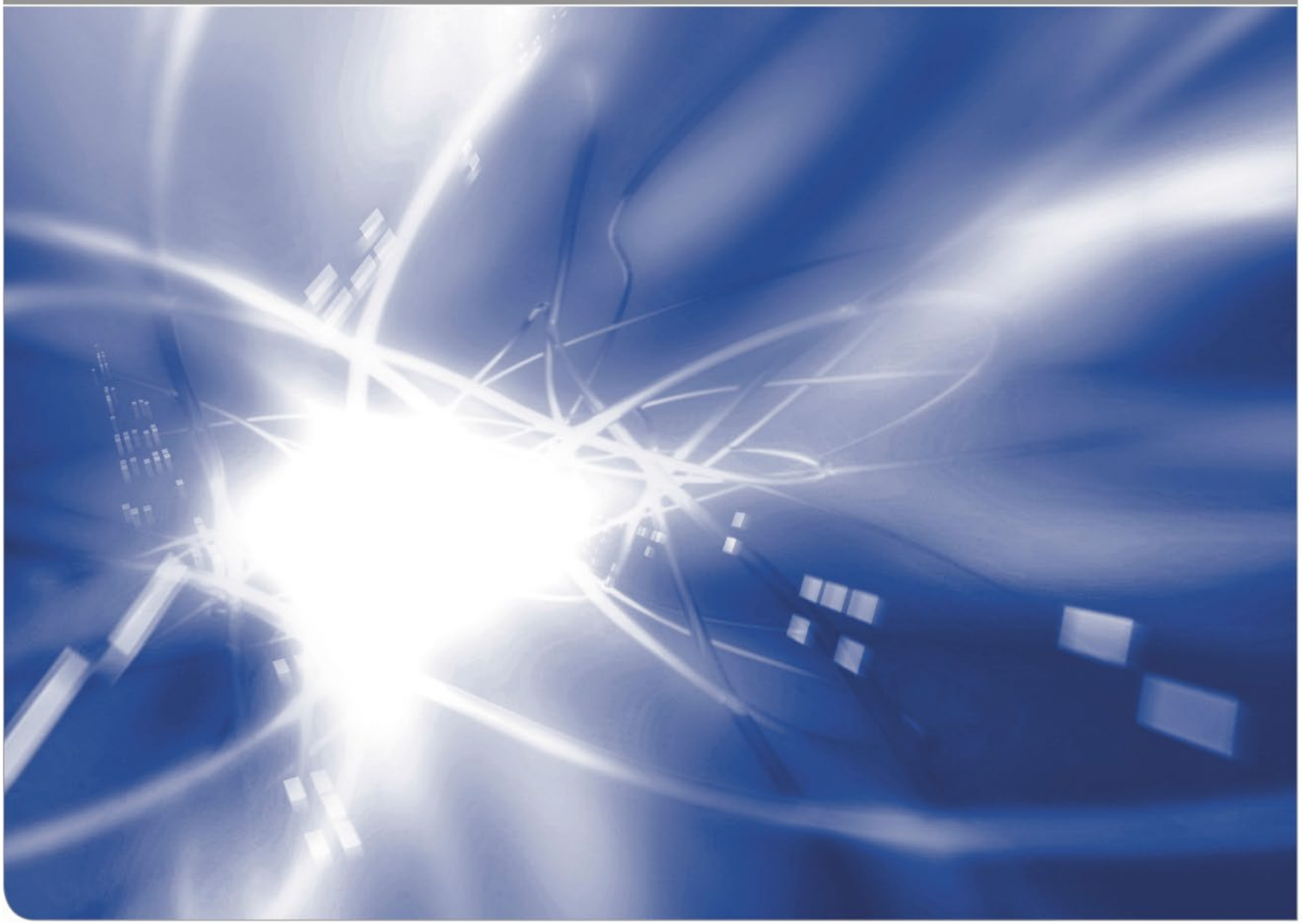
Karlsruhe Institute of Technology

Neutron displacement cross-sections for ZrH_2

A.Yu. Konobeyev[1], D. Leichtle[1], P. Pereslavtsev[2]

KIT SCIENTIFIC WORKING PAPERS 259



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Impressum

Karlsruher Institut für Technologie (KIT)
www.kit.edu

2025

ISSN: 2194-1629

Abstract

The atomic displacement cross-sections were obtained for neutron irradiation of zirconium hydride ZrH_2. The number of stable defects was calculated using the SRIM/TRIM code with corrections.

The recoil energy spectra were obtained using nuclear data from the JEFF-4T4, ENDF/B-VIII.1, and JENDL-5 libraries. As a result, three different versions of displacement cross sections were prepared for ZrH_2.

In addition, 100 sets of cross-sections with SRIM parameters generated by Monte Carlo method (random files) were obtained for each of the libraries.

All obtained data in ENDF and ACE formats can be downloaded from the link https://bwsyncandshare.kit.edu/s/54dyKZS8M4pdFjc.

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1. Introduction

Zirconium hydride ZrH_2 is used in the industry such as nuclear power, aerospace, and metallurgy. In nuclear industry, zirconium hydride is utilized as a moderator or neutron absorber in nuclear reactors [1]. Particularly for fusion reactors, ZrH_2 is considered as one of the promising shield materials [2].

In this paper, the neutron displacement cross-sections for ZrH_2 were obtained for the first time based on the modelling of the number of defects using the BCA approach [3].

The calculations were performed using the SRIM code [3-5] with a modified calculation procedure recommended in the Ref. [6].

The nuclear data required for calculating the recoil spectra were taken from various data libraries: JEFF-4T4 [7], ENDF/B-VIII.1 [8], and JENDL-5 [9]. The displacement cross-sections were calculated using the NJOY code [10,11] with changes made to allow the use of external data files containing the numbers of stable atom displacements, i.e., the results of the modelling.

