On the use of SRIM for calculating arc-dpa exposure

E. Mitsi[a,b], K. Koutsomitis[b], G. Apostolopoulos[b,*]

[a]*Department of Physics, National Technical University of Athens, Zografou Campus, EL-15780 Athens, Greece*
[b]*Institute of Nuclear and Radiological Science and Technology, Energy, and Safety, N.C.S.R. "Demokritos", EL-15310 Agia Paraskevi, Greece*

Abstract

We propose two methods for evaluating athermal recombination corrected (arc) displacement damage parameters in ion irradiations employing the computer code SRIM (Stopping and Range of Ions in Matter). The first method consists of post-processing the detailed SRIM output for all simulated damage events and re-calculating according to the arc damage model. In the second method, an approximate empirical formula is devised which gives the average displacements in the arc damage model as a function of the corresponding quantity according to the standard Norgett-Robinson-Torrens model, which is readily obtained from SRIM.

Keywords: Displacements per atom (dpa), Athermal recombination corrected dpa, Ion irradiation, SRIM

1. Introduction

In studies of radiation effects in materials it is generally desirable to have a standardized parameter to quantify radiation damage exposure, that would provide a common basis for comparison of data obtained under different irradiation conditions in terms of impinging particle type and energy. Currently, the internationally accepted standard parameter for this purpose is the number of displacements per atom (dpa) calculated according to the Norgett-Robinson-Torrens (NRT) model [1]. In the case of ion irradiation, one of the most widely used software tools for estimating the NRT-dpa exposure is the Monte Carlo code SRIM (Stopping and Range of Ions in Matter) [2]. SRIM incorporates the NRT model and readily provides the NRT-dpa value for a given ion irradiation. Its popularity is based on the fact that it employs accurate ion stopping powers and on its user-friendly interface. Several authors [3–8] have discussed the application of SRIM for accurate NRT-dpa calculations.

Recently, a modification to the NRT model has been proposed, the athermal recombination corrected dpa (arc-dpa) [9, 10]. It addresses a well known issue of NRT, namely, the overestimation of the number of stable defects generated by high energy displacement cascades. The arc-dpa model is based on evidence from experimental studies and computer simulations, which indicates that significant defect recombination takes place during the cascade cool-down phase leading to reduced numbers of remaining stable defects. Currently, there is no standardized way to compute arc-dpa exposure in ion irradiations as the model has not yet been implemented in any of the widely used software tools. In their original publication introducing the new model, Nordlund et al. [9] already proposed a method to indirectly estimate the arc-dpa parameter based on the output of standard SRIM simulations. Their implementation consisted of two main parts. First, a series of SRIM simulations were performed to evaluate the energy deposited by primary knock-on atom (PKA) recoils as target displacements. This is also called damage energy, T_d, and must be obtained as a function of the initial PKA recoil energy, E_R, for a given target material. In [9] this was done for Fe and an interpolating function was devised to obtain T_d as a function of E_R continuously for recoil energies up to 300 keV. In the second part of the calculation, the information obtained on T_d is used in post-processing of the SRIM output file "COLLISON.TXT" to finally obtain the arc-dpa values.

In this paper, we propose two alternative methods to calculate arc-dpa exposure using SRIM. The first one is also based on the COLLISON.txt file, similarly to the method in [9]. However, instead of separately computing T_d by interpolation, we use the damage energy values that are internally calculated in SRIM with the Lindhard-Scharff-Schiøtt (LSS) approximation [11]. Thus, the damage energy interpolation for different target materials is not required. The second method is based on an approximate formula that we propose, which can be employed to estimate directly the arc-dpa exposure based on the corresponding NRT-dpa value. Thus, the cumbersome handling of the COLLISON.txt file is avoided. The two methods are tested on all targets for which arc-dpa model parameters are available and for a range of projectile ions.

*Corresponding author
Email address: gapost@ipta.demokritos.gr (G. Apostolopoulos)

Ion	H	He	Al	Fe	Au
E_0 (MeV)	1	1	3	5	10

Table 1: Projectile ions and corresponding incident energies E_0.

Target	Fe	Ni	Cu	Pd	W	Pt
E_d (eV) [9]	40	40	29	41	90	44
b [12]	-0.568	-1.01	-0.68	-0.88	-0.56	-1.12
c [12]	0.286	0.23	0.16	0.15	0.12	0.11

Table 2: Displacement threshold, E_d, and arc-dpa model parameters, (b, c), of simulated targets.

