Predicting displacement damage for ion irradiation: Origin of the overestimation of vacancy production in SRIM full-cascade calculations

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Predicting displacement damage for ion irradiation: Origin of the overestimation of vacancy production in full-cascade calculations[☆]

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Highlights

- Improper thresholds in vacancy production calculations lead to excessive vacancies and minimal replacements.
- Overestimation of vacancies in SRIM F-C vacancy text file is likely caused by a coding error or incorrect threshold energy.
- Modifying the SRIM and Iradina codes by setting final and replacement energies to the displacement energy can reconcile vacancy calculations.
- A new open-source software for vacancy production calculations, based on a modified version of Iradina, has been developed. (IRAD: https://code.ornl.gov/liny/irad)

Abstract

Ion irradiation and implantation have wide applications that demand accurate determination of displacement damage profile and distribution of implanted ion concentration. The prediction of vacancies is especially important to determine displacement per atom (dpa), the standard parameter of primary radiation damage in materials. However, significant discrepancies exist in estimations of vacancies between full-cascade (F-C) and quick calculation (Q-C) options in the popular computer code SRIM. This study inspected the SRIM code and a relatively new code called Iradina which uses a similar methodology, to develop an understanding of the origin of vacancy overestimation in SRIM F-C. We found that using the default values of thresholds (namely final energy in SRIM and replacement energy in Iradina) in displacement production calculations results in excessively large number of calculated vacancies and very few replacements. After conducting multiple calculations using SRIM, Iradina, and MARLOWE (all based on the binary collision approximation), a comparison of the results indicates that there may be a coding error and improper threshold energy in SRIM F-C. This issue is responsible for the deficiency of replacements observed in the SRIM F-C results. Drawing on the principles of collision physics, we propose recommendations for modifying the source codes to address these issues.

Keywords: ion irradiation; dpa (displacements per atom); radiation damage; SRIM; nuclear materials

1 Introduction

SRIM, first developed by Ziegler et al. [1], is widely used to simulate the interaction of energetic ions in matter. It has been applied in ion irradiation effects research [2], even though it was developed primarily for use in other ion beam applications such as ion implantation for semiconductor doping [3], ion beam materials modification [4], ion beam analysis of materials [5] and ion beam therapy [6]. However, studies have found that SRIM's full-cascade mode prediction for vacancy production is much higher than obtained with other simulations [7-10]. This discrepancy in SRIM was discovered by comparing the full-cascade (F-C) and quick calculation (Q-C) modes using the standard "vacancy.txt" method [7]; significant discrepancy did not occur when using the SRIM F-C damage energy method [7, 9]. Furthermore, no error was found for the Q-C mode in either the vacancy.txt or damage energy methods. The excessive number of vacancies (by more than a factor of 2) predicted by the SRIM F-C "vacancy.txt" method is inconsistent with results from the MARLOWE binary collision approximation code [11] and molecular dynamics (MD) simulations [12]. This discrepancy is significant because it results in errors in the calculation of displacement per atom (dpa), the international standardized parameter of primary radiation damage in materials [13]. A recent extensive evaluation recommended applying the damage energy method if calculations are performed using the SRIM F-C mode [9]. Evidence that the SRIM F-C vacancy.txt file was incorrectly classifying replacement events as vacancies was also presented in Ref. [9]. However, the origin of the overestimation of vacancy production in SRIM F-C calculation has remained unclear as the SRIM source code is not available for public inspection.

SRIM uses Monte Carlo simulation methods based on the binary collision approximation, considering the path of incident and recoil ions in each collision and assuming a straight path

between collisions [1]. It provides valuable predictions on the distribution of implanted ion concentration, energy loss depth profiles (partitioned between electronic and nuclear processes), dpa depth profiles, and other relevant information like sputtering rate, and the total energy dissipated by ionization and in phonon production. For irradiation effects research, SRIM can be used to calculate the average damage energy (T_d) or number of vacancies (ν_{NRT}) at a specific penetration depth for dpa calculation. Based on the NRT model [13], for $\frac{2E_d}{\kappa} < T_d < \infty$, the total number of Frenkel pairs (vacancies or displacements) can be calculated using the equation

$$\nu_{NRT} = \frac{\kappa\, T_d}{2E_d} \tag{1}$$

where κ is the displacement efficiency with a value of 0.8, and E_d is the displacement energy.

Despite the problem of vacancy overestimation, the F-C option is desirable due to the use of an advanced stopping power database for both primary ions and recoil atoms, and is also advantageous since it provides a detailed record of all collisions. Because the SRIM code has not been open to the public since it was developed in the 1980s, the source code could not be inspected or modified by general users. Recently, several alternative vacancy production and ion range codes (e.g., Iradina [14], IM3D [15], RaT [10], BCA-MD [16]) have been developed. Among these codes, the calculations of Iradina (an open-source code modified from the Corteo code [17]) showed good agreement with SRIM for both Q-C and F-C options [14]. The objective of this study is to conclusively determine the source of vacancy overestimation in SRIM F-C vacancy.txt calculations and provide a reliable physics-based method for dpa calculation based on the binary collision approximation. The numbers of vacancies and replacements estimated by SRIM and Iradina are compared to the results from MD and MARLOWE [18] (a versatile benchmark binary collision approximation code) using different values of the Frenkel pair

spontaneous recombination radius. A new graphical user interface, IRAD, has been developed for a revised Iradina code to quickly perform dpa and ion concentration calculations. In a broader perspective, an accurate standard method for converting ion fluence to a quantitatively comparable damage parameter (e.g., displacements, vacancies, and replacements) for various materials is critically important to understand the fundamentals of ion-matter interaction and radiation damage of materials.

2 Methodology

This study used SRIM-2013 and Iradina-CEA with either Q-C or F-C options for computations. Input parameters for a given projectile and target were kept consistent across all calculations with 10,000 injected ions to ensure good statistics. We conducted irradiation calculations for a UO_2 composite target using 1 MeV Xe ions, and for various targets (atomic numbers 3-92) using 2, 5, or 10 MeV Fe ions. The ion beam was directed perpendicular to the surface and all ions were stopped within the target. Table 1 lists the input parameters for each SRIM and Iradina calculation. The displacement energies (E_d), lattice binding energies (E_b), and surface binding energies (E_s) were taken from Agarwal et al. [9]. According to SRIM documents [19], E_d is the minimum energy required to displace a target atom far enough from its lattice site to prevent immediate return, while E_b is the minimum energy needed to remove an atom from its lattice site, taking into account the energy required to break electronic bonds. Additionally, E_s has been defined to reflect the fact that the energy required to remove an atom from its lattice site on the target surface is lower than that needed if it were located inside the solid, surrounded by other atoms. Agarwal et al. [9] reported that the calculations using the Q-C option were not influenced by E_b, whereas the vacancy production moderately decreased as E_b increased (from 0

to 5 eV) when using the F-C option. The effective displacement energy (E_d^{eff}) of multi-elemental targets for the damage energy method was calculated using Ghoniem and Chou's [20] empirical equation:

$$E_d^{eff} = \left[\sum_i S_i / E_d^i\right]^{-1} \quad (2)$$

where S_i and E_d^i are the stoichiometric fraction and displacement energy of the ith target elements, respectively. As an example, for UO_2, the calculation results in an effective displacement energy of approximately 26 eV, which is calculated as $E_d^{eff} = 1/\left[\left(\frac{1}{3}\times\frac{1}{60}\right)+\left(\frac{2}{3}\times\frac{1}{20}\right)\right] \cong 25.7\ eV$.

Table 1. Input parameters for SRIM and Iradina calculations for various targets.

Target	Atomic number (Z)	Mass (amu)	Atomic density ($\times 10^{22}$ atoms/cm^3)	Displacement energy (eV)	Surface binding energy (eV)	Lattice binding energy (eV)
Li	3	7.02	4.63	25	1.6	1.1
C	6	12.00	11.29	40	7.4	11.0
Al	13	26.98	6.03	25	3.4	2.3
Si	14	27.98	4.97	33	4.7	7.0
V	23	50.94	7.05	40	5.3	5.4
Fe	26	55.94	8.48	40	4.3	5.8
Ni	28	57.94	9.13	40	4.5	5.9
Cu	29	62.93	8.45	20	3.5	4.4
Se	34	79.92	3.67	40	2.4	3.0
Mo	42	97.91	6.41	60	6.8	10.5
Nd	60	141.91	2.93	40	3.2	3.0
W	74	183.95	6.34	90	8.6	13.2
Au	79	196.96	5.90	40	3.8	3.8
Pb	82	207.97	3.29	25	2.0	2.1

U	92	238.05	4.82	60	5.4	2.6
UO_2	92/8	238/16	7.38	26	4.0	2.0

Based on the recommendation in Ref. [9], three different methods were used to calculate dpa or number of vacancies in SRIM. The first method, called the vacancy.txt method, involves using the SRIM output file "VACANCY.txt" to obtain vacancy numbers, which are calculated using Eq. 1 for SRIM Q-C. Note that SRIM F-C vacancy.txt method disregards the use of Eq. 1 for calculating the vacancy number. Instead, it evaluates the results for each collision by moving ions in the solid. If the energies of both the incident ion after the collision and the recoiling target atom are above E_c (the required kinetic energy to be imparted to the struck atom), then a vacancy is produced at that lattice site. The second and third methods in Table 2 are classified as damage energy methods and require manual computation of the damage energy (T_d) in Eq. 1. These values can be determined by subtracting the recoil ionization from the kinetic energy transferred to the recoil ions (hereafter called “recoil damage energy”) or by using the phonon energy calculated by SRIM for the recoil ions (hereafter called “phonon energy”). Table 2 provides a summary of the three methods and the necessary SRIM output files for calculating the number of vacancies. The Appendix of the present study provides a detailed comparison of different methods for calculating damage energy.

Table 2. Summary of three methods used for dpa or vacancy calculations using SRIM

Methods	Required SRIM output files	Calculations
Vacancy.txt	“VACANCY.txt”	Add the “Ion Element Knock-Ons” column and the “Target Element Vacancies” column together to obtain the number of vacancies (ν_{NRT})

Recoil damage energy	"E2RECOIL.txt" and "IONIZ.txt"	Subtract the integration of "IONIZ. by RECOILS" column from the "Energy Absorbed by Target Element" column to manually calculate the damage energy (T_d) for Eq. 1
Phonon energy	"PHONON.txt"	Subtract the integration of "PHONONS by ION" column from the "PHONONS by RECOILS" column to manually calculate the damage energy (T_d) in Eq. 1

As summarized in Table 3, the definition of a replacement collision and the conditions that must be met for the production of replacements in SRIM and Iradina are similar. As illustrated in Fig. 1, the energy of the projectile atom is denoted as E_1 and that of the recoil atom as E_2. Their corresponding atomic species are represented as Z_1 and Z_2, respectively. In the same figure, the pink dashed arrow represents a potential path for replacement production. If the energy of E_1 is less than E_d, the projectile atom will return to the position of the stuck atom via path "a" and produce a replacement. If E_2 is less than E_d, the recoil atom will return to its original position through path "b" (orange dashed arrow) but this is described as a subthreshold displacement event. This is because the atom that hops into the struck target atom position is the same atom that initially occupied that lattice position, resulting in no discernible change in the lattice compared to the situation prior to the collision.