In addition to the main results, for each general-purpose data library 100 random data files with varied SRIM calculation parameters were obtained, which can be used to estimate the uncertainty of calculating the radiation damage rate.

Section 2 briefly describes the calculation method, including the choice of calculation parameters, Section 3 discusses the calculation results.

2. Brief description of calculations

The calculation of the number of stable defects is discussed in Subsection 2.1 and the calculation of recoil nucleus spectra in Subsection 2.2.

2.1 *Calculation of the number of stable displacements*

2.1.1 *General details of calculation*

The main calculations were carried out using the SRIM/TRIM code [5]. As is known, the code overestimates the number of calculated defects in irradiated materials in *Full Damage Cascade* calculations. The reasons and solutions to this problem were discussed in the works [6,12-16].

The present calculations use the recommendations [6], according to which the method “Modified vacancy.txt” (Table 2, Ref.[6]) is applied to calculate the number of stable defects. In this case, the so-called final energy, E_f, below which an ion is considered to be stopped [17], is chosen equal to average threshold displacement energy E_d, the same one that is included in the NRT formula [18,19].

For this, the following procedure is used:

- after the start of the simulation, the calculation is stopped with the data saved, the file TDATA.SAV is created,
- the TDATA.SAV file is edited as follows: a) all commas in the numbers are replaced with dots which ensures further smooth operation of the code, b) the final energy, the *“Lowest E.”* in the file, is replaced by effective E_d value for the composite material,
- the calculations are continued using the modified TDATA.SAV file.

To calculate the effective values of E_d for the composite material, the empirical formula from the Ref.[20] is used:

$$E_d^{eff} = \left[\sum_i S_i \, E_{d,i}^{-n} \right]^{-1/n},$$

where S_i is the stoichiometry of the material element (i) with a displacement energy $E_{d,i}$, the value of n- value is assumed to be 1 [20]. In the case of ZrH_2, the value of S_{Zr} is equal to 0.3333 and for S_H - 0.6666.

The above procedure was automated to work with a list of primary ion energies, i.e. in the case of ZrH_2 with the energies of zirconium and hydrogen ions. The scripts and necessary programs used in this work are available upon request [21].

Using these programs [21] requires installing the SRIM-2013 program on a PC with the Windows 10 or 11 operating systems.

It is important to note that for the successful operation of SRIM-2013, one must first install an earlier version of the code SRIM-2008 [22]. Installing SRIM-2008 solves all the problems that are partly mentioned in the "SRIM Install Problems" section [5].

2.1.2 *Parameters*

An important calculation parameter is the average value of the threshold displacement energy E_d for zirconium and hydrogen in zirconium hydride ZrH_2.

There appears to be no literature on measuring or modelling these values. One can point to Ref. [23], where threshold displacement energy was obtained by modelling for three crystalline directions.

The averaged E_d value, however, may differ markedly from the values [23]. An illustration is paper [24] in which the E_d value was obtained, however, for a different material.

Table 1 illustrates the threshold displacement energies for various zirconium compounds. The table is purely illustrative, does not pretend to be complete and contains data not only on average but also on other threshold values. It is important to note that the value reported as “averaged threshold displacement energy” by different authors may differ in meaning.

In the present work, the following E_d values were used as a first step to obtain displacement cross sections for ZrH_2: 40 eV for Zr, and 10 eV for H. The rationale for the 40 eV value for zirconium is rather intuitive, and 10 eV for hydrogen is the default value in the SRIM code. The effective threshold energy E_d^{eff} value for ZrH_2 in this case is equal to 13.33 eV.

Standard SRIM values of 3 eV and 6.3 eV were used for lattice binding energy, E_{latt} and surface binding energy, E_{surf} [17], correspondingly. The density of ZrH_2 was assumed to be 5.56 g/cm^3.

The sensitivity of the calculation results to changes in the E_d value for zirconium and hydrogen and the E_{latt} value was also investigated. The values were generated randomly, the value of E_d for zirconium – 40 ± 10 eV, E_d for hydrogen – 10 ± 5 eV, and the value of E_{latt} – 3 ± 1.5 eV. In all cases, the values were sampled with a flat distribution within the specified limits.

2.2 *Calculation of the recoil energy distributions*

The program NJOY [10] was used to calculate the recoil spectra. The HEATR module was modified to use external data files [33] for calculating the displacement numbers. These files were prepared using the SRIM code for Zr and H- ions moving in ZrH_2, as described in the previous section. The modified NJOY code is available on request [11].

Table 1

Threshold displacement energies for zirconium compounds used or obtained by different authors. The “Comment” column indicates the type of value reported in the article or assumed here. The value given by different authors as “average” may differ in meaning.

Material	Component	Threshold energy (eV)	Comment	Reference
ZrC	Zr	35	averaged threshold displacement energy	Gosset [25]
	C	25		
ZrC	Zr	41.5	averaged threshold displacement energy	Jiang [26]
	C	34.5		
ZrC	Zr	37	averaged threshold displacement energies along the main crystallographic directions on the C and Zr sublattices	Zheng [27]
	C	16		
ZrN	Zr	33	Zr and N sublattice weighted average	Rahman [28]
	N	29		
Zr-1at.%Nb	Zr	30.04±11.08	calculated effective threshold displacement energies	Pan [29]
	Nb	21.24±6.02		
$ZrSiO_4$	Zr	98…163	minimum values for different crystallographic directions	Park [30]
	Si	48…100		
	O	23…107		
$Gd_2Zr_2O_7$	Gd	72 ± 13	averaged values for different crystallographic directions	Devanathan [31]
	Zr	121 ± 27		
	O	41 ± 19		
$La_2Zr_2O_7$	La	153	mean values obtained over fourteen different crystallographic directions O: stoichiometric mean value	Chartier [32]
	Zr	188		
	O	42		
ZrH_2	Zr	22.7, 21.5, 24.5	directions [100], [101], [111], correspondingly	Wang [23]
	H	4.6, 5.2, 4.8		

