the updated d–Li cross section data is well able to reproduce the experimental results over the entire deuteron energy range from threshold up to 40 MeV. This is a clear improvement over the original 2001 d–Li evaluation [3] which gave an underestimation of the experimental yields below 20 MeV and some deviations from the recent measurements of Baba and co-workers [6] at 25 and 40 MeV. With the updated d–Li cross section data, the average deviation of calculated and measured forward neutron yield data is around 10%. The approaches of the McDeLi and the MCNPX codes give significant worse agreement with the experimental neutron yields. McDeLi is not capable of prediction below 15 MeV deuteron energy while MCNPX underesti-

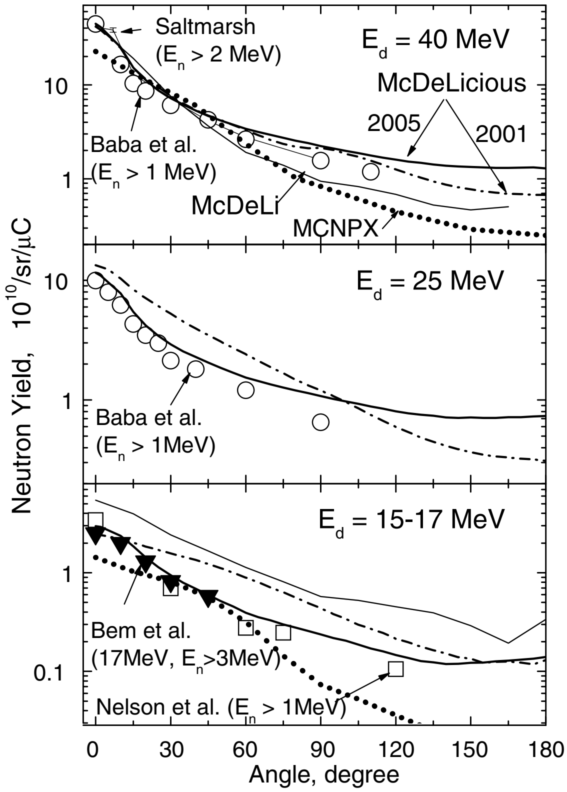

Fig. 4. Angular neutron yields from thick lithium target at different incident deuteron energies. Symbols – experimental data; curves – calculations with McDeLicious (2005 and 2001 d–Li data), McDeLi and MCNPX codes.

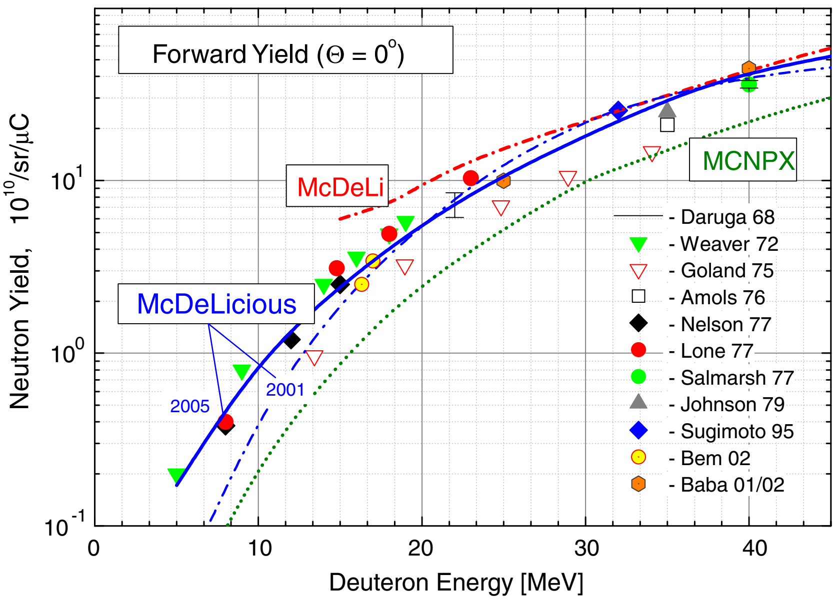

Fig. 3. Comparisons of measured and calculated thick lithium target forward neutron yields as a function of deuteron incidence energies.

mates the neutron yields by a factor 2 over the entire deuteron energy range.

Neutron angular differential yields were measured from 15 to 40 MeV deuteron energy in several experiments, in most cases, however, only in the forward directed hemisphere. The comparison of McDeLicious calculations using the new d–Li evaluation shows that the angular dependence can be satisfactorily predicted over the whole range of measured deuteron energies and secondary neutron angles, see Fig. 4. The other approaches show again a worse reproduction of the experimental data set, especially below 20 MeV.