Table 3. Comparison of replacement collision calculations in SRIM and Iradina. The energies of the projectile and recoil atoms are indicated as E_1 and E_2, and their atomic species are identified as Z_1 and Z_2, respectively.

	SRIM [19]	Iradina [14, 21]
Definition of replacements	"If the incident atom is the same element as the atom that it hits, then the incident atom might transfer its energy to the target atom, knock it out of its lattice site, and the incident atom will then take its place in the lattice, while the hit atom moves on."	Projectile and recoil are of the same type, and the projectile loses so much energy to the recoil that its remaining kinetic energy is below E_d, then the projectile is assumed to replace the recoil on its lattice site.
Related threshold energy	Final energy (E_f)	Replacement energy (E_r)
Conditions for producing replacements	(1) The projectile and recoil atoms are of the same type ($Z_1 = Z_2$). (2) Neither the projectile nor the recoil atoms are classified as subthreshold displacements (3) The projectile atom must have less energy than the final energy ($E_1 < E_f$) when it stops. (4) The recoil atom must have sufficient energy to create a stable vacancy ($E_2 > E_d$).	(1) The projectile and recoil atoms are of the same type ($Z_1 = Z_2$). (2) Neither the projectile nor the recoil atoms are classified as subthreshold displacements (3) The projectile has energy less than lattice energy ($E_1 < E_r$) (4) The value of E_r is set to be equal to E_b. The value of E_r is -1 eV by default, which serves as a flag for the code to assign E_r the same value as E_b.

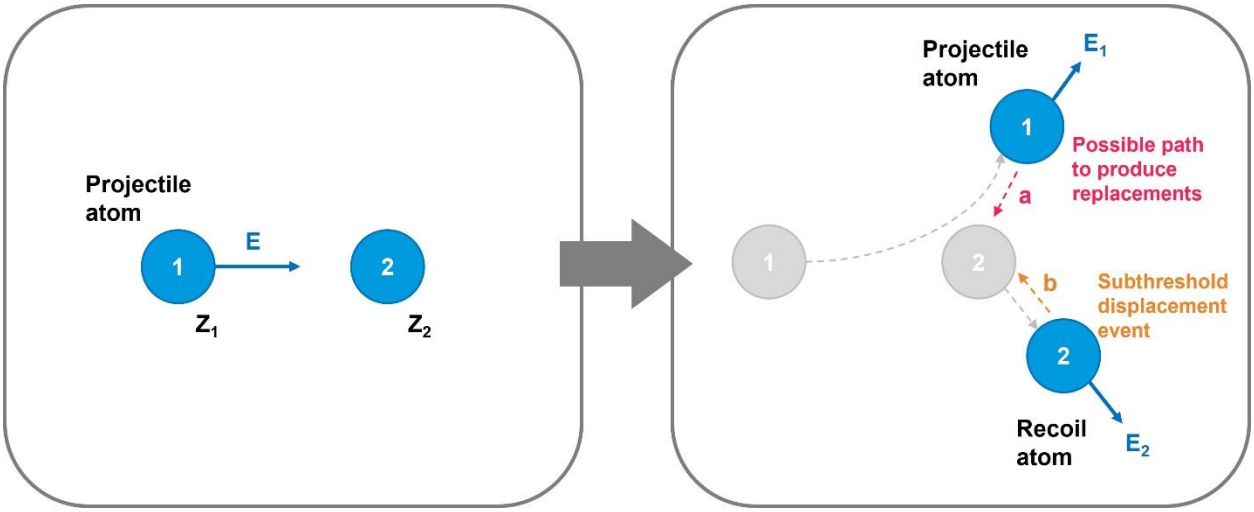


Fig 1. Schematic showing collision between initial incident ion with energy E and resulting energies of projectile atom (E_1) and recoil atom (E_2), with atomic species represented by Z_1 and Z_2. Pink and orange arrows denote (a) possible paths for replacement productions and (b) subthreshold displacement event, respectively.

In SRIM simulations, the final energy (E_f) plays a role in determining the number of vacancies and replacements. E_f represents the energy threshold below which a moving atom is considered to be at rest [19]; this parameter is assigned a value of E_f= 1 eV in the SRIM F-C program and is not a user-provided variable. Iradina uses the replacement energy (E_r) as a new parameter defined in the CEA version [14], whereas earlier versions used E_d for the replacement calculations instead of E_r [21]. The Iradina parameter E_r is assigned a default value of -1 eV which serves as a flag for the code to assign E_r the same value as E_b (which by default is 3eV). E_r has a distinct meaning from E_f and is exclusively used for replacement calculations in Iradina. In Iradina, there is another parameter known as the minimum energy (E_m) that has been defined to represent the energy threshold at which a moving atom is considered to come to a complete stop. The default minimum energy value in Iradina is 2 eV. From a kinematics perspective, E_f in SRIM and E_r in Iradina serve the same purpose in the replacement calculation

algorithm of both codes. A replacement can be generated when E_1 is less than E_f or E_r for SRIM and Iradina, respectively.

From a physics perspective, ions with energies below E_d are not capable of inducing a displacement, although they could induce a replacement. In both the SRIM F-C and Iradina codes, a vacancy is subtracted every time a replacement is produced. To check the accuracy of these codes, we manually changed the limits for E_f and E_r to E_d to examine their impact on calculated vacancies and replacements. If the codes are correctly written, this change should have no effect on the calculated vacancy production. The default values of E_r in Iradina and E_f in SRIM are -1 eV and 1 eV, respectively. In SRIM-2013, the steps to reset the E_f value to E_d or another value are: (1) start a simulation, then exit and save the data. (2) edit the TDATA.SAV file where a line "Lowest E, Ed (min) (eV)" will list two values "x, y". (3) change the "x" value to reset the E_f value to the desired value, e.g., E_d. (4) re-run the saved SRIM calculation. For the Iradina code, E_r can be changed in the "Materials.in" input file before starting a simulation. Note that in Iradina code, E_r is set to E_b (lattice binding energies) if it is below E_b. Default E_r value of -1 eV signals the code to assign it the same value as E_b.

For the MARLOWE calculations, 2 MeV Fe ions were launched at 0 K onto a monocrystal Fe target in 1,000 cascades, with an incident angle of 7° to avoid channeling. Recombination radius (r_v), the distance at which a Frenkel pair recombines spontaneously, was systematically varied in the range of 0 to $3.3a_0$ (where a_0 is the lattice parameter of BCC Fe) for the MARLOWE calculations. Note that SRIM and Iradina do not rely on the Frenkel pair separation distance criterion when determining whether vacancies or replacements occur. Instead, they base their evaluations simply on the recoil energies of the incident particle and recoiling lattice atom (compared to E_d). The threshold displacement energy and recombination

distance concepts are closely related, as the threshold displacement energy for production of a stable Frenkel pair primarily depends on the energy required to separate a Frenkel pair beyond the spontaneous recombination distance (i.e., E_d is several times larger than the sum of the vacancy and interstitial formation energies). For the ion energy used in this study, the kinetic energy of Fe ions exceeds 25 keV/amu, and the default model in MARLOWE cannot accurately predict the electronic stopping power. To address this issue, we used a specialized module within MARLOWE that accounts for a wide range of velocities and masses. For more information about this module, please refer to Ref. [22].

3 Results

Fig. 2 compares the predicted vacancy production profiles of 2 MeV Fe into Fe (Fig. 2a) and 1 MeV Xe into UO_2 (Fig. 2b) using the SRIM F-C simulation. The results show the difference between the default final energy $E_f = 1\ eV$ and revised $E_f = E_d$ using both the vacancy.txt method (V) and recoil damage energy method (E). The results indicate that using the full cascade option in SRIM with default E_f, the vacancy.txt method calculated 1.4-1.7 times more vacancies near the peak damage region (~625 nm and ~ 100 nm for Fe and UO_2, respectively) compared to the damage energy method. However, when E_f was set to E_d, the vacancy.txt method (filled squares) produced fewer vacancies compared to the default E_f (open squares) and became comparable to the values calculated by the recoil damage energy method. No significant (>5%) difference was observed between the two profiles using the recoil damage energy method with the default $E_f = 1\ eV$ (open circles) and revised $E_f = E_d$ (filled circles). Therefore, the workaround approach to terminate the SRIM calculations for energy below E_d largely fixes the SRIM F-C problem with overestimation of vacancies. It is worth noting that the

near-surface (<120 nm depth for UO_2) anomaly of the vacancy profiles using the recoil damage energy method was not found in the profile predicted by the F-C(V) method with revised E_f.

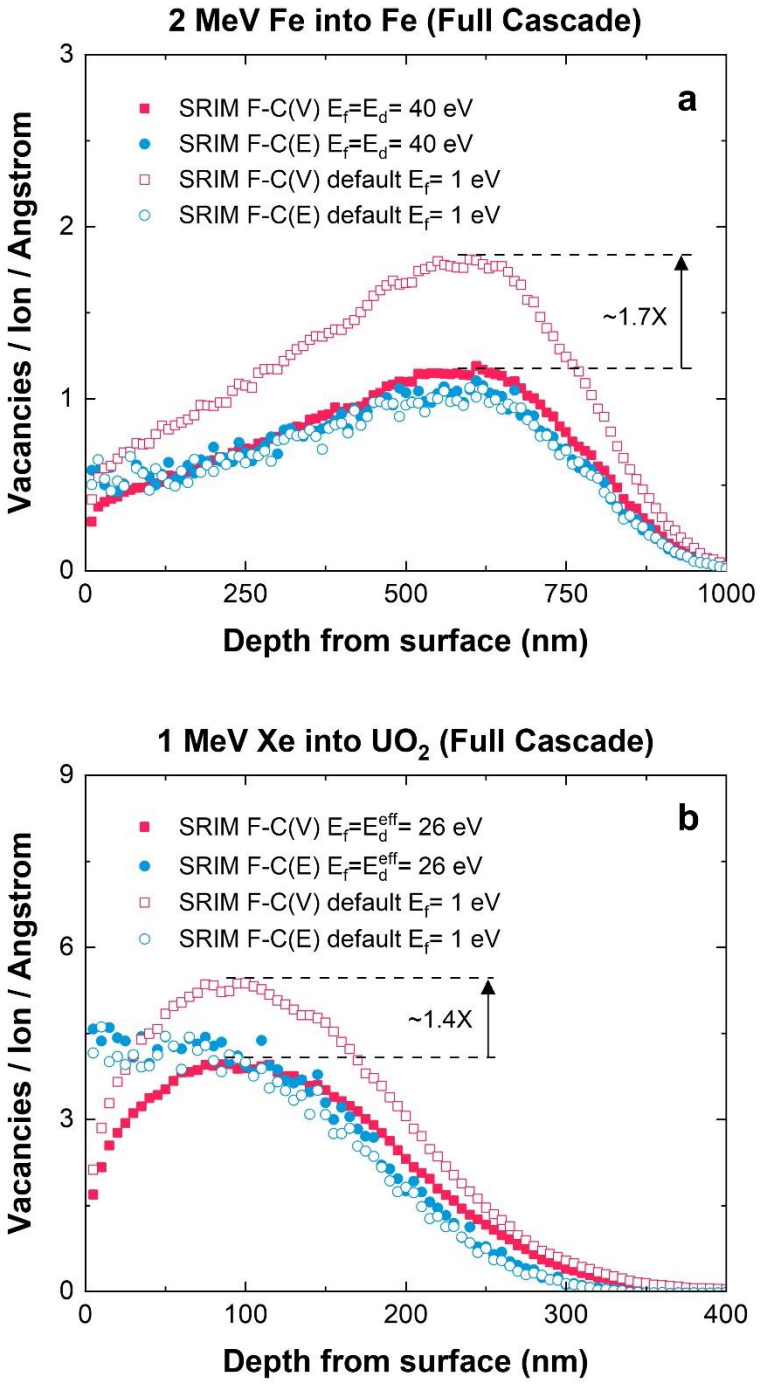


Fig 2. Depth-dependent vacancy production for (a) 2 MeV Fe in Fe and (b) 1 MeV Xe in UO_2 estimated with SRIM full cascade calculations. Comparison between SRIM vacancy.txt (F-C(V); square) and recoil damage energy (F-C(E); circle) methods, with default E_f = 1 eV (open symbol) and revised $E_f = E_d$

(filled symbol). E_f and E_d are the final energy and displacement energy, respectively. Effective displacement energy E_d^{eff} calculated using the empirical equation from Ghoniem and Chou (U: 60 eV, O: 20 eV).