3. Results and discussion

3.1 *Number of stable defects*

The number of defects calculated in different ways for the motion of hydrogen and zirconium ions in ZrH_2 are shown in Fig.1 and Fig.2, respectively. A brief explanation of the figure designations is given below:

- "*SRIM: Full cascades modelling, default, E_f=1 MeV*": the number of stable defects was calculated with SRIM using the default value of the final energy E_f,
- "*SRIM: Full cascades modelling, corrected*": the number of defects was obtained using SRIM, as recommended in Ref.[6] and described above with the value of E_f equal to the effective value E_d^{eff} value 13.33 eV,
- "*SRIM: Quick calculations*": the number of defects was calculated by SRIM using a simplified procedure. In this case, the motion of primary ions is modelled with BCA and the number of defects produced in the material is estimated approximately based on the Kinchin-Pease approach [34]. Despite the fact that the SRIM authors refer to the work [18] when explaining how the number of defects is estimated, it can be assumed that they probably use one of Robinson's formulas [19, 35], which distinguishes between the Z, A values of the ion and the material. Considering that Robinson's formula was obtained for monoatomic materials, its application to a composite material probably introduces additional uncertainty into the calculated number of defects,
- "*IOTA*": the simulation was performed using the IOTA code [36,37].

The figures show that the corrected SRIM calculations are lower than those performed with E_f equal to 1 eV. The results of "*Quick calculations"* are noticeably lower than both of these calculations. The number of defects produced in $H+ZrH_2$ interactions is naturally lower than the number of defects for $Zr+ZrH_2$ irradiation.

Figure 3 shows, at different scales, the number of defects calculated by SRIM with unperturbed and perturbed parameters, as discussed in Section 2. A total of 100 calculations for each of the $H+ZrH_2$ and $Zr+ZrH_2$ interactions were performed with the generated parameters.

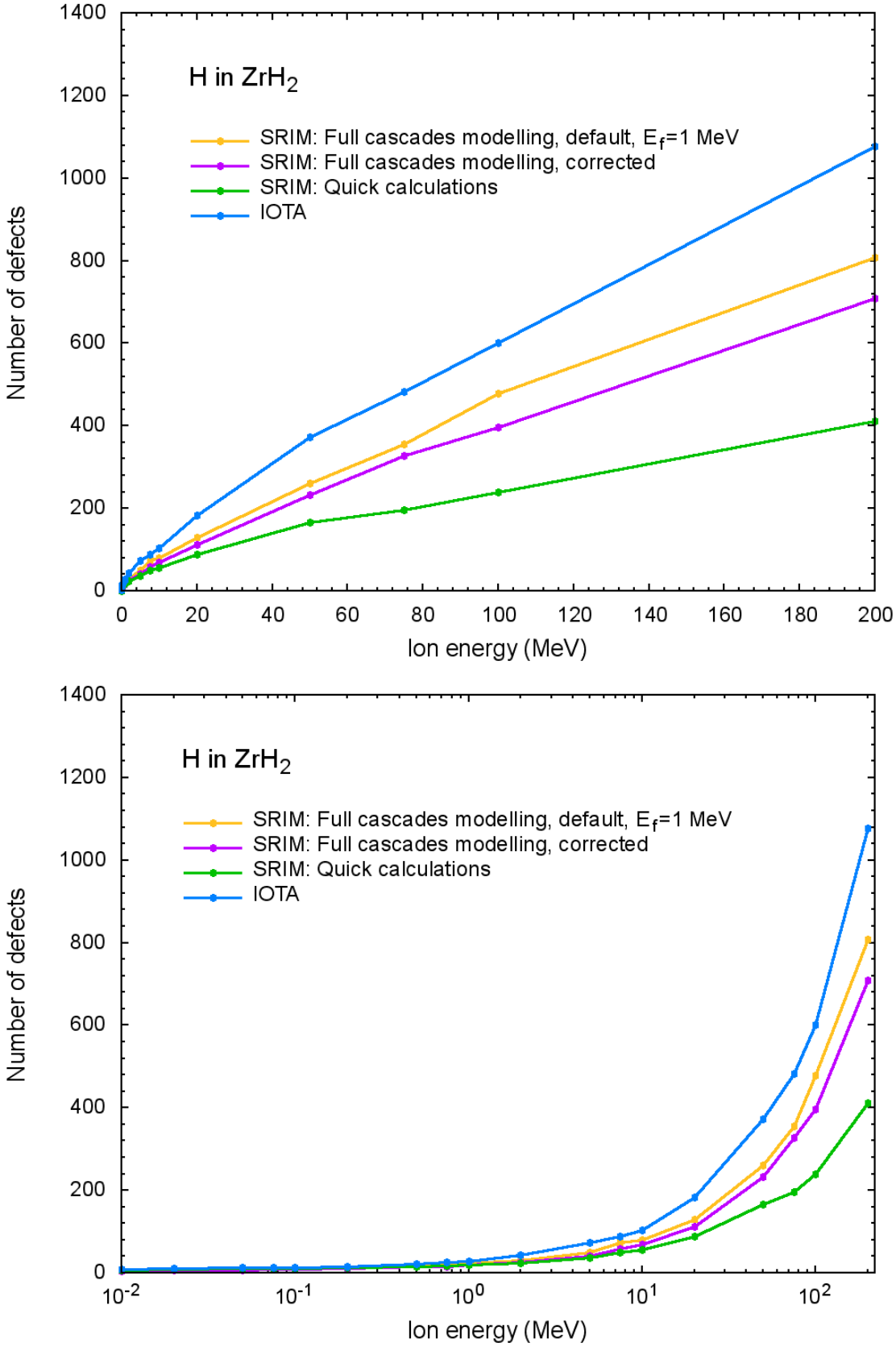

Fig.1 The number of stable defects for H+ZrH_2 interactions calculated using different approaches. The upper figure is in linear-linear scale, in the lower figure the energy is in logarithmic scale. See details in the text.