2. Radiation Damage Models

The NRT model gives the number of stable displacements, ν_d, produced by a PKA recoil with damage energy T_d as:

$$\nu_d(T_d) = \begin{cases} 0 & \text{for } T_d \leq E_d \\ 1 & \text{for } E_d < T_d \leq L \\ T_d/L & \text{for } T_d > L \end{cases} \quad (1)$$

where E_d is the displacement threshold energy, i.e., the minimum energy required to displace an atom from its lattice position. $L = 2E_d/0.8$ denotes the cascade multiplication threshold above which more than one stable displacements are generated by the PKA.

In the arc-dpa model, the 3^{rd} branch of (1) is multiplied by an energy dependent efficiency factor, $\xi \leq 1$. The model definition is summarized in the following two relations:

$$\nu_{d,\mathrm{arc}}(T_d) = \begin{cases} 0 & \text{for } T_d \leq E_d, \\ 1 & \text{for } E_d < T_d \leq L, \\ \xi(T_d/L) \cdot T_d/L & \text{for } T_d > L, \end{cases} \quad (2)$$

$$\xi(x) = (1-c)\, x^b + c, \quad \text{for } x \geq 1. \quad (3)$$

The parameters b and c are material constants that have been determined for a number of target materials by Nordlund et al. [12]. Their values are given in table 2.

We note that for damage energies above the displacement threshold, $T_d > E_d$, $\nu_{d,\mathrm{arc}}(T_d)$ can be compactly written as

$$\nu_{d,\mathrm{arc}}(T_d) = \nu_d(T_d) \cdot \xi\left[\nu_d(T_d)\right]. \quad (4)$$

This definition will be utilized in the following paragraphs.

3. SRIM simulation conditions and data handling

All simulations were performed utilizing SRIM-2013 and employing the option "Ion distribution and Quick calculation of damage" (Q-C). Lattice and surface binding energies were set equal to zero according to the recommendation in [3]. A range of projectile ions were employed, with atomic numbers varying from $Z = 1$ (H) to 79 (Au) and energies ranging from $E_0 = 1$ to 10 MeV, similarly to the work of Agarwal et al. [8]. The ions and corresponding energies are listed in Table 1. Table 2 shows all the targets that we tested, which are essentially all materials whose arc-dpa parameters were estimated in [12]. Target thickness was chosen appropriately in order to ensure that the impinging ions stop within the examined region. The target displacement energies, E_d, are based on internationally recommended standard values and are also given in Table 2. In the case of Fe self-ion irradiation, an extra simulation with $E_0 = 78.7$ keV was also performed in order to directly compare with results from [9]. For each ion/target combination 10,000 ion histories were run.

Damage parameters were extracted from the SRIM output files, either VACANCY.txt or COLLISON.txt. Table 3 lists all quantities of interest and the way they are calculated depending on the damage model and the output file used.

The number of PKAs per ion, N_{PKA}, is obtained by integrating the 2nd data column of VACANCY.txt ("vacancies by ions", ν_i) or by dividing the number of data rows, N_{rows}, in COLLISON.txt by the number of simulated ions, N_{ions}. N_{PKA} is independent of the damage model.

The NRT displacements per ion, N_d, is obtained as follows. In the case of VACANCY.txt, N_d is found by summing the 2^{nd} and 3^{rd} column of the data table, i.e., "vacancies by ions", ν_i, and "vacancies by recoils", ν_r, respectively. Regarding the COLLISON.txt file, N_d is calculated by adding up the "Target vacancies", ν_d, of all PKAs and dividing by N_{ions}. Finally, the average displacements per PKA, $\langle\nu_d\rangle$, is equal to N_d/N_{PKA}.

The calculation of arc-dpa damage parameters is described in the next section.

All evaluations and the parsing of SRIM output files were performed in the OCTAVE computing environment [13]. The open source python code PYSRIM [14] was employed to automate the SRIM calculations. All relevant data and code are available in ZENODO.

4. Methods and Results

In this section, we present the two different methods to obtain arc-dpa damage parameters from SRIM output.