The Iradina code was further used to examine the vacancy production discrepancy between $E_f = 1\ eV$ and $E_f = E_d$ observed in SRIM calculations (Fig. 2). The replacement energy (E_r) in Iradina, which seems to be identical (only for vacancy calculation) to the final energy (E_f) parameter in SRIM, was changed from the default value of -1 eV to E_d. The comparison between Iradina and SRIM full cascade calculations for the Fe and UO_2 test cases with default and revised E_r and E_f values is given in Fig. 3. The results from Iradina and SRIM clearly show similar trends for the default and revised E_r and E_f values. The Iradina F-C predictions with $E_r = -1\ eV$ (filled squares) and $E_r = E_d$ (filled circles) agreed with the SRIM calculation with the default $E_f = 1\ eV$ using vacancy.txt method (open squares) and recoil damage energy method (open circles), respectively. Similar to the depth profiles in Fig. 2, Fig. 3 shows a notable variance between the default and revised E_r calculations up to a factor of 1.4-1.7. The recoil damage energy method could not be easily evaluated for the Iradina calculations because the depth profile of beam energy lost to target atoms and ionization energy cannot be directly obtained from the Iradina output files. All vacancy production profiles predicted by Iradina in this study were plotted directly using the Iradina output files for the calculated number of vacancies.

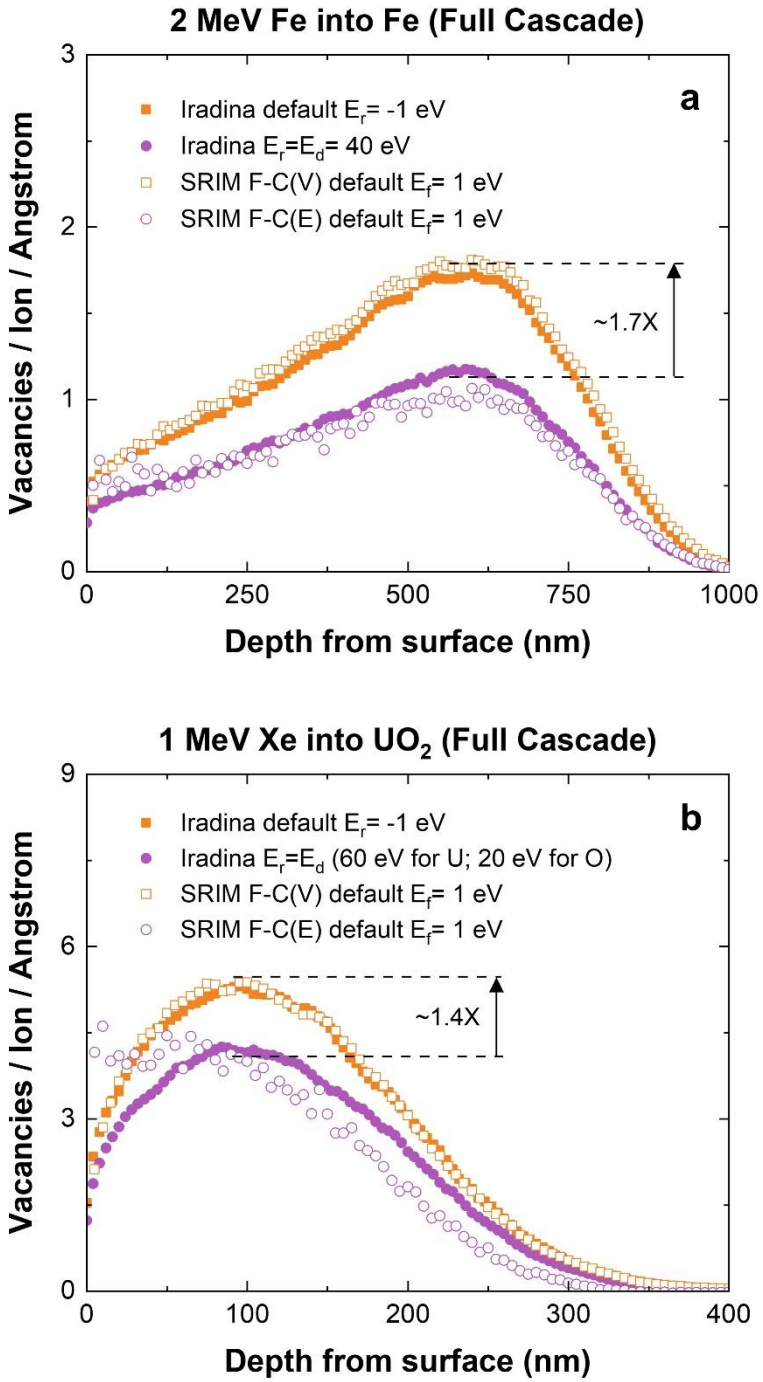
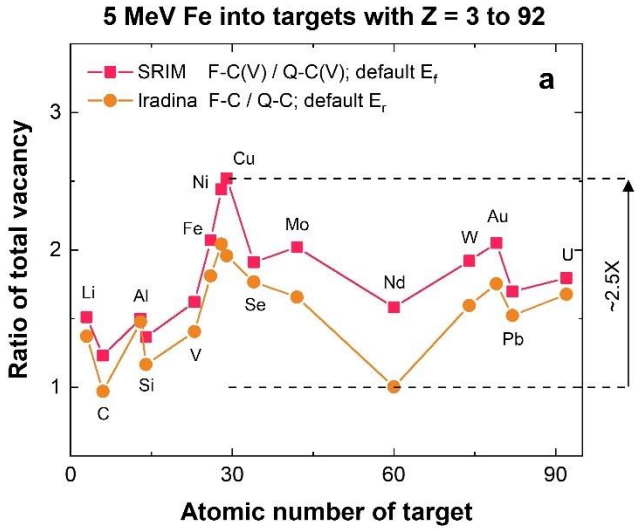
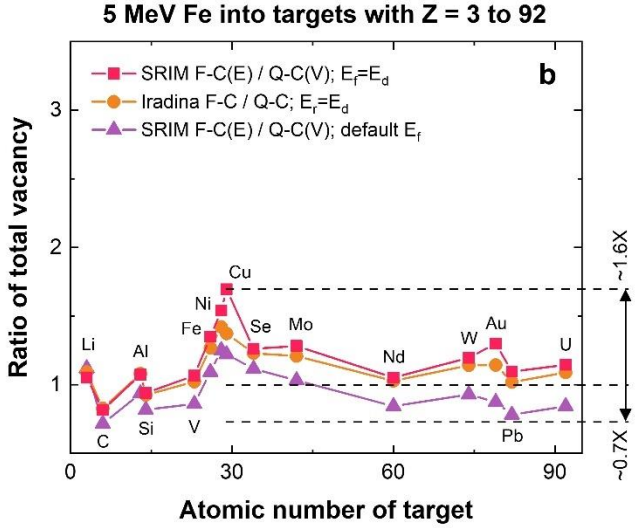


Fig 3. Depth-dependent vacancy production profiles for (a) 2 MeV Fe in Fe and (b) 1 MeV Xe in UO_2 estimated with full cascade calculation. Iradina results with default E_r = -1 eV (filled square) and revised E_r = E_d (filled circle) are compared to SRIM vacancy.txt method (F-C(V); open square) and recoil damage energy method (F-C(E); open circle). E_r and E_d represent the replacement energy and displacement energy, respectively.

To confirm the impact of the proposed correction of E_f and E_r, SRIM and Iradina calculations were performed with 5 MeV Fe on 15 different elemental targets (atomic numbers 3-92). Fig. 4 compares the F-C to Q-C total vacancy ratio (integrated over the full ion range) using the vacancy.txt method and recoil damage energy method, and with default and revised E_f and E_r values. Using the default E_f and E_r values (Fig. 4a), both SRIM F-C(V) and Iradina overpredicted vacancy production compared to the damage energy method (ratios up to 2.5 and 2, respectively). With revised E_f and E_r values (Fig. 4b), the ratios decreased to a maximum of ~1.6 and ~1.4 for SRIM F-C(V) and Iradina, respectively. The overall ratios are between 0.7-1.6 with some systematic oscillations with respect to the target atomic number (Z). In Fig. 4b, the SRIM F-C(V) and Iradina F-C ratios tend to be slightly higher than the SRIM F-C(E) (filled triangle). Excluding Cu and Ni, all targets had ratios between 0.8 to 1.2 for the SRIM F-C(V) and Iradina F-C calculations with revised E_f and E_r (Fig. 4b). This indicates there is only minor deviation between F-C and Q-C options when the proposed correction of the E_f and E_r terms is applied. The results depicted in Figs. 3 and 4 also suggest that Iradina and SRIM generally were in good agreement for the two cases. Nevertheless, certain targets, such as Ni, Cu, and Nd, show a relatively large disparity. According to the findings in Ref. [9], the Z-oscillation observed in Fig. 4a are primarily attributed to discrepancies in stopping power. Similarly, in Fig. 4b, this variability stems from disparities between the analytical LSS stopping powers in Q-C mode and more precise SRIM stopping powers in F-C mode. Consequently, when the SRIM F-C(E) method is chosen as the reference condition, depicted in Fig. 4c, the ratio of calculated vacancies obtained from SRIM F-C(V) to SRIM F-C(E) (represented by pink squares) is significantly reduced. Overall, the ratio generally exhibits an increase from 0.9 to 1.2 with increasing atomic number of the target.