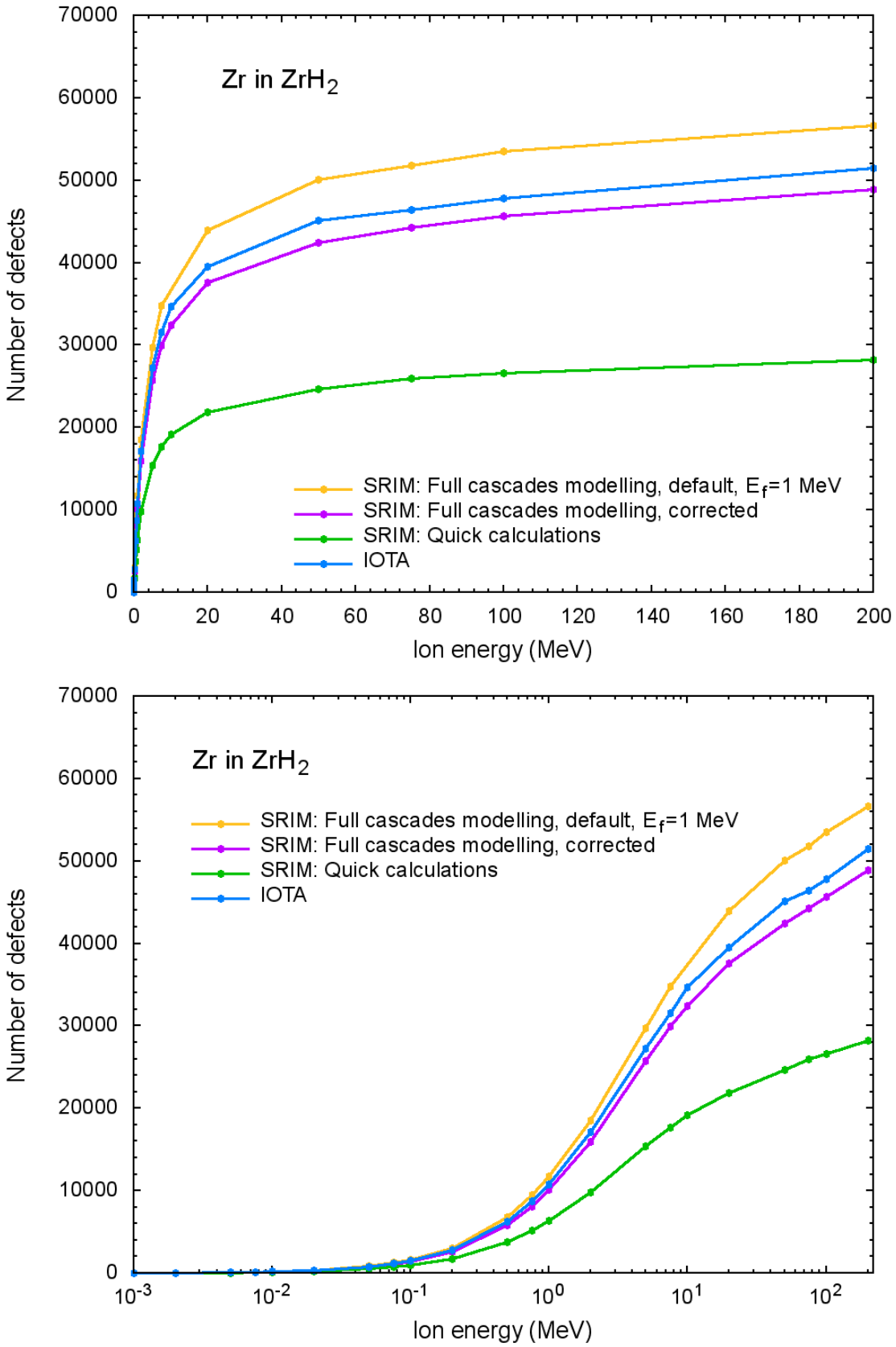

Fig.2 The same as in Fig.1, but for Zr+ZrH_2 interactions.