Measured double-differential neutron yields from thick lithium targets are available from the experiments of Baba and co-workers [6] (25 and 40 MeV deuteron incidence energy), Bém et al. [5] (17 MeV) and Sugimoto [20] (32 MeV). The comparison of McDeLicious calculations with the measured energy distributions (double-differential thick target neutron yields) demonstrates significant improvements achieved with the updated d–Li evaluation. As shown in Figs. 5 and 6 for the Baba experiments, both the absolute values and the shape of the energy spectra are reproduced with better accuracy. In particular it is seen that the humps in the high energy part of the neutron spectra, corresponding to the population of low lying states in ^{8}Be due to the ^{7}Li(d,n) reaction, are well represented by the McDeLicious calculations with the newly evaluated d–Li cross section data.

The accuracy of the thick Li target neutron yield data has a direct impact on the IFMIF irradiation parameters. IFMIF will be operated at 40 MeV deuteron energy and the material irradiation specimens will be located in the deuteron beam direction subjected to an angle of ±80°. An uncertainty assessment of the related thick target neutron yields for IFMIF neutronics calculations was performed on the basis of the recent experiment of Baba and co-workers

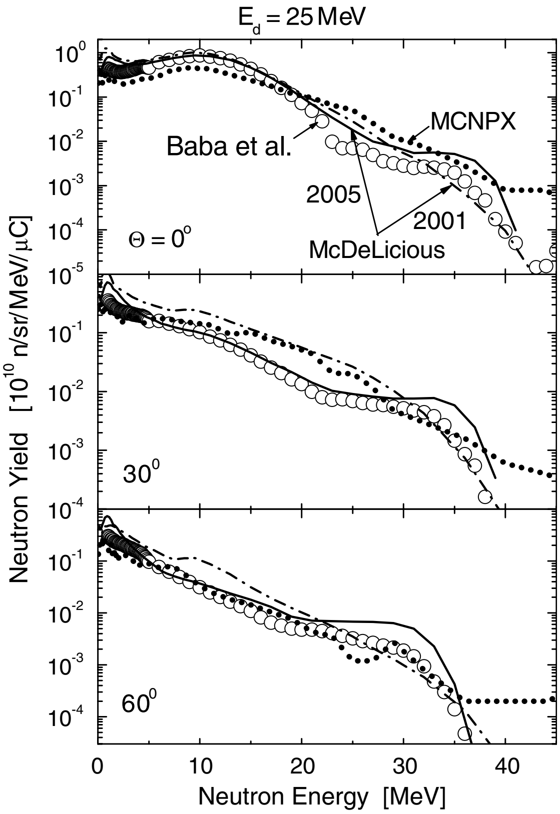

Fig. 5. Energy differential neutron yields from thick lithium target at 25 MeV deuteron incidence energy. Symbols – experimental data of Baba and co-workers [6]; curves – calculations with McDeLicious (2005 and 2001 d–Li data) and MCNPX codes.

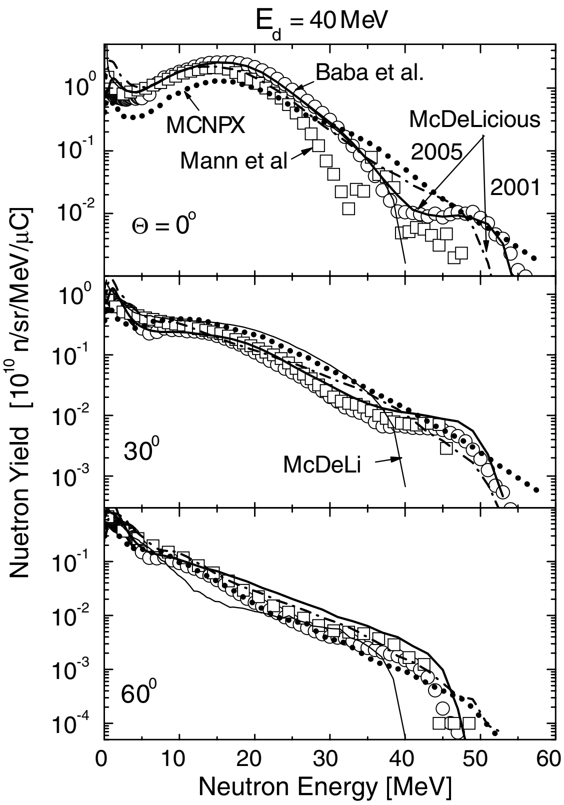

Fig. 6. Energy differential neutron yields from thick lithium targets at 40 MeV deuteron incidence energy. Symbols – experimental data of Mann et al. [21] and Baba and co-workers [6]; curves – calculations with McDeLicious (2005 and 2001 d–Li data), McDeLi and MCNPX codes.

[6] performed at the Tohoku University using the AVF cyclotron and applying the time-of-flight (TOF) technique for the measurement of the neutron spectra at various angles between 0° and 110° at 40 MeV deuteron incidence energy. These measurements are considered state-of-the-art with the highest experimental accuracy currently achievable. An uncertainty of 20% was assessed for the double-differential neutron yields at 40 MeV deuteron incidence energy when using the McDeLicious code with the newly evaluated d–Li cross section data.