5 MeV Fe into targets with Z = 3 to 92
SRIM F-C(V) / Q-C(V); default E_f
Iradina F-C / Q-C; default E_r
a
Ratio of total vacancy
Atomic number of target
~2.5X
Li
C
Al
Si
V
Fe
Ni
Cu
Se
Mo
Nd
W
Au
Pb
U


5 MeV Fe into targets with Z = 3 to 92
SRIM F-C(E) / Q-C(V); E_f=E_d
Iradina F-C / Q-C; E_r=E_d
SRIM F-C(E) / Q-C(V); default E_f
b
Ratio of total vacancy
Atomic number of target
~1.6X
~0.7X
Li
C
Al
Si
V
Fe
Ni
Cu
Se
Mo
Nd
W
Au
Pb
U

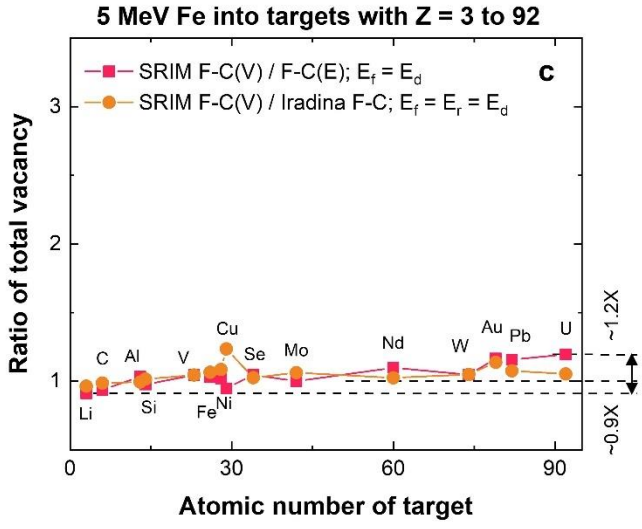

5 MeV Fe into targets with Z = 3 to 92
SRIM F-C(V) / F-C(E); E_f = E_d
SRIM F-C(V) / Iradina F-C; E_f = E_r = E_d
c
Ratio of total vacancy
Atomic number of target
~1.2X
~0.9X
Li
C
Al
Si
V
Fe
Ni
Cu
Se
Mo
Nd
W
Au
Pb
U

Fig 4. Comparison of vacancy production ratios between (a) SRIM F-C(V) to Q-C(V) and Iradina F-C to Q-C using default final energy (E_f=1 eV) and default replacement energy (E_r=-1 eV); (b) SRIM F-C to Q-C and Iradina F-C to Q-C using displacement energy as final/replacement energy. (c) SRIM F-C(V) to F-C(E) with Ef = Ed and SRIM F-C(V) to Iradina F-C with $E_f = E_r = E_d$ (F-C: full cascade option, Q-C: quick calculation option, "(V)": vacancy.txt method, "(E)": recoil damage energy method, E_f: final energy, E_r: replacement energy, E_d: displacement energy)"

4 Discussion

4.1 The use of thresholds in displacement calculations

Since the 1950s, models for damage energy were developed based on the elementary binary collision theory to gain a better understanding of the damage production process [23]. Two main factors can influence the estimation of the number of displaced atoms. The first factor is the electronic stopping power, which causes energy loss through electron excitation. The second factor is the specified conditions required for permanently displacing an atom from its lattice site. In general, there are two models used to determine the threshold for the production of displacements: the displacement energy (E_d) [24] and recombination radius (r_v) [25] models. The E_d model involves a threshold energy level, above which a lattice atom that receives kinetic energy E > E_d can be permanently displaced. On the other hand, the r_v model specifies an instability volume of radius, within which a displaced atom that comes to rest will subsequently spontaneously recombine with the vacancy. If the range of a recoil atom exceeds r_v, a stable defect pair is formed, but if not, the recoil eventually returns to its lattice site. These two models are closely related, as r_v can be viewed as the range of a recoiling atom with an initial kinetic energy of E_d. It is also worth noting that both E_d and r_v can be dependent on the crystallographic orientation. For the calculations used in this study, the SRIM and Iradina codes applied the E_d model, while the MARLOWE code applied the r_v model.

Robinson and Oen [26] noted an inconsistency in the original NRT formulation that arises from using a damage energy calculated from other models that is independent of any consideration of a threshold in a threshold-based displacement model. They pointed out a flaw in the model proposed by Lindhard et al. [27], where it was assumed that the initial energy of the primary recoil was entirely dissipated without considering any displacement threshold energy. Because the NRT model uses a displacement threshold, a correction is needed to account for electronic losses that occur at low energies. Their solution can be understood as correcting the threshold energy for inelastic losses [23, 26]. These references also discuss the development of the NRT and alternate models with various energy parameters related to displacement production (see the Appendix for details). It is possible that the coding of the F-C option in SRIM may have been influenced by some of these alternate models. Although the SRIM book indicates that a threshold energy E_d is assigned for vacancy or displacement calculation in F-C mode [19], it is suspected that the SRIM F-C vacancy.txt algorithm actually uses a model without an introduced threshold, or there is simply a coding error. Therefore, when we set $E_f = E_d$, it alters the boundary conditions and appears to fix the SRIM F-C vacancy.txt overestimation problem, giving an estimation closer to the SRIM F-C damage energy method, as shown in Figs. 2 and 4. If the codes are correctly written and a proper damage energy model with threshold energy were used, the change from 1 eV to E_d for E_f should have no effect on the number of produced vacancies, since no vacancy should be produced for recoil energies below E_d. The significant change observed after setting $E_f = E_d$ in Figs. 2 and 4 indicates a possible coding error and missing threshold energy for vacancy calculation in the SRIM F-C vacancy text mode. Additional investigation and revision of the vacancy calculation algorithm within the SRIM F-C source code are required to effectively address this issue.

In addition, the concept of E_d has caused confusion in the past. E_d is defined as the minimum energy required to displace the struck atom a distance equal to the spontaneous recombination distance (r_v~2 a_0 in most metals [28]). It can be calculated as $E_d = E_f^i + E_f^v + E_c$, where E_f^i and E_f^v are the formation energies for an interstitial and a vacancy, and E_c is the kinetic energy needed to be imparted to the struck atom so that it moves a distance beyond the spontaneous recombination distance r_v (this energy can be estimated from low-energy nuclear and electronic stopping powers). To ensure accuracy in SRIM and Iradina, the lattice binding energy used in these codes should be comparable to $E_f^i + E_f^v$.

4.2 Number of Replacements

Table 4 calculations for 2 MeV Fe ion irradiated Fe shows that, when E_f and E_r are set equal to E_d in SRIM and Iradina calculations, the number of replacements increased and the number of vacancies decreased compared to the default conditions of 1 eV and -1 eV, respectively. We are unaware of any physical mechanism where the number of vacancies would decrease and replacements would increase by prematurely terminating the displacement collision evolution at a kinetic energy of E_d. This scenario would require conversion of replacements to vacancies during recoil atom motion at energies below the displacement threshold energy. It is worth noting that the decrease in vacancies between the SRIM default (E_f=1 eV) and revised (E_f=E_d) cases is almost identical to the increase in calculated replacements for these two cases (4234 vs. 4246). A similar correspondence is observed for the Iradina default and revised E_r cases (2807 less vacancies vs. 2805 more replacements). This phenomenon is primarily caused by an apparent flaw in the default SRIM and Iradina source codes for the treatment of collisions

involving recoil energies below E_d that misclassifies replacements as vacancies, resulting in an overestimation of vacancies and underestimation of replacements in both codes.

Table 4. Number of vacancies and replacements for 2 MeV self-ion irradiated Fe. (E_f: final energy, E_r: replacement energy, E_d: displacement energy, r_v: recombination radius, a_0: lattice constant of bcc Fe)

Calculation code	Conditions	Number of vacancies	Number of replacements	Replacement to vacancy ratio
SRIM (default E_f=1 eV)	F-C (vacancy.txt)	11,095	519	0.05
	F-C (damage energy)	6,464	--	--
SRIM (E_f=E_d)	F-C (vacancy.txt)	6,861	4,765	0.69
	F-C (damage energy)	6,699	--	--
Iradina	F-C (E_r= -1 eV)	9,676	815	0.08
	F-C (E_r=E_d)	6,869	3,620	0.53
MARLOWE	r_v=0	31,982	4,829	0.15
	r_v=0.5a_0	14,370		0.34
	r_v=1.0a_0	7,104		0.68
	r_v=1.5a_0	2,808		1.72
	r_v=2.0a_0	1,681		2.87
	r_v=3.3a_0	708		6.82

To provide further information on vacancy production and replacements calculated by binary collision approximation methods, the well-known historic MARLOWE code was used; the results are summarized in Table 4. The corrected number of replacements (4,765 and 3,620 for SRIM and Iradina, respectively) are in approximate agreement with the MARLOWE estimation (4,829), whereas the default value SRIM (519) and Iradina F-C (815) calculations dramatically underpredict the number of replacements compared to MARLOWE. The

MARLOWE calculations were performed for Frenkel pair spontaneous recombination distances (r_v) ranging from zero to 3.3 a_0. The MARLOWE-calculated replacements were independent of recombination distance, whereas the calculated vacancies decrease with increasing recombination distance. For the MARLOWE calculation with a recombination radius of 1 a_0, the number of vacancies (7,104) is comparable to the corrected SRIM (6,861) and Iradina (6,869) estimations (Table 4 and Fig. 5). In Fig. 5a, a recombination radius near 1 a_0 provides self-consistent calculated values of the displacement threshold energy and was recommended for self-ion irradiation in previous MARLOWE calculations [18] that became the basis for the NRT dpa [13]. Comparing the MARLOWE vacancy production calculations with SRIM and Iradina, Fig. 5b demonstrates a satisfactory agreement between the revised SRIM and Iradina values and the MARLOWE result when employing a recombination radius of 1 a_0. Conversely, when using default values of E_f=1 eV and E_r=-1 eV, both SRIM and Iradina F-C vacancy production values exhibit a significant overestimation, ranging from 1.4 to 1.6 times higher compared to the other values.