4.1. Method 1 (M1)

This method utilizes the COLLISON.txt output file. In SRIM Q-C mode, this file lists all simulated PKA scattering events and reports, among other data, the number of displacements, ν_d, generated per event. These ν_d values, labelled "Target vacancies", are calculated according to the NRT model, eq. (1), with the damage energy, T_d, obtained from the approximate LSS theory [15]. For the ν_d values in COLLISON.txt that satisfy $\nu_d > 1$, we can easily recover the LSS damage energy by multiplying ν_d with the cascade multiplication factor, L (cf. eq. (1)). Then, the obtained T_d can be used in eq. (2) to evaluate the displacements according to the arc-dpa model. This is

Quantity	Symbol	Method 2 (M2) VACANCY.txt	Method 1 (M1) COLLISON.txt
PKAs per ion	N_{PKA}	$\sum_k [\nu_i]_k \, \Delta x$ †	$N_{\mathrm{rows}}/N_{\mathrm{ions}}$
		NRT-dpa model	
Displacements per ion	N_d	$\sum_k [\nu_i + \nu_r]_k \, \Delta x$ †	$N_{\mathrm{PKA}} \langle \nu_d \rangle$
Mean displacements per PKA	$\langle \nu_d \rangle$	N_d/N_{PKA}	$N_{\mathrm{rows}}^{-1} \sum_k [\nu_d]_k$ ‡
		arc-dpa model	
Displacements per ion	$N_{d,arc}$	$\langle \nu_{d,arc} \rangle \cdot N_{\mathrm{PKA}}$	
Mean displacements per PKA	$\langle \nu_{d,arc} \rangle$	eq. (7) with $\langle \nu_d \rangle$ as above	$N_{\mathrm{rows}}^{-1} \sum_k [\nu_d]_k \, \xi([\nu_d]_k)$ ‡

† $[\nu_i]_k$ and $[\nu_r]_k$ are the "vacancies by ions" and "vacancies by recoils", respectively, in the k-th target depth bin, with Δx denoting the bin width.

‡ $[\nu_d]_k$ denotes the number of vacancies estimated by SRIM for the k-th PKA event. The sum is over all events.

Table 3: Calculation of damage parameters from SRIM output files

essentially what is done in M1, however, instead of actually evaluating T_d we employ ν_d directly in the equivalent arc-dpa definition, eq. (4). Thus, the steps to calculate the arc-dpa parameters are as follows:

1. Run SRIM with the "Quick calculation of damage" (Q-C) option.
2. Parse the COLLISON.txt output file to obtain the NRT displacements per PKA event, ν_d.
3. Calculate the corresponding $\nu_{d,\mathrm{arc}}$ per PKA from eq. (4), $\nu_{d,\mathrm{arc}} = \nu_d \cdot \xi(\nu_d)$.
4. Take the average of the $\nu_{d,\mathrm{arc}}$ values to obtain the mean displacements per PKA according to the arc-dpa model, $\langle \nu_{d,\mathrm{arc}} \rangle$ (cf. Table 3).
5. Multiply by the number of PKAs per ion, N_{PKA}, to obtain the number of displacements per ion, $N_{d,arc} = \langle \nu_{d,\mathrm{arc}} \rangle \cdot N_{\mathrm{PKA}}$

M1 is very similar to the method proposed by Nordlund et al. [9]. The main difference lies in the derivation of damage energy. In [9], T_d is obtained by separate SRIM simulations employing the "Detailed Calculation with Full Damage Cascades" (F-C) option. In this case, SRIM utilizes detailed stopping power calculations for all secondary recoils in the PKA cascade, thus, the value of T_d is potentially more accurate. Agarwal et al. [8] have made a detailed comparison of SRIM damage calculations in Q-C and F-C modes. They found that there is a difference of up to ±25% in the amount of NRT vacancies predicted by the two modes, when vacancy production is estimated by the SRIM damage energy. The authors attributed the difference to the use of the LSS approximation in Q-C mode. It is expected that also in the present case, where the arc-dpa damage estimation in M1 is based on the Q-C damage energy, there will be similar differences with respect to the procedure described in [9], where the F-C mode was employed.