4. Conclusions

A new evaluation of the $d + {}^{6,7}Li$ interaction cross sections up to 50 MeV has been performed applying a new methodology which takes into account compound nucleus reactions, pre-equilibrium processes, stripping and direct interactions. Microscopic and global optical model potentials were developed to describe elastic cross sections and transmission coefficients for deuterons, neutrons and protons. The re-evaluated $d + {}^{6,7}Li$ cross section data were prepared in the laboratory frame, stored in standard ENDF-6 data format and processed by the NJOY code system. The new data evaluations show an improved agreement with measured differential cross sections and thin target neutron yields.

A series of benchmark calculations was performed with the McDeLicious code to test the new data against experimental thick lithium target neutron yields. It was shown that the experimental thick target yields can be well reproduced over the entire deuteron energy range up to 40 MeV. Other methodological approaches as available with the McDeLi and MCNPX codes which use built-in semi-empirical analytical models for the d–Li cross sections give significant worse agreement. Thus there is a clear improvement of the prediction accuracy for the IFMIF neutron source term simulation with the new $d + {}^{6,7}Li$ cross section data evaluations.

Acknowledgements

This work, supported by the European Communities under the contract of Association between EURATOM and Forschungszentrum Karlsruhe, was carried out within the framework of the European Fusion Development Agreement.

References

[1] IFMIF International Team, IFMIF Comprehensive Design Report, January 2004.
[2] S.P. Simakov, U. Fischer, U. von Möllendorff, I. Schmuck, A. Konobeev, P. Pereslavtsev, J. Nucl. Mater. 307–311 (2002) 1710.
[3] A. Konobeyev, Yu. Korovin, P. Pereslavtsev, U. Fischer, U. von Möllendorff, Nucl. Sci. Eng. 139 (2001) 1.
[4] U. Fischer, S.P. Simakov, U. von Möllendorff, P. Pereslavtsev, P. Bem, P.P.H. Wilson, AccApp'03 ANS Embedded Topical Meeting, San Diego, CA, June 1–5, 2003.
[5] P. Bém, V. Burjan, M. Götz, U. Fischer, V. Kroha, U. v. Möllendorff, J. Novák, S. Simakov, E. Šimečková, D–Li reaction source term: experimental verification of neutron yield based on thick and thin Li-targets. Report NPI ASCR Řež EXP(EFDA)-05/2004.
[6] M. Hagiwara, M. Baba, N. Kawata, N. Hirabayashi, T. Itoga, in: JAERI Nuclear Data Symposium, December 2002.
[7] R. Serber, Phys. Rev. 72 (11) (1947) 1008.
[8] A.G. Sitenko, Theory of Nuclear Reactions, Energoatomizdat, Moscow, 1982.
[9] M. Avrigeanu, W. von Oertzen, U. Fischer, V. Avrigeanu, Nucl. Phys. A 759 (2005) S.327.
[10] A.J. Koning, J.P. Delaroche, Nucl. Phys. A 713 (2003) 231.
[11] S. Chiba, K. Togasaki, M. Ibaraki, et al., Phys. Rev. C 58 (1998) 2205.
[12] F.D. Bechetti, G.W. Greenlees, in: H.H. Barschall, W. Haeberly (Eds.), Polarization Phenomena in Nuclear Reactions, The University of Wisconsin, 1971, p. 682.
[13] V. Avrigeanu, P.E. Hodgson, Phys. Rev. C 49 (1994) 2136.
[14] P.G. Young, E.D. Arthur, M.B. Chadwick, in: A. Gandiny, G. Reffo (Eds.), Proc. IAEA Workshop Nuclear Reaction data and Nuclear Reactors-Physics, Design and Safety, Trieste, Italy, April 15–May-17, 1996, World Scientific Publishing, Ltd., Singapore, 1998, p. 227.
[15] J. Raynal, Notes on ECIS94, CEA Saclay Report No. CEA-N-2772, 1994.
[16] P.D. Kunz, DWUCK4 user's manual, available from the NEA data bank, France. <http://www.nea.fr/abs/html/nesc9872.html>.
[17] R.E. McFarlane, D.W. Muir, R.M. Boicourt, NJOY99.00 – Code System for Producing Pointwise and Multigroup Neutron and Photon Cross Sections from ENDF/B Data. RSICC Code Package PSR-480, Oak Ridge, 1999.
[18] P.P.H. Wilson, Neutronics of the IFMIF neutron source: development and analysis. Report FZKA 6218, Karlsruhe 1999.
[19] L.S. Waters (Ed.), MCNPX User's Manual Version 2.1.5, available from <http://mcnpx.lanl.gov>.
[20] M. Sugimoto, JAERI, Double differential neutron yields from Li(d,n) experiments, private communication, 1995.
[21] F.M. Mann, F. Schmittroth, L.L. Carter, Neutrons from d + Li and the FMIT irradiation environment. Report HEDL-TC-1459, Richland, 1981.