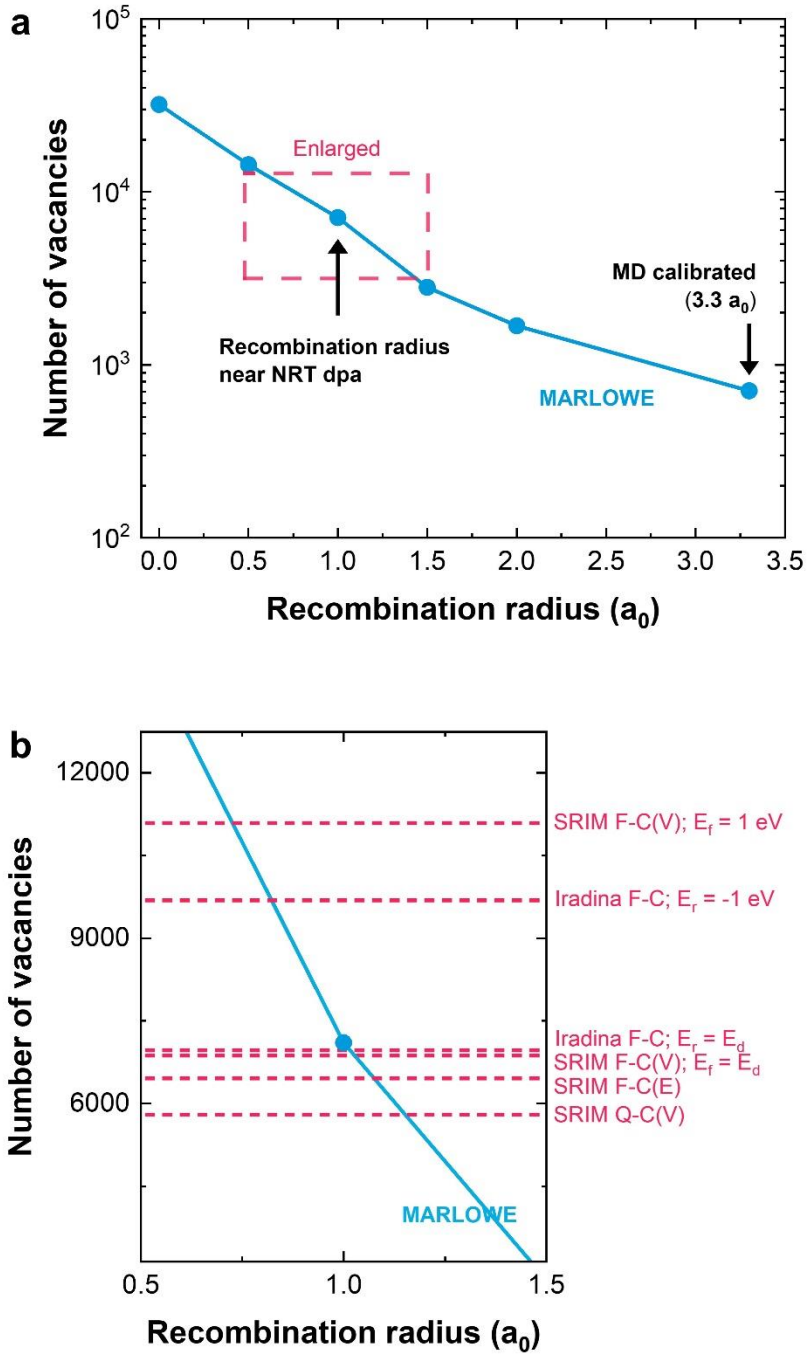


Fig 5. MARLOWE estimation of the number of vacancies as a function of recombination radius for 2 MeV self-ion irradiated Fe. The number of vacancies predicted by SRIM and Iradina with the same irradiation condition is indicated by the short lines. (F-C: full cascade option, Q-C: quick calculation option, "(V)": vacancy.txt method, "(E)": recoil damage energy method, E_f: final energy, E_r: replacement energy, E_d: displacement energy)

Considering prior calculational and experimental studies, a replacement-to-vacancy ratio below ~1 for the Fe test case seems physically incorrect. An early approximate analysis by Kinchin and Pease predicted that the replacement per vacancy ratio should always be larger than one [24]. For binary collision approximation calculations, the replacement to vacancy ratio calculated by MARLOWE (Table 3) is around 1 to 7 for reasonable values of the spontaneous recombination distance (1-3.3 a_0). In Table 4 and Fig. 5, the recombination radius of 3.3 a_0 is a value calibrated using MD results in Fe at different energies to achieve similar vacancy production values between MARLOWE and MD [29, 30], with a corresponding MARLOWE replacement to vacancy ratio of 6.8. Experimental [31-33] and computational [28, 34-37] studies have provided estimates of the spontaneous recombination distance for Fe and other mid-atomic number elements. These studies suggest that the appropriate value falls within the range of ~2.0-3.4 a_0, with the most recommended value for Fe being around 2.2 a_0 [28]. Therefore, the replacement-to-vacancy ratio for 2 MeV self-ion irradiated Fe as calculated by MARLOWE is ~3. Demange et al. [38] obtained higher replacement values in Cu by using MARLOWE and a recombination radius of 2.2 a_0, but it is unclear what other modifications they made to attain these results.

Evaluations of the replacement per vacancy ratio from experimental order-disorder studies [39] and MD simulations [40] indicate much higher values than calculated using binary collision approximation codes. For example, Fig. 6 shows the average atomic displacements obtained in 10 keV cascades in Fe estimated by MD simulations as reported in Ref. [12]. The average number of Frenkel pairs produced was 34, and the total number of atoms displaced more than one-half of the nearest neighbor distance (0.248 nm) was 342. One can assume that the atoms displaced more than one-half of the nearest neighbor distance comprise both replacements

and stable interstitials. In this case, the number of replacements is (342-34) =308, and the replacement to vacancy ratio would be 9.1. Higher ratios were observed for higher energies and higher temperatures. As reviewed in Ref. [39], typical experimental estimates of replacement per vacancy ratios are ~2 for near-threshold electron irradiations and ~50 for energetic displacement cascade irradiations; the latter value is relevant for 2 MeV Fe irradiated Fe. This quantitative underestimation of replacement events by binary collision approximation codes may be attributed to the lack of consideration of replacement events from different branches of the displacement cascade; such effects are correctly evaluated in MD simulations. In summary, the expected replacement per vacancy ratio for energetic cascades in Fe as calculated by binary collision approximation codes is ~1 (using revised SRIM and Iradina F-C calculations with $E_f = E_r = E_d$ as well as MARLOWE calculations with a recombination radius near 1 a_0). This is well below the value of ~50 (estimated from experimental and MD studies) and is attributed to shortcomings of binary collision approximation codes to simulate multi-body in-cascade recombination events. Even greater discrepancies regarding the number of replacements per dpa are produced if the current SRIM and Iradina default values for E_f and E_r are used for the calculations.

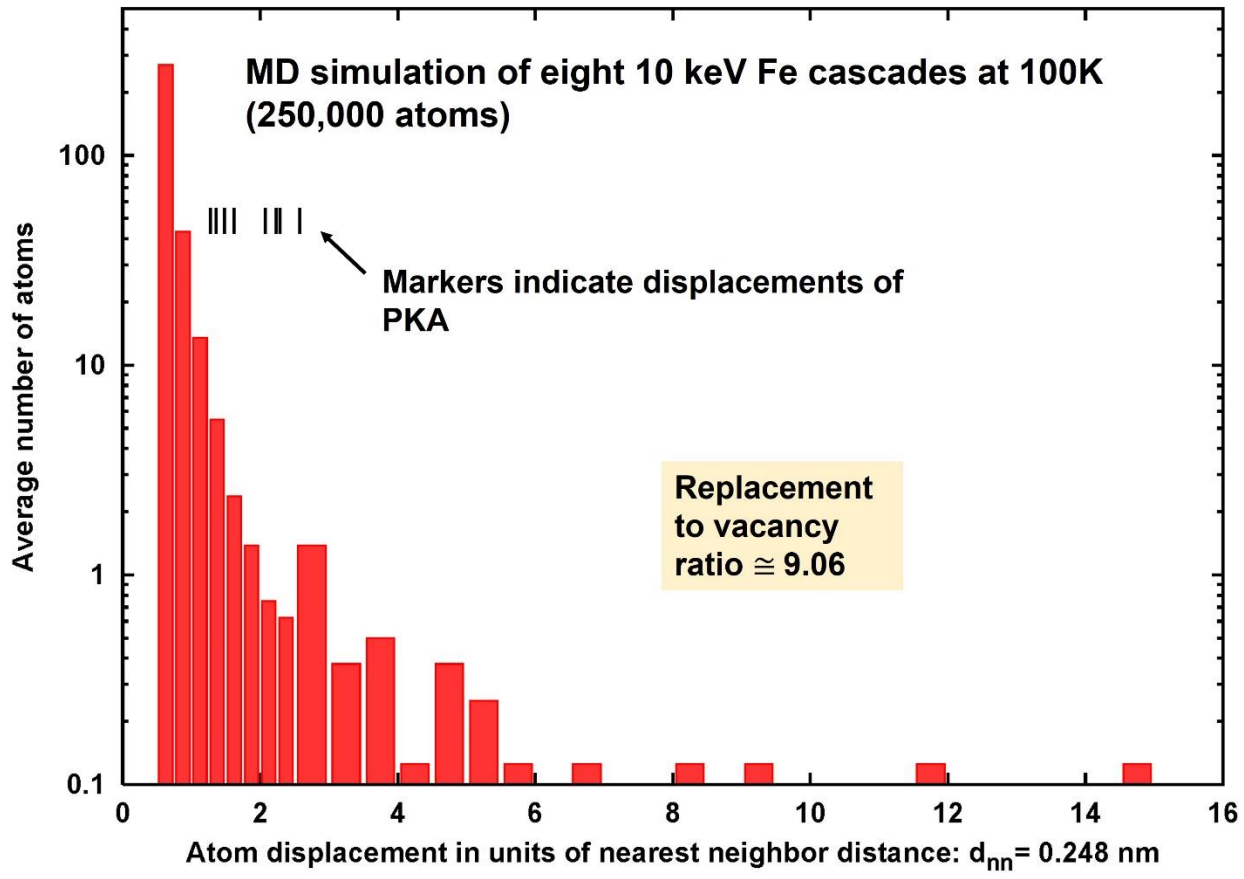


Fig 6. MD simulation depicting the average atom movement during atomic displacement cascades in Fe, specifically for eight 10 keV cascades at a temperature of 100K. The vertical black bars represent the total movement of the primary knock-on atom (PKA). Out of the total of 250,000 atoms, 249,658 atoms have been displaced below $0.5d_{nn}$ (0.124 nm). (Adapted from Ref. [12].)

In general, radiation mixing and replacements can occur if any bombarding ion ends up being located in the original struck atom site [41]. SRIM and Iradina use a narrow definition for replacements (Table 2). It is indeed true that a replacement can be generated when E_1 is less than E_f or E_r. However, replacements will also occur when $E_1<E_d$. Therefore, the criterion $E_1<E_d$ should be the dominant factor for replacement reactions. Consequently, by assigning the default values of E_f and E_r to E_d, the underestimation of replacements in SRIM and Iradina can be partially corrected. To improve the accuracy of vacancy, replacement, and subthreshold collision evaluations, we propose the following recommendations for new codes or modifications to

existing ones. The code should assess the collision outcome (vacancy, replacement, and subthreshold collision) based on the energy E_1 and E_2 relative to the criterion $E_{1,2} \geq E_d$ for vacancy generation. If both E_1 and E_2 are less than E_d, and E_1 is smaller than E_2, a replacement should be generated. This occurs because the recoiling projectile ion will come to rest closer to the dislodged lattice atom's site, enabling it to spontaneously migrate back to the dislodged atom site faster than the recoiling lattice atom would (Fig. 1). A replacement would also occur if E_1 is less than E_d and E_2 is greater than or equal to E_d. In the case where both E_1 and E_2 are less than E_d, and E_1 is greater than E_2, a subthreshold collision would be produced. A subthreshold collision would also occur when E_1 is greater than E_d, as long as E_2 is below E_d.