To make a quantitative comparison of the two approaches, we repeated the simulation of 78.7 keV Fe ions incident on an Fe target that was employed in [9]. Table 4 shows the results from the two approaches. It is seen that there is only a small 2% difference in the NRT parameters, N_d and $\langle \nu_d \rangle$, obtained with the present method in comparison to the values reported in [9], while the corresponding arc-dpa parameters almost coincide. We attribute the good agreement to the low damage energies occurring in this simulation. To have a more meaningful comparison, we simulated self-ion Fe irradiation with a much higher projectile energy, $E_0 = 5$ MeV, and evaluated the results with both our proposed method M1 and the one by Nordlund et al. [9]. In the latter case, we used the data from their fig. 1.2 to extend the interpolation of T_d to target recoil energies up to 10 MeV. The results are also listed in Table 4. As seen from the table, there is a 10% difference between the NRT parameters obtained by our M1 and the evaluation according to [9]. This difference is comparable to the observations of [8] and thus can be attributed to the use of approximate LSS damage energy in the Q-C simulation mode. The corresponding arc-dpa parameters exhibit a similar but slightly lower difference of about 8%. This is due to the fact that the arc-dpa efficiency lowers the significance of high energy damage events, where the errors due to the LSS approximation are more pronounced.

Method 2 (M2)

The objective of M2 is to provide a quick estimate of the arc-dpa damage parameters, without having to resort

	E_0	N_{PKA}	N_d	$\langle\nu_d\rangle$	$N_{d,arc}$	$\langle\nu_{d,\mathrm{arc}}\rangle$
Nordlund et al. [9]			539	12.2†	217	4.93†
This study - Method 1	78.7 keV	44.1	530	12.0	217	4.92
This study - Method 2			530	12.0	209	4.74
Method of Nordlund et al. [9]			8800	20.0	3150	7.14
This study - Method 1	5 MeV	442	7870	17.9	2900	6.56
This study - Method 2			7870	17.9	2890	6.54

† Mean values are calculated by dividing N_d and $N_{d,arc}$ from [9] by N_{PKA} as obtained in the present study.

Table 4: Damage parameters obtained by different methods for the irradiation of an Fe target with Fe ions of energy E_0.

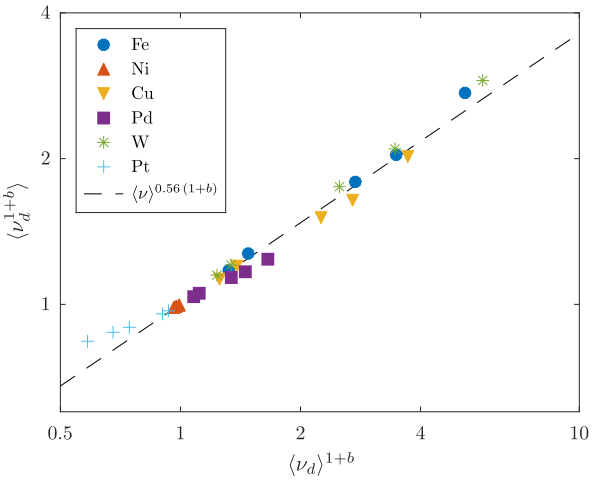

Figure 1: $\langle\nu_d^{1+b}\rangle$ as a function of $\langle\nu_d\rangle^{1+b}$, where ν_d denotes the NRT displacements and b is the arc-dpa model parameter of the corresponding target material. Both quantities were obtained by post-processing the output of SRIM simulations and averaging over all PKA events. Results for the different target materials are depicted with different symbol and color. The dashed line corresponds to the approximate relation (6).

to the cumbersome processing of COLLISON.txt. For this, we note that from eq. (4) the average arc-dpa can be written:

$$\langle\nu_{d,\mathrm{arc}}\rangle = (1-c)\langle\nu_d^{1+b}\rangle + c\cdot\langle\nu_d\rangle. \tag{5}$$

Thus, to obtain $\langle\nu_{d,\mathrm{arc}}\rangle$ the value of $\langle\nu_d^{1+b}\rangle$ is needed. We performed an approximate calculation of this quantity, employing a power-law cross-section for the ion-target atom interaction and ignoring the effect of ionization losses, i.e., setting $T_d \approx T$. As shown in Appendix A, the following approximation

$$\langle\nu_d^{1+b}\rangle \approx \langle\nu_d\rangle^{\lambda(1+b)}, \tag{6}$$

where $\lambda \approx 0.56$, gives adequate results for a wide range of incident ion energies and ion-target combinations. This can be seen in fig. 1, where $\langle\nu_d^{1+b}\rangle$ is plotted as a function of $\langle\nu_d\rangle^{1+b}$ for all the ion/target combinations simulated in the current work. The data shown in the figure have been obtained by taking the ν_d values per PKA event listed in COLLISON.txt and evaluating the required averages. As seen from the figure, the data from all simulated targets lie within $\pm 10\%$ of the approximate eq. (6), which is depicted by the dashed line.