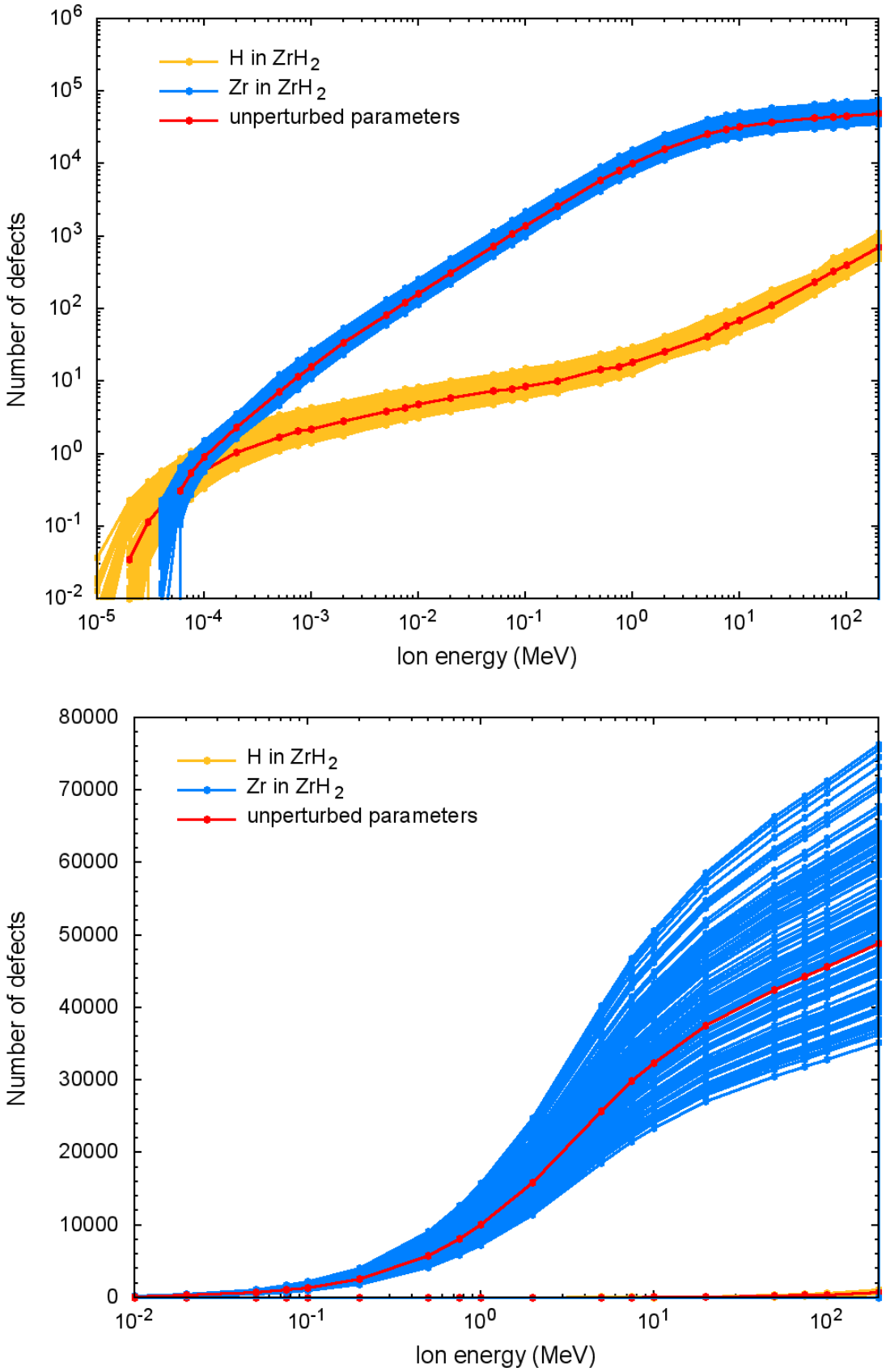

Fig.3 The number of stable defects for $H+ZrH_2$ and $H+ZrH_2$ interactions calculated with perturbed and unperturbed parameters, as discussed in Section 2. The upper figure is in log-log scale, in the lower figure the energy is in logarithmic scale. The number of calculations with perturbed parameters is 100.

3.2 *Components of displacement cross-section*

Using the obtained data for the number of produced defects, the different components of the neutron displacement cross-sections for the zirconium hydride were calculated.

Figure 4 shows the parts of displacement cross-sections for neutron irradiation of zirconium hydride corresponding to the motion of hydrogen ions and zirconium ions in ZrH_2. The neutron data were taken from the JEFF-4T4 library.

The following curves are shown in Figure 4: the calculation results for 100 different sets of generated SRIM parameters; the results corresponding to the unperturbed parameters; the displacement cross-sections obtained using the "usual" NJOY procedure, in which the ion motion in the compound material was not simulated. The green curves in Fig. 4 correspond to the displacement cross-sections calculated for neutron irradiation of hydrogen and zirconium. In this case, hydrogen ions move in hydrogen, and zirconium ions in zirconium. Data for all components were multiplied by 0.3333 for zirconium and by 0.6667 for hydrogen. The results of ordinary NJOY processing are markedly different from more advanced calculations.

It is seen that at neutron energies up to 0.01 MeV the displacement cross-section components for hydrogen PKA exceed the corresponding components for zirconium.

3.3 *Displacement cross-section for zirconium hydride*

The displacement cross-sections for ZrH_2 were calculated using the obtained data for the number of defects and the data from the JEFF-4T4 [7], ENDF/B-VIII.1 [8], and JENDL-5 [9] libraries.

Figure 5 shows the cross-section calculated using the JEFF-4T4 library. The following data are shown:

- "*Data with perturbed parameters*" correspond to 100 different data sets obtained using the SRIM parameters generated by Monte Carlo, as described in Section 2,
- "*Averaged value*" presents the average cross-section calculated using the 100 different displacement cross-sections,