4.3 Evaluation of SRIM code for dpa calculation

4.3.1 Collision Details

An examination of the "collision.txt" files in the SRIM F-C reveals a noticeable error in the calculation of vacancy production for near-threshold collisions when using the default value of E_f (as shown in Fig. 7a). This serves as clear evidence that the vacancy counting algorithm in SRIM F-C is flawed. However, setting E_f equal to E_d (Fig. 7b) results in a reasonable number of produced vacancies for near-threshold collisions, which should be zero for $E_2 < E_d$ and one for $E_d < E_2 < 2.5E_d$ (with $\kappa = 0.8$). For higher energies ($E_2 \geq 2.5E_d$) and ignoring parasitic ionization energy losses, the maximum vacancy production is limited by Eq. 1. In Figs. 7a and 7b, the pink dashed lines show the boundary above where no vacancies can be produced (yellow shaded areas). The calculated plot of vacancies vs. recoil energy with the default E_f (Fig. 7c) also shows an unreasonable trend of excessive vacancy production and underestimated

replacements, while the plot for the corrected E_f equal to E_d (Fig. 7d) reflects SRIM F-C calculated vacancy production in general agreement with the NRT damage model and a higher dependence of replacement production on the recoil energy.

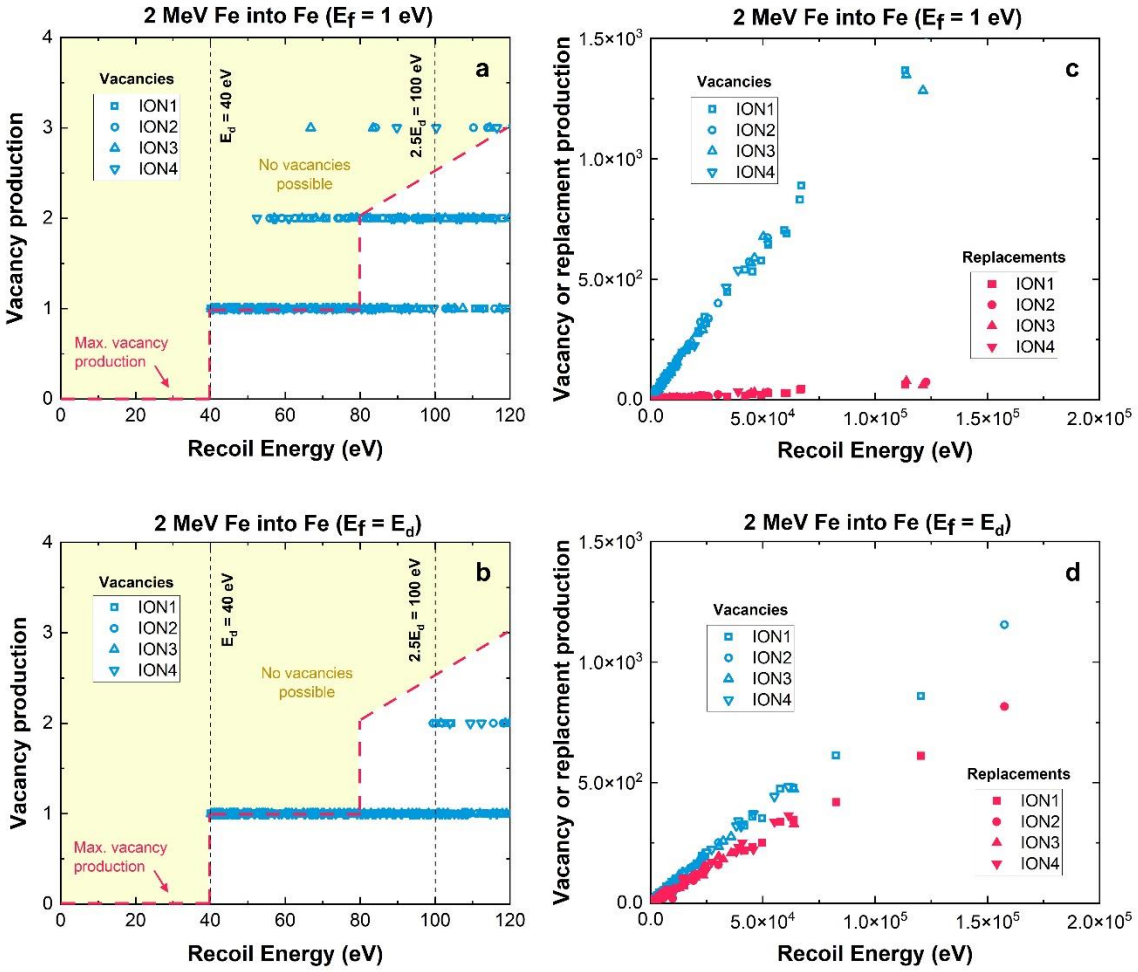


Fig 7. Comparison of vacancy production and recoil energy for 2 MeV Fe ions in Fe target. The data is obtained from the SRIM "collision.txt" file using the F-C option. The plot includes near-threshold events (a-b) and events with recoil energy up to 0.2 MeV (c-d), with final energy values of 1 eV (default) and E_d.

With SRIM F-C calculation, it is possible to track the detailed energy losses associated with ionization (including primary ion and recoil target atoms), and thereby obtain an integrated damage energy for all of the simulated ions. This method is superior to the SRIM Q-C mode, which is based on an approximate analytic function fitted the LSS stopping power [27] and is

only strictly valid for Z_1=Z_2. The F-C method uses the generally more accurate SRIM stopping power database and should calculate the effective damage energy for compound targets (e.g., UO_2 and SiC) more accurately. In principle, the vacancy production calculated by the damage energy method should be equal to the value provided in the vacancy.txt file in SRIM. Therefore, comparing the values obtained from the vacancy.txt file to those calculated using the damage energy method serves as a valuable cross-check to ensure the proper functioning of the code. It is worth noting that using Eq. 1 to convert damage energy to vacancies may slightly underestimate the vacancy production, as the NRT defect production equation at damage energies between E_d and 2.5E_d is greater than this linear expression. However, the differences observed in Fig. 4c are primarily attributed to the distinct algorithms employed by SRIM for vacancy and energy transfer calculations. Although setting E_f equal to E_d in SRIM may address the overestimation of vacancies (as demonstrated in Fig. 7), it may create problems in energy transfer because E_f corresponds to the energy below which SRIM no longer tracks collision processes. In this case, the sum of the final dissipated energy values will not equal the initial particle energy. Physically, an atom with energy below E_d should still be capable of transferring energy to electrons and subthreshold nuclear collisions before stopping (reaching its final energy). Assigning too low of an E_f value shouldn't lead to an underestimation of replacements if the collision outcomes are correctly evaluated by the code.

4.3.2 Different methods for vacancy calculation

In the present study, although revising the final energy (E_f) appears to correct the overestimation of vacancy production in SRIM full-cascade vacancy.txt calculations (with minor impact on the F-C damage energy vacancy calculation), minor deviation still persists between the

SRIM F-C(V) method to SRIM F-C(E) method with $E_f = E_d$ (Fig. 4c). Stoller et al. [7] reported that SRIM's phonon output files can also be used for damage energy calculations. Agarwal et al. [9] suggested that that the "phonon" energy is equal to the beam energy minus the energy used for ionization (Table 2), which is referred to as the damage energy in the NRT model. The term "phonon" in SRIM is ambiguous. In the SRIM document [19], "phonons" are mentioned as if they represent the number of phonons, but the output files show that they represent an energy - supposedly, the energy dissipated during the production of phonons. The unit for the phonon table in the SRIM output file was given as phonons/Angstrom-ion (as stated above the column headings in the phonon.txt file). However, the damage energy equations appear to function adequately when assuming units of eV/Angstrom-ion (or alternatively assuming all phonons to possess an energy of 1 eV). Ultimately, most of this energy is distributed as lattice vibrations or phonons.

A comprehensive comparison of various methods for calculating the damage energy is presented in the Appendix. Through extensive experimentation with different incident ion and target elements, we have verified the agreement between damage energy-calculated vacancies and the values in the vacancy.txt file when the final energy (E_f) is set to E_d in SRIM. In contrast, a significant discrepancy arises when using SRIM's default value of $E_f = 1\ eV$. This discrepancy is due to SRIM incorrectly identifying subthreshold collisions (which should result in replacements) as vacancies as discussed in the previous section. A thorough analysis of the output files (detailed in the Appendix) has enabled us to identify the three most recommended calculation methods for the F-C option, as summarized in Table 5. Given that the original definition of damage energy (T_d) relates to the portion of PKA energy dissipated through elastic collisions with lattice atoms, the most straightforward method to determine damage energy (T_d)

is to subtract the ionization energy of the incident ion and target from the incident ion energy. While this approach proves useful in verifying the calculation's accuracy in terms of the total number of vacancies, it cannot provide an estimation of the vacancy/dpa depth profile.

Table 5. Summary of three modified methods recommended for dpa or vacancy calculations using SRIM-F-C option.

Methods	Required SRIM output files	Calculations
Modified vacancy.txt	"VACANCY.txt"	To obtain the number of vacancies, first set E_f=E_d, and use the sum of the "Target Element Vacancies" column and the "Ion Element Knock-Ons" (1st modification method) or use the "Target Element Vacancies" column (2nd modification method).
Modified recoil damage energy	"E2RECOIL.txt", "IONIZ.txt", and "PHONON.txt"	Subtract the integration of the "IONIZ. by RECOILS" column from the "Energy Absorbed by Target Element" column. Next, add the "PHONONS by ION" column to manually calculate the damage energy (T_d) for Eq. 1
Modified phonon energy	"PHONON.txt" and "VACANCY.txt"	To manually calculate the damage energy for Eq. 1, use the default value of $E_f = 1\ eV$. Add the values from the "PHONONS by RECOILS" column and the "Target Element Vacancies" column, multiplied by the lattice binding energy (E_b).

Fig. 8 presents a comparison between the methods recommended in Ref. [9], as summarized in Table 2, and the modified methods proposed in the present study, as summarized in Table 5. Additionally, the figure includes a comparison of SRIM's calculated phonon and

recoil damage energy values with corrected E_f in order to validate SRIM's calculations and definition of phonon energies. In Fig. 8, for the 10 MeV Fe into Fe case, the F-C(V) method with the default E_f (1 eV) shows a significant discrepancy compared to the modified F-C(V) method with E_f=E_d, and also versus the recoil damage energy (E) and phonon energy (P) methods with or without E_f correction. When normalizing the total number of vacancies to the F-C(E) method with default E_f, the F-C(V) method with default E_f shows the highest value of 1.75, while other methods have values ranging from 0.91 to 1.11. Overall, no significant difference was observed between the F-C (V) and F-C (P) methods and the modified F-C (V) and modified F-C (P) methods in Figs. 8b and 8c. A slight increase in the total number of vacancies was observed in the F-C(E) and F-C(P) methods when changing E_f from 1 eV to E_d= 40 eV. This increase is due to the decrease of "IONIZ. by RECOILS" in the "IONIZ.txt" file and the increase of "PHONONS by RECOILS" in the "PHONON.txt" file. According to the SRIM tutorial, the projectile energy of E_1 (see Fig. 1) is released as phonons after a replacement collision. Therefore, changing E_f from 1 eV to E_d may have a slight impact on vacancy profiles as predicted by the F-C(E) and F-C(P) methods, as seen in Figs. 9b and 9c. This suggests that although setting E_f=E_d may correct the F-C(V) method, it causes energy problems for the F-C(E) and F-C(P) methods since all atoms were stopped at a minimum energy of 40 eV. Following the physics of recoil cascades, SRIM should assess the energies of the projectile and recoil atom (see Fig. 1) and prevent additional vacancies if either E_1 or E_2 is below E_d (the vacancy would have already been counted in the prior collision). If either recoil energy falls below E_d, then no further replacements can be generated in subsequent collisions. Eventually, all of the remaining energy should be deposited as phonon heat.