Utilizing the above approximation, the arc-dpa damage parameters can be obtained by the following prescription:

1. Run SRIM with the "Quick calculation of damage" (Q-C) option.
2. Calculate the NRT-$\langle\nu_d\rangle$ from VACANCY.txt as described in Table 3.
3. Obtain $\langle\nu_{d,\mathrm{arc}}\rangle$ from eq. (5), substituting the approximate relation (6):

$$\langle\nu_{d,\mathrm{arc}}\rangle \approx (1-c)\langle\nu_d\rangle^{0.56(1+b)} + c\cdot\langle\nu_d\rangle \tag{7}$$

4. The number of displacements per ion is $\langle\nu_{d,arc}\rangle \cdot N_{\mathrm{PKA}}$

Fig. 2 depicts the ratio of $\langle\nu_{d,\mathrm{arc}}\rangle$ calculated by the two methods, M2 and M1, respectively, for all simulated ion/target combinations. It is seen that the results of the approximate method M2 deviate by at most 3% from those of M1. A similar small deviation can be observed in Table 4 between the arc-dpa damage parameters obtained by methods M1 and M2 in the two simulated Fe self-ion irradiations. In the low energy case the arc-dpa parameters obtained by M2 are 4% lower than those of M1 while in the high energy example the two methods produce essentially equivalent results. Thus, the method M2 can be employed for a quick, approximate evaluation of arc-dpa damage, introducing an error of not more than a few percent compared to the more detailed method M1.

5. Conclusions

In this work, we present two methods for evaluating arc-dpa damage parameters in ion irradiations employing the SRIM simulation code with the option "Quick calculation of damage" (Q-C).

The first method is based on SRIM's COLLISON.txt output file, which lists the NRT displacements, ν_d, produced in each simulated primary knock-on atom (PKA) recoil event. The ν_d values are converted to the corresponding arc-dpa model prediction, $\nu_{d,\mathrm{arc}}$, by means of eq.

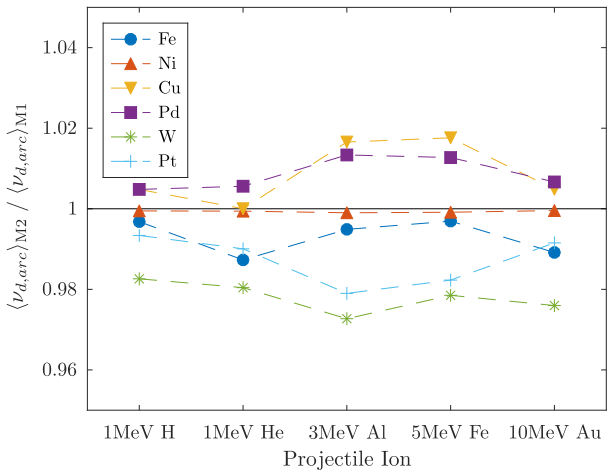

Figure 2: The ratio of the average displacements per PKA according to the arc-dpa model, $\langle \nu_{d,\mathrm{arc}} \rangle$, obtained by methods M2 and M1. Results for the different target materials are depicted with different symbol and color.

(4) and then averaged to obtain the total damage parameters. This procedure is similar to the one proposed by Nordlund et al. [9] only in our case the damage energy is essentially obtained by the LSS approximation employed in SRIM's Q-C mode, whereas in [9] the damage energy was interpolated from the results of separate detailed SRIM simulations. Thus, our method gains in simplicity but can lead to errors due to the approximation in the damage energy calculation. The errors in the estimated damage could be up to $\sim 30\%$ [8].

In the second method, we devise an approximate relation, which gives $\langle \nu_{d,\mathrm{arc}} \rangle$ directly as a function of $\langle \nu_d \rangle$. Thus, the cumbersome processing of the COLLISON.txt file is not needed since the NRT damage parameter $\langle \nu_d \rangle$ can be easily obtained from VACANCY.txt. We found that the arc-dpa parameters obtained by this approximate method differ by not more than a few percent from those calculated by the first method.

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). 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.