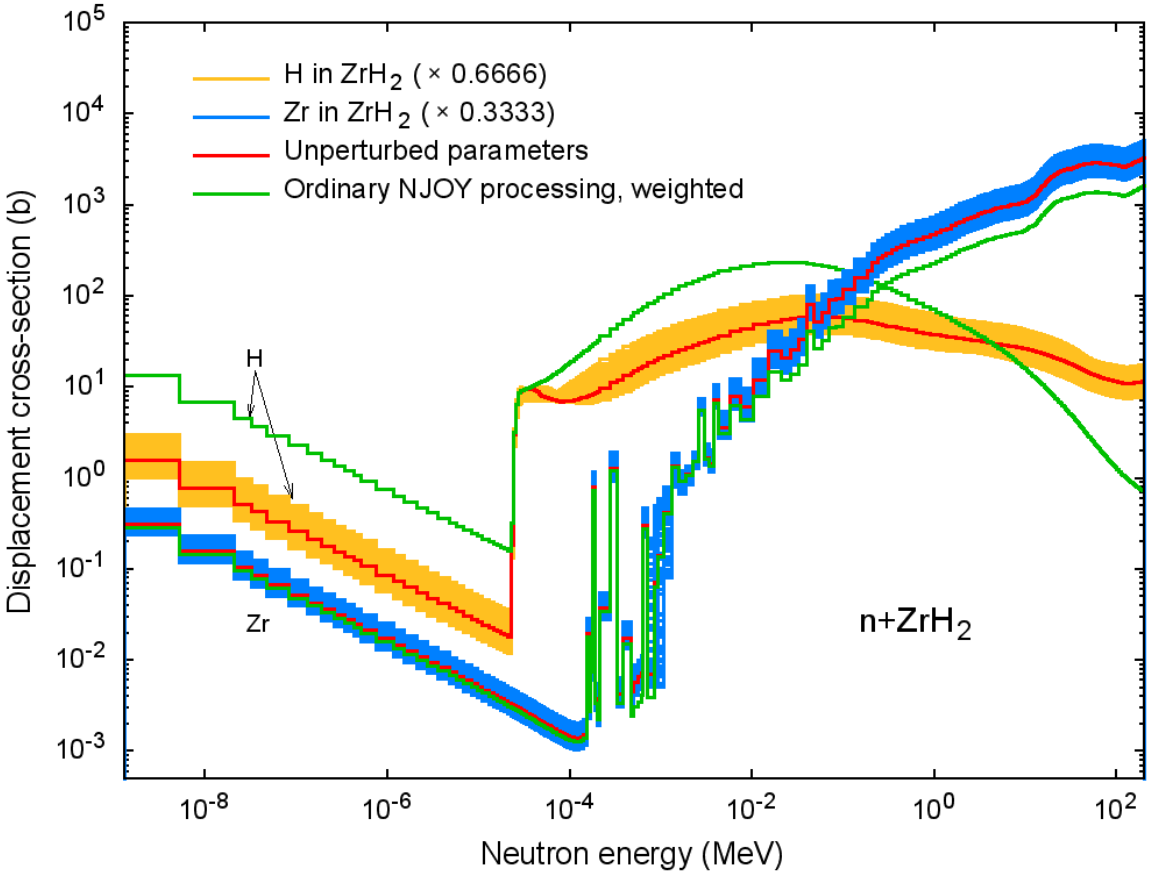

Fig.4 Components of displacement cross-sections for neutron irradiation of zirconium hydride. Nuclear data were taken from JEFF-4T4. See explanations in the text.

- "*Data with unperturbed parameters*" shows the displacement cross-section calculated using SRIM parameters specified in Section 2,

- "*Ordinary NJOY processing*" corresponds to the "usual" procedure for the preparation of displacement cross-section for compounds using NJOY. In this case the weighted sum of the cross-sections for n + H and n + Zr was calculated without taking into account the modelling of the motion of the hydrogen and zirconium PKA in the ZrH_2 compound.

The obtained displacement cross-sections can be downloaded from the site [38]. For each library, data are given in ENDF and ACE formats. The folders contain the following data

\No_SRIM_simulation: The data were obtained using NJOY only. No SRIM calculations were performed. The cross sections were obtained by simple summation of displacement cross-sections calculated separately for different components of the target. The calculation of the number of defects produced by ions in the alloy were not performed. The NRT model was used for each component of the alloy independently of the other parts;

\Unperturbed_parameters: The number of stable displacements was calculated using the SRIM code with corrections proposed in Ref.[6] and described in Section 2. These SRIM parameters were considered as "basic" and were used to obtain random data files recorded in the \Random_files folder.

\Random_files: The SRIM was used to get numbers of stable displacements. The parameters were defined using the MC procedure. The folder also contains a file with displacement cross-sections obtained by averaging data from all random files.