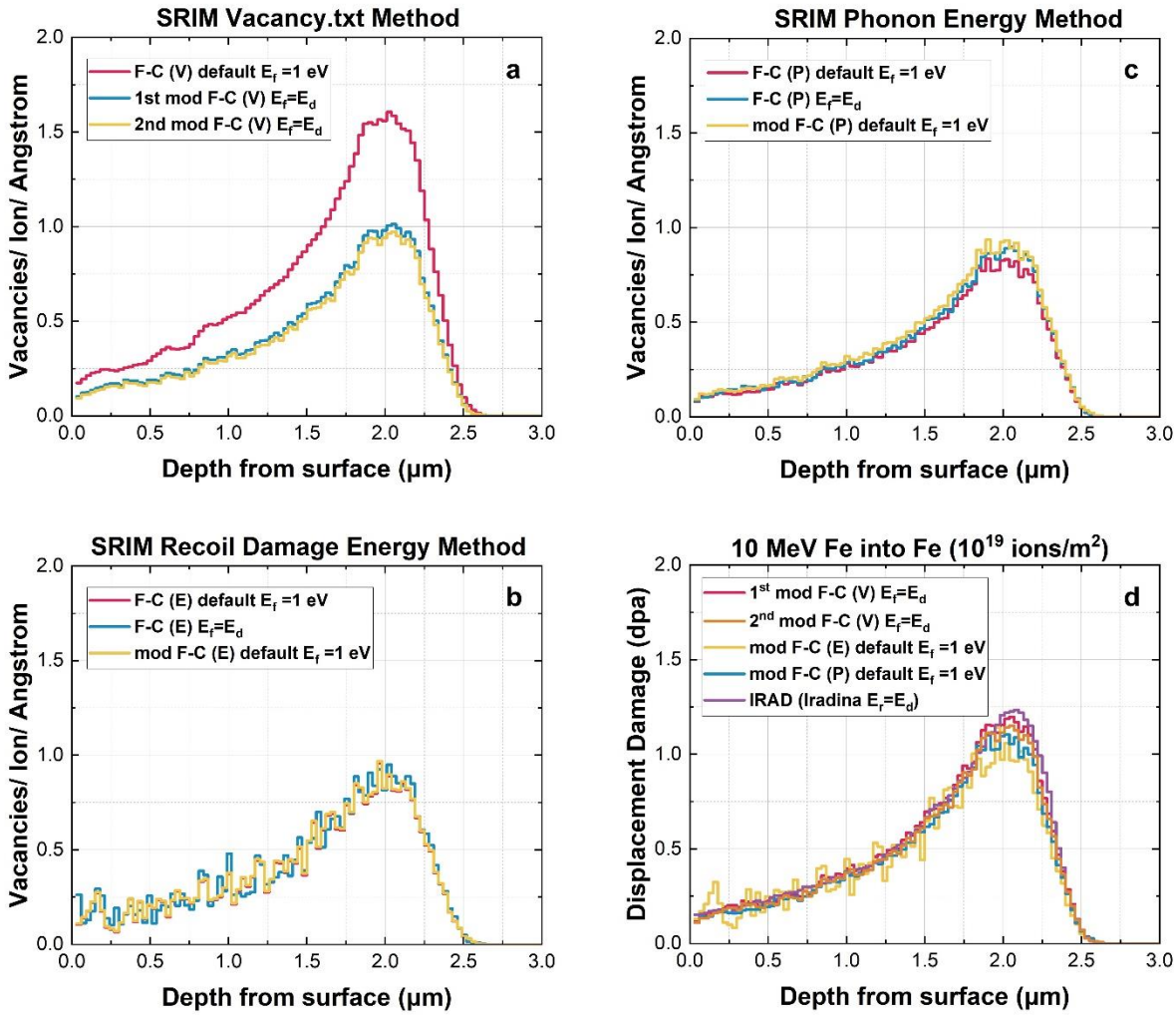


Fig 8. Comparison of various SRIM vacancy calculation methods for 10 MeV Fe ions in a Fe target: (a) Vacancy.txt methods, (b) Recoil damage energy methods, (c) Phonon energy methods, and (d) dpa depth profiles. (F-C: full cascade option, Q-C: quick calculation option, "(V)": vacancy.txt method, "(E)": recoil damage energy method, "(P)": phonon energy method, mod: modified)

Compared to SRIM F-C(V), Q-C(V), and Q-C(E) methods, Agarwal et al. [9] suggested that the SRIM F-C(E) method generally provides better accuracy for vacancy production. Their suggestion was made to provide a way to use the more accurate SRIM stopping power database (vs. the analytical LSS stopping powers), and to avoid the vacancy overestimation of the SRIM F-C(V) method. Unfortunately, there appear to be certain noticeable problems with the depth-dependent profile in the SRIM F-C(E) method, particularly near the surface and near the ion's

end of range for particular combinations of projectile and target masses. These issues can also be observed in Figs. 2 and 3, and they arise from interval binning problems in SRIM [9]. For the modified phonon energy method, if the lattice binding energy is not set to zero in SRIM calculations, the binding energy loss terms (vacancies×E_b) should also be taken into account when calculating T_d. This consideration, which was not addressed in Ref. [9], would slightly impact the values obtained through the SRIM F-C(P) method (Fig. 8c), ensuring the energy balance is maintained. Based on our investigation, we recommend manually computing the damage energy using the methods summarized in Table 5 with the default $E_f = 1\ eV$ value to obtain depth profiles for dpa. However, using either E_f= 1 eV or E_d will produce acceptable accuracy for the damage energy method.

The modified SRIM F-C(V) method with the corrected $E_f = E_d$ effectively eliminates the need for manual damage energy calculations and is expected to yield a negligible difference compared to the dpa profile obtained from the other two methods calculating the damage energy. However, our investigation revealed a disparity in how the "vacancy.txt" file summarizes the total number of vacancies for Q-C and F-C. In the case of Q-C, the calculation involves integrating the values found in the 1st (primary vacancies) and 2nd columns (recoil vacancies) of the "vacancy.txt" file. Conversely, in the case of F-C (after applying the $E_f = E_d$ correction), only the sum of the values in the 2nd column (labeled “recoil vacancies”) is considered for the total number of vacancies summarized in the vacancy.txt file. This raises the suspicion that the 2nd column may include the values from the 1st column for SRIM F-C. When comparing the total number of vacancies using the sum of the 2nd column in vacancy.txt to the values obtained from the damage energy methods, a closer alignment between the numbers is observed (refer to Appendix). Moreover, using the sum of the 2nd column in vacancy.txt further reduces the

discrepancy between the E_f-corrected SRIM F-C(V) method and the E_r-corrected Iradina method, as illustrated in Fig. 4c and 8d. For SRIM simulations with heavy incident ions, the number of primary vacancies (1st column) is generally much lower compared to the recoil vacancies (2nd column). Consequently, for calculations with heavy incident ions, the differences between the 1st modified F-C(V) method (1st column + 2nd column) and the 2nd modified F-C(C) method (only using the 2nd column) are negligible, as exemplified in Fig. 8d. However, for irradiations with light incident ions (such as protons), the differences can be significant, necessitating a careful comparison with the damage energy methods (see Appendix for the details).

To prevent misleading comparisons of data obtained from different experiments, it is crucial for future studies to thoroughly describe how they calculated the reported dpa values. This description should include the simulation code and mode used (F-C or Q-C option), the total ion fluences, the incident ion energy, and the displacement energy, all of which should be clearly listed in the reports.

4.4 Evaluation of Iradina code for dpa calculation

In Fig. 4c, the E_f-corrected SRIM and E_r-corrected Iradina F-C vacancy text file calculations are generally in agreement with the SRIM F-C(E) method. Besides, near-surface and end-of-range anomalies observed in rare cases when using SRIM F-C(E) method [9] were not noticeable in the E_f-corrected SRIM F-C(V) and E_r-corrected Iradina predictions (Figs. 2 and 3). Overall, the ratio of vacancy from SRIM F-C(V) to Iradina F-C was between 0.95-1.09. The only exceptions were the Ni, Cu, and Au targets, with ratios between 1.09-1.25. This discrepancy is likely due to an error in the stopping power model used in SRIM-2013. Previous studies with

energy dispersive X-ray spectroscopy (EDS) and secondary ion mass spectrometry (SIMS) experimental methods found that SRIM-2013 overestimates the peak position of implanted 8 MeV Ni ions in Fe, causing a shift of ~700 nm toward the sample surface [42, 43]. However, this discrepancy was not observed when using the earlier stopping power database in SRIM-1998. Nevertheless, given that both SRIM and Iradina codes use similar stopping power databases and presumably use similar calculational methods, it is expected that the differences should be minimal. A possible reason for the slight difference could be the use of different stopping power versions for certain targets (such as Cu, Mo, Nd, Pb, and U) between SRIM and Iradina. SRIM has updated its database over time, while Iradina has relied on the Corteo database, which was derived from the SRIM 2003 database.

It is important to note that while SRIM only allows for a single assignment of E_f per calculation, Iradina allows for individual E_r values for each element in the target. This discrepancy may result in differences for compounds composed of multiple elements with varying displacement energies. Further research into the impact of replacement energy on replacement production in multi-element targets, such as high-entropy alloys, would shed light on the complexities of collision events in these materials. Additionally, Iradina defines a minimum energy (E_m) below which a moving atom is considered stopped, similar to E_f in SRIM. If E_r only impacts the counting of vacancies/replacements and E_m serves for energy transfer calculation, both F-C(V) and F-C(E) methods may produce similar outcomes in Iradina. Extracting energy transfer information from Iradina to calculate damage energy and conducting F-C(E) calculations could verify the accuracy of Iradina's energy transfer algorithm and improve the accuracy of vacancy or dpa calculations.

We have developed IRAD, a new open-source graphical user interface (GUI), for performing SRIM-like calculations based on our analysis. The IRAD package, which includes the application software, source code, installation instructions, and user manuals, can be found at https://code.ornl.gov/liny/irad. Currently, the application software is only available for Windows systems. IRAD performs E_r-corrected Iradina calculations and automatically calculates the dpa and implanted ion concentration, taking the total ion fluence into account. Additional results, such as ion and recoil trajectories, final ion positions, stopping power distribution, etc. can also be obtained. Advanced manual settings allow changing the stopping power database, incident ion angle, 3D target simulations, etc. The IRAD GUI only sets parameters for Iradina calculations and runs them. Major changes to the vacancy/replacement counting or energy transfer algorithms must be done in the Iradina source code. Fig. 8d displays an example of the depth profile of dpa calculated using IRAD for 10 MeV Fe ions into a Fe target, at a total fluence of 10^{19} ions/m^2. The results demonstrate a good agreement with the modified SRIM F-C(V) method and the two damage energy methods, exhibiting an error <10%. IRAD and the Iradina code are works in progress and are expected to be improved in the future. Iradina CEA GUI on sourcefoge will be updated to incorporate easily the two choices of $E_r = E_b$ for consistency with past SRIM calculations or $E_r = E_d$ to correct the replacement problem. Feedback and suggestions from users are welcome.