Appendix A. Approximation of $\langle \nu_d^{1+b} \rangle$

The general expression for the average $\langle \nu_d^n \rangle$ is given by

$$\langle \nu_d^n \rangle = \frac{\int_{Ed}^{T_m} [\nu_d(T_d)]^n \, d\sigma(E,T)}{\int_{Ed}^{T_m} d\sigma(E,T)}, \tag{A.1}$$

where $d\sigma(E,T)$ denotes the cross-section for scattering of an ion with initial energy E producing a PKA with recoil energy T. T_m is the maximum PKA recoil energy. Making the following assumptions:

(i) A power-law cross-section, $d\sigma(E,T) \propto dT/T^{1+p}$, where p ranges from 0.5 (heavy ions) to 1 (light ions) [16]
(ii) Ionization losses can be ignored ($T_d \approx T$)

and performing the integrations in eq. (A.1) we obtain the following analytical expression:

$$\langle \nu_d^n \rangle = \frac{(L/E_d)^p - 1 + \frac{p}{p-n}\left[1 - (L/T_m)^{p-n}\right]}{(L/E_d)^p - (L/T_m)^p}, \tag{A.2}$$

which is valid for $T_m \geq L$ and $n \neq p$. In the special case $n = p$ it becomes

$$\langle \nu_d^n \rangle = \frac{(L/E_d)^n - 1 - n\log(L/T_m)}{(L/E_d)^n - (L/T_m)^n}. \tag{A.3}$$

Based on eqs. (A.2)-(A.3) we calculate $\langle \nu_d^{1+b} \rangle$ for several representative (b,p) combinations and for T_m values in the range $L < T_m < 10^4 L$. This corresponds to a maximum T_m of $\sim 10^6$ eV in Fe and similar values for other metals. The results are shown in fig. A.3 as a function of $\langle \nu_d \rangle^{1+b}$, where $\langle \nu_d \rangle$ is also obtained from (A.2). It is apparent from the figure that all curves follow roughly a central line. Fitting a power law of the form:

$$\langle \nu_d^{1+b} \rangle \approx A \, \langle \nu_d \rangle^{\lambda\,(1+b)}, \tag{A.4}$$

to the data, with A and λ as adjustable parameters, we obtain the values $\lambda \approx 0.56$ and $A \approx 1.0$. This is denoted by the dashed line in fig. A.3. The deviation of the analytically calculated $\langle \nu_d^{1+b} \rangle$ from the fitted power law is within ± 0.2, which corresponds to the shaded area in fig. A.3.

References

[1] M. J. Norgett, M. T. Robinson, I. M. Torrens, A proposed method of calculating displacement dose rates, Nuclear Engineering and Design 33 (1975) 50–54. URL: http://www.sciencedirect.com/science/article/pii/0029549375900357. doi:10.1016/0029-5493(75)90035-7.

[2] J. F. Ziegler, M. D. Ziegler, J. P. Biersack, SRIM – The stopping and range of ions in matter (2010), Nuclear Instruments and Methods in Physics Research Section B: Beam Interactions with Materials and Atoms 268 (2010) 1818–1823. URL: http://www.sciencedirect.com/science/article/pii/S0168583X10001862. doi:10.1016/j.nimb.2010.02.091.

[3] R. E. Stoller, M. Toloczko, G. S. Was, A. Certain, S. Dwaraknath, F. Garner, On the use of SRIM for computing radiation damage exposure, Nuclear Instruments and Methods in Physics Research Section B: Beam Interactions with Materials and Atoms 310 (2013) 75–80. URL: http://www.sciencedirect.com/science/article/pii/S0168583X13005053. doi:10.1016/j.nimb.2013.05.008.

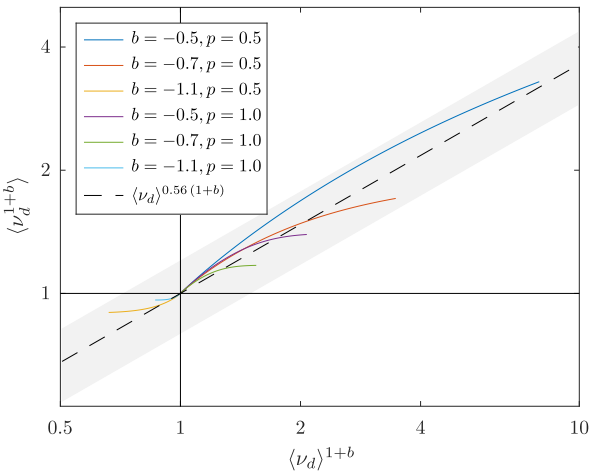

Figure A.3: Curves of $\langle \nu_d^{1+b} \rangle$ from eqs. (A.2)-(A.3) as a function of $\langle \nu \rangle^{1+b}$ for different values of the parameter b and the power-law cross-section exponent, p. The dashed line is a fit to eq. (A.4).