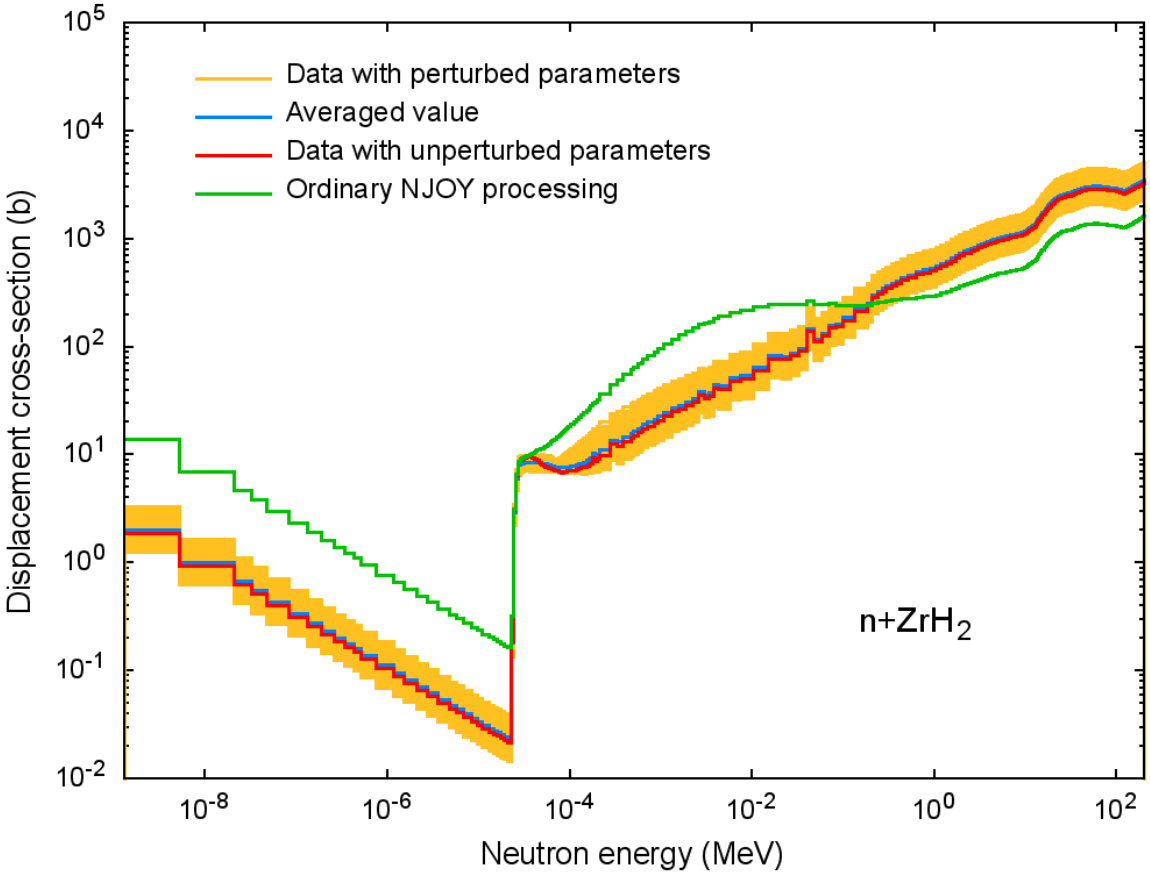

Fig.5 Displacement cross-sections for neutron irradiation of zirconium hydride. Nuclear data were taken from JEFF-4T4. See explanations in the text.

4. Conclusion

The displacement cross-sections for neutron irradiation of zirconium hydride ZrH_2 were obtained. The number of stable defects was calculated using the SRIM program taking into account the recommendations of Ref. [6]. The threshold displacement energy values for zirconium and hydrogen were chosen based on intuitive considerations, Section 2.

The nuclear data were taken from the JEFF-4T4, ENDF/B-VIII.1, and JENDL-5, and thus three different versions of the displacement cross-sections for ZrH_2 were prepared.

Additionally, 100 sets of cross-sections with SRIM parameters generated by MC (random data files) were obtained for each of the libraries.

The obtained data in ENDF and ACE formats can be downloaded from the website [38].

References

[1] Zirconium hydride (ZrH2) powder, www.samaterials.com/zirconia-ceramic/1428-zirconium-hydride.html

[2] T. Hayashi, K. Tobita, S. Nishio, K. Ikeda, Y. Nakamori, S. Orimo, Neutronics assessment of advanced shield materials using metal hydride and borohydride for fusion reactors, *Fusion Engineering and Design* 81, 1285 (2006)

[3] J.F. Ziegler, J.P. Biersack, The stopping and range of ions in matter. In: Bromley, D.A. (eds) Treatise on Heavy-Ion Science. Springer, Boston, MA. (1985) https://doi.org/10.1007/978-1-4615-8103-1_3

[4] J.F. Ziegler, M.D. Ziegler, J.P. Biersack, SRIM – The stopping and range of ions in matter (2010), *Nucl. Instr. Meth. Phys. Res*. B268, 1818 (2010)

[5] J.F. Ziegler, SRIM - The stopping and range of ions in matter (2013) http://www.srim.org/

[6] Y.-R. Lin, S.J. Zinkle, C.J. Ortiz, J.-P. Crocombette, R. Webb, R.E. Stoller, Predicting displacement damage for ion irradiation: Origin of the overestimation of vacancy production in SRIM full-cascade calculations, *Current Opinion in Solid State & Materials Science* 23 100757 (2019)

[7] Joint evaluated fission and fusion (JEFF), nuclear data library, JEFF-4T4 Downloads (2024), https://www.oecd-nea.org/dbdata/jeff/jeff40/t4/

[8] G. Nobre, D. Brown, R. Arcilla, R. Coles, B. Shu, Progress towards the ENDF/B-VIII.1 release, *EPJ Web of Conferences* 294, 04004 (2024)

[9] O. Iwamoto, N. Iwamoto, S. Kunieda, F. Minato, S. Nakayama, Y. Abe, K. Tsubakihara, S. Okumura, C. Ishizuka,T. Yoshida, S. Chiba, N. Otuka, J.-C. Sublet, H. Iwamoto, K. Yamamoto, Y. Nagaya, K. Tada, C. Konno, N. Matsuda, K. Yokoyama, H. Taninaka, A. Oizumi, M. Fukushima, S. Okita, G. Chiba, S. Sato, M. Ohta, S. Kwon, Japanese evaluated nuclear data library version 5: JENDL-5, *Journal of Nuclear Science and Technology* 60, 1 (2023)

[10] NJOY nuclear data processing system (2024), https://github.com/njoy/NJOY2016

[11] A.Yu. Konobeyev, D. Leichtle, Module HEATR of NJOY, with changes for calculating the arc-dpa displacement cross-sections and using external files with the results of modelling the number of stable defects (2024); available upon request at the email: alexander.konobeev@kit.edu

[12] R.E. Stoller, M.B. Toloczko, G.S. Was, A.G. Certain, S. Dwaraknath, F.A. Garner, On the use of SRIM for computing radiation damage exposure, *Nucl. Instr. Meth. Phys. Res*. B310, 75 (2013); Erratum: *Nucl. Instr. Meth. Phys. Res*. B459, 196 (2019)

[13] J.-P. Crocombette, C. Van Wambeke, Quick calculation of damage for ion irradiation: implementation in Iradina and comparisons to SRIM, *EPJ Nuclear Sci. Technol.* 5, 7 (2019); https://doi.org/10.1051/epjn/2019003

[14] W.J. Weber, Y. Zhang, Predicting damage production in monoatomic and multi-elemental targets using stopping and range of ions in matter code: Challenges and recommendations, *Current Opinion in Solid State and Materials Science* 23, 100757 (2019)

[15] S. Agarwal, Y. Lin, C. Li, R.E. Stoller, S.J. Zinkle, On the use of SRIM for calculating vacancy production: Quick calculation and full-cascade options, *Nucl. Instr. Meth. Phys. Res*. B503, 11 (2021)

[16] Y. Sun, S.Z. Diao, P.P. Liu, Q. Zhan , F.R. Wan, Anomalies in the calculation of dpa by using damage energy method based on full-cascades option of SRIM, *Annals of Nuclear Energy* 183, 109667 (2023)

[17] SRIM - Lessons and Tutorials, #4- Calculations of Target Damage, http://www.srim.org/SRIM/Tutorials/SRIM%20Tutorial%204%20-%20Target%20Damage.pdf

[18] M.J. Norgett, M.T. Robinson, I.M. Torrens, A proposed method of calculating displacement dose rates, *Nuclear Engineering and Design* 33, 50 (1975)

[19] M.T. Robinson, Basic physics of radiation damage production, *J. Nucl. Mater.* 216, 1 (1994)

[20] N.M. Ghoniem, S.P. Chou, Binary collision Monte Carlo simulations of cascades in polyatomic ceramics, *J. Nucl. Mater.* 155–157, 1263 (1988)

[21] A.Yu. Konobeyev, D. Leichtle, Scripts and auxiliary programs for performing calculations using the SRIM code with a list of primary ion energies (2024); available upon request at the email: alexander.konobeev@kit.edu

[22] J.F. Ziegler, Download SRIM software. See “DOWNLOAD SRIM-2008” on the page http://www.srim.org/SRIM/SRIMLEGL.htm

[23] X. Wang, M. Tang, M.-X. Jiang, Y.-C. Chen, Z.-X. Liu, H.-Q. Deng, Properties of radiation defects and threshold energy of displacement in zirconium hydride obtained by new deep-learning potential, *Chinese Physics* B33, 076103 (2024)

[24] K. Nordlund, J. Wallenius, L. Malerba, Molecular dynamics simulations of threshold displacement energies in Fe, *Nucl. Instr. Meth. Phys. Res*. B246, 322 (2006)

[25] D. Gosset, M. Dolle, D. Simeone, G. Baldinozzi, L. Thome, Structural evolution of zirconium carbide under ion irradiation, *J. Nucl. Mater.* 373, 123 (2008)

[26] M. Jiang, H.Y. Xiao, H.B. Zhang, S.M. Peng, C.H. Xu, Z.J. Liu, X.T. Zu, A comparative study of low energy radiation responses of SiC, TiC and ZrC, *Acta Materialia* 110, 192 (2016),

[27] M.-J. Zheng, I. Szlufarska, D. Morgan, Ab initio prediction of threshold displacement energies in ZrC, *J. Nucl. Mater.* 471, 214 (2016)

[28] M.M. Rahman, T. Yamamoto, S. Matsumura, J.M. Costantini, K. Yasuda, Ab Initio molecular dynamics study of threshold displacement energy in Zirconium Nitride, *J. Nucl. Mater.* 554, 153076 (2021)

[29] R. Pan, M. Zhou, J. Cui, B. Fu, Q. Hou, J. Qin, X. Kong, C. Ma, Q. Wang, L. Wu, Unveiling the characteristics of the residual point defects of collision cascade in Zr-xNb binary system: A molecular dynamics study, *J. Nucl. Mater.* 584, 154546 (2023)

[30] B. Park, W.J. Weber, L.R. Corrales, Molecular-dynamics simulation study of threshold displacements and defect formation in zircon, *Phys. Rev.* B64, 174108 (2001)

[31] R. Devanathan, W.J. Weber, Insights into the radiation response of pyrochlores from calculations of threshold displacement events, *Journal of Applied Physics* 98, 086110 (2005)

[32] A. Chartier, C. Meis, J.-P. Crocombette, Atomistic modeling of displacement cascades in $La_2Zr_2O_7$ pyrochlore, *Phys. Rev.* B67, 174102 (2003)

[33] A.Yu. Konobeyev, D. Leichtle, Neutron NRT and arc-dpa displacement cross-sections for JEFF-4, EFFDOC-1540, (2024), https://www.oecd-nea.org/dbdata/nds_effdoc/effdoc-1540.pdf

[34] G.H. Kinchin, R.S. Pease, The displacement of atoms in solids by radiation, *Rep. Prog. Phys.* 18, 1 (1955)

[35] M. Robinson, The dependence of radiation effects on primary recoil energy, radiation induced voids in metals, US Atomic Energy Commission, *AEC Symposium Series* 26, 397 (1972)

[36] C.H.M. Broeders, A.Yu. Konobeyev, K. Voukelatou, IOTA - a code to study ion transport and radiation damage in composite materials, FZKA-6984 (2004); https://publikationen.bibliothek.kit.edu/270058614

[37] A.Yu. Konobeyev, U. Fischer, Yu.A. Korovin, S.P. Simakov, IOTA-2017: a code for the simulation of ion transport in materials, KIT Scientific Working Papers 63 (2017), https://publikationen.bibliothek.kit.edu/1000077011

[38] A.Yu. Konobeyev, D. Leichtle, P. Pereslavtsev, Neutron displacement cross-sections for ZrH_2, KIT (2025): https://bwsyncandshare.kit.edu/s/54dyKZS8M4pdFjc

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