[4] Y. G. Li, Y. Yang, M. P. Short, Z. J. Ding, Z. Zeng, J. Li, IM3D: A parallel Monte Carlo code for efficient simulations of primary radiation displacements and damage in 3D geometry, Scientific Reports 5 (2015). URL: https://doi.org/10.1038%2Fsrep18130. doi:10.1038/srep18130.

[5] 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 (2019). doi:10.1016/j.cossms.2019.06.001.

[6] J.-P. Crocombette, C. Van Wambeke, Quick calculation of damage for ion irradiation: implementation in Iradina and comparisons to SRIM, EPJ Nuclear Sciences & Technologies 5 (2019) 7. URL: https://doi.org/10.1051%2Fepjn%2F2019003. doi:10.1051/epjn/2019003.

[7] R. E. Stoller, M. Toloczko, G. S. Was, A. Certain, S. Dwaraknath, F. Garner, Erratum to "On the use of SRIM for computing radiation damage exposure" [Nucl. Instrum. Methods Phys. Res. B 310 (2013) 75–80], Nuclear Instruments and Methods in Physics Research Section B: Beam Interactions with Materials and Atoms 459 (2019) 196–197. doi:10.1016/j.nimb.2019.08.015.

[8] 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, Nuclear Instruments and Methods in Physics Research Section B: Beam Interactions with Materials and Atoms 503 (2021) 11–29. URL: https://doi.org/10.1016%2Fj.nimb.2021.06.018. doi:10.1016/j.nimb.2021.06.018.

[9] K. Nordlund, A. E. Sand, F. Granberg, S. J. Zinkle, R. E. Stoller, R. S. Averback, T. Suzudo, L. Malerba, F. Banhart, W. J. Weber, F. Willaime, S. L. Dudarev, D. Simeone, Primary radiation damage in materials: Review of current understanding and proposed new standard displacement damage model to incorporate in cascade defect production efficiency and mixing effects, Technical Report, IAEA, 2015. URL: https://www.oecd-nea.org/science/docs/2015/.

[10] K. Nordlund, S. J. Zinkle, A. E. Sand, F. Granberg, R. S. Averback, R. E. Stoller, T. Suzudo, L. Malerba, F. Banhart, W. J. Weber, F. Willaime, S. L. Dudarev, D. Simeone, Primary radiation damage: A review of current understanding and models, Journal of Nuclear Materials 512 (2018) 450–479. URL: http://adsabs.harvard.edu/abs/2018JNuM..512..450N. doi:10.1016/j.jnucmat.2018.10.027.

[11] J. Lindhard, M. Scharff, H. E. Schiøtt, RANGE CONCEPTS AND HEAVY ION RANGES (NOTES ON ATOMIC COLLISIONS, II), Kgl. Danske Videnskab. Selskab. Mat. Fys. Medd. 33, no. 14 (1963).

[12] K. Nordlund, S. J. Zinkle, A. E. Sand, F. Granberg, R. S. Averback, R. E. Stoller, T. Suzudo, L. Malerba, F. Banhart, W. J. Weber, F. Willaime, S. L. Dudarev, D. Simeone, Improving atomic displacement and replacement calculations with physically realistic damage models, Nature 9 (2018). URL: https://doi.org/10.1038/s41467-018-03415-5. doi:10.1038/s41467-018-03415-5.

[13] J. W. Eaton, D. Bateman, S. Hauberg, R. Wehbring, GNU Octave version 7.1.0 manual: a high-level interactive language for numerical computations, 2022. URL: https://www.gnu.org/software/octave/doc/v7.1.0/.

[14] C. Ostrouchov, Y. Zhang, W. J. Weber, pysrim: Automation, analysis, and plotting of srim calculations, Journal of Open Source Software 3 (2018) 829. doi:10.21105/joss.00829.

[15] J. F. Ziegler, M. D. Ziegler, J. P. Biersack, SRIM–The stopping and range of ions in matter (2008).

[16] G. S. Was, Fundamentals of Radiation Materials Science, Springer, 2017. doi:10.1007/978-1-4939-3438-6.