5 Conclusions

The SRIM code is widely used in studies involving ion irradiation to predict the depth profile of injected ion concentration as well as the number of vacancies, which is an indicator of

radiation damage. However, there is an issue with the SRIM F-C vacancy.txt method as it predicts approximately 2-2.5 times more vacancies than the SRIM F-C recoil damage energy or phonon energy methods, as well as MARLOWE binary collision calculations. This discrepancy can create confusion when reporting SRIM dpa values. While the physics equations presented in the SRIM book and user manual are generally accurate, a coding error exists within the "black box" SRIM code. Based on our inspection of the SRIM and Iradina codes, it is proposed that the final energy (E_f) in SRIM and replacement energy (E_r) in Iradina should be set equal to the displacement energy to address the overestimation of vacancy production in full-cascade calculations. Without a displacement, there can be no replacement (only an injected interstitial). When using the SRIM full cascade vacancy.txt method for vacancy production (or dpa) calculations, setting $E_f = E_d$ is necessary to correct the SRIM code error that considerably underestimates the number of replacements and correspondingly overestimates the number of vacancies. IRAD, a new GUI that takes the total ion fluence into account and automatically calculates the dpa and implanted ion concentration, was developed to perform E_r-corrected Iradina calculations. Good agreement is obtained between the E_f-corrected SRIM and E_r-corrected Iradina calculations. If the SRIM source code cannot be released to the public, Iradina (as an open-source code) may be a prospective platform that can be continually improved and revised to support the research field of ion irradiation and radiation effects in materials. To avoid misleading data comparisons, future studies must clearly describe how they calculated the reported dpa values.

6 Appendices

6.1 Evolution of displacement calculations

The Kinchin and Pease model [24] and the original NRT model [13] (modified Kinchin-Pease model) are two of the most renowned models in displacement calculations. The following equations (Eqs. A-1 and A-2) present a summary of the number of displacements generated by recoil with a specified PKA energy using both models. The definition of terms in these equations are summarized in Table A.1.

I. Kinchin and Pease [24]

$$\eta(E_p) = \begin{cases} 0, & 0 < E_p < E_d & (A-1a) \\ 1, & E_d \le E_p < 2E_d & (A-1b) \\ \dfrac{E_p}{2E_d}, & E_p \ge 2E_d & (A-1c) \\ \dfrac{E_c}{2E_d}, & E_p \ge E_c & (A-1d) \end{cases}$$

II. Original NRT (modified Kinchin-Pease) [13]

$$\eta(E_p) = \begin{cases} 0, & 0 < T_d < E_d & & & (A-2a) \\ 1, & E_d \le T_d < \dfrac{2E_d}{\kappa} & \text{or} & 1, \quad E_d \le T_d < L & (A-2b) \\ \dfrac{\kappa T_d}{2E_d}, & T_d \ge \dfrac{2E_d}{\kappa} & \text{or} & \dfrac{\kappa}{L}, \quad T_d \ge L & (A-2c) \end{cases}$$

Table A.1. Definition of symbols used for the Kinchin-Pease and NRT models

Term	Definition	Typical or recommended value
E_p	atomic recoil energy, PKA energy	--
T_d	damage energy, amount of PKA energy dissipated in elastic collisions	calculate from LSS stopping powers
ν	number of displacements created by recoil with specified PKA energy	--
κ	correction factor to account for realistic (as opposed to hard sphere) atomic scattering	0.8
L^*	cascade multiplication threshold	$2E_d/\kappa$ or 100 eV in NRT model
E_d	atomic displacement threshold energy	40 eV (for Fe)
E_c	maximum energy below which a vacancy will capture an atom	40 eV (for Fe)
E_b	atomic binding energy to lattice site	0*

* Model dependent: $L = (E_d + E_c + E_b)/\kappa$, K-P and NRT use $E_d = E_c$ and $E_b = 0$

Robinson and Oen [26] noted an inconsistency in the original NRT formulation that arises from using damage energy calculated from a model that is independent of any consideration of a threshold in a threshold-based displacement model. They argue that $\nu(L)$ in Eq. A-2c should equal 1. However, since $T_d(100)$=86.63 eV and L=100, $\nu(L) < 1$. This can be corrected by replacing L with $T_d(L)$ in Eq. A-2. This increases the number of displacements in Eq. A-2c by the ratio of 100/86.63=1.15430.

Alternately, if 40 eV is the actual displacement threshold measured in an experiment (e.g., by HVEM irradiation), this implies that E_p =40 eV is the minimum PKA energy for a stable displacement. However, note that for E_p=40 eV, $T_d(E_p)$=35.33 eV and the requirement for a stable displacement in Eq. A-2b is that the damage energy, not the PKA energy, exceed 40 eV. This can be corrected by using $T_d(E_d)$ as the effective displacement threshold in Eq. A-2. This increases the number of displacements in Eq. A-2c by the ratio of 40/35.33=1.13233.

6.2 Comparison of different damage energy methods using SRIM for displacement calculations

In SRIM, there are six types of energy loss as summarized in Table A.2. According to the SRIM documentation [1, 19], the total energy loss equals the incident ion energy (E_i^0) when all ions come to a stop within the sample and presumably no sputtered ions carry away any kinetic energy. This can be expressed as the sum of individual energy losses, $E_i^0 = E_i^I + E_T^I + E_i^B + E_T^B + E_i^P + E_T^P$. This relationship should hold true for both SRIM F-C and Q-C modes. However, upon manually calculating the sum of the six energy loss terms (E_{total}), we found that the sum is slightly larger than the input ion energy (E_i^0), that is, $E_i^I + E_T^I + E_i^B + E_T^B + E_i^P + E_T^P = E_{total} > E_i^0$. In other words, the sum of the six energy loss terms does not equal the incident ion energy as stated in the SRIM documentation. In general, for the SRIM F-C mode, such errors are minimized when subtracting the energy lost to vacancy binding energy (E_i^B) and phonons (E_i^P) from the total beam energy (E_{total}), resulting in $E_i^0 \cong E_{total} - E_i^B - E_i^P$. This implies that the beam energy loss terms associated with vacancy binding energy (E_i^B) and phonons (E_i^P) are included in the target atom energy loss terms (E_T^B and E_T^P, respectively). In the case of the Q-C option, $E_i^0 \cong E_{total} - E_i^P$, without an additional subtraction of E_i^B. Table A.3 summarizes the energy balance for various cases. The parentheses in the tables indicate the total energy ratio, which is obtained by dividing the calculated total energy loss by the input incident ion energy.

Table A.2. Definition of symbols used for the damage energy methods.

Term	Definition	Notes
E_i^I	Beam energy lost to ionization	"Ioniz. by ions" in IONIZ.txt
E_T^I	Target atom energy lost to ionization	"Ioniz. by recoils" in IONIZ.txt
E_i^B	Beam energy lost to lattice binding energy	"Ion knock-ons" in VACANCY.txt. ($E_i^B = E_b \times v_i$)

E_T^B	Target atom energy lost to lattice binding energy	"Target vacancies" in VACANCY.txt. ($E_T^B = E_b \times v_T$)
E_i^P	Beam energy lost to phonons	"Phonons by ions" in PHONON.txt
E_T^P	Target atom energy lost to phonons	"Phonons by recoils" in PHONON.txt
E_i^0	Incident ion or beam energy	SRIM input parameter
E_{total}	Sum of the six types of energy loss in SRIM	The integration of energies and depths is needed
E_T^0	Beam energy lost to target atoms	"Energy from ions" in E2RECOIL.txt
E_i^T	Beam energy absorbed by target atoms	"Energy absorbed by target" in E2RECOIL.txt

* E_b and v represent the binding energy and the number of vacancies, respectively

Table A.3. Summary of energy balance for the various SRIM calculation cases.

SRIM calculations	FC (E_f=1)		FC (E_f=E_d)		QC	
	$E_{total} - E_i^B - E_i^P$	$E_{total} - E_i^P$	$E_{total} - E_i^B - E_i^P$	$E_{total} - E_i^P$	$E_{total} - E_i^B - E_i^P$	$E_{total} - E_i^P$
10 MeV Fe into Fe	10,009,191 (1.0009)	10,012,446 (1.0012)	10,001,047 (1.0001)	10,004,306 (1.0004)	9,996,915 (0.9997)	9,999,999 (1.0000)
10 MeV Au into Au	10,090,117 (1.0090)	10,091,942 (1.0092)	10,017,904 (1.0018)	10,019,737 (1.0020)	9,998,220 (0.9998)	9,999,999 (1.0000)
10 MeV Au into Li	9,976,486 (0.9976)	9,978,905 (0.9979)	9,999,534 (1.0000)	10001952 (1.0002)	9,997,749 (0.9998)	9,999,999 (1.0000)
1 MeV H into Li	999,739 (0.9997)	999,745 (0.9997)	999,964 (1.0000)	999970 (1.0000)	999,994 (1.0000)	999,999 (1.0000)
1 MeV H into Au	999,936 (0.9999)	999,963 (1.0000)	999,663 (0.9997)	999,689 (0.9997)	999,690 (0.9997)	999,714 (1.0000)

The SRIM energy output files can be used to obtain the damage energy for the NRT model. There are several variant expressions than can potentially be used for this purpose, but because of the discrepancies in the energy balance shown in Table A.2, they may not all be equivalent. To investigate the variations among different methods of calculating damage energy, we performed 21 additional SRIM calculations using F-C and Q-C options. These calculations involved Fe ions into Fe, Au ions into Au, Au ions into Li, H ions into Au, and H ions into Li (Tables A.3-A.9). The final energy (E_f) was set to the displacement energy (E_d), deviating from the default 1 eV,

and the binding energy (E_b) was set to zero in certain cases to assess changes in energy loss. The purpose of examining the damage energy values is primarily to demonstrate that the modification using E_f=E_d yields self-consistent results between the vacancy.txt file and the various expressions for damage energy. After conducting a thorough analysis of the output files, we have identified the two most appropriate damage energy calculation methods to recommend for the F-C option:

(1) D_2^{**}: $T_d = E_i^0 - E_i^I - E_T^I$

(2) D_1^{*}: $T_d = E_i^T - E_T^I + E_i^P$

For most cases, D_2^{**}=D_1^{*}. However, since the original definition of damage energy (T_d) pertains to the fraction of PKA energy that dissipates through elastic collisions with lattice atoms, D2** appears to be the most unambiguous reference case for damage energy in SRIM. To provide a detailed explanation of how we arrived at these recommendations, we will elaborate in the following paragraphs.

The user documentation for the SRIM program lacks precise definitions for several of the parameters summarized in the SRIM output files. This ambiguity makes it challenging to determine the appropriate SRIM output file parameters to use for damage energy calculations. From the output files of these SRIM calculations, we employed nine different methods to calculate the damage energy (T_d). In the supplemental file of Ref. [9], Agarwal et al. proposed three methods for calculating damage energies:

(1) D_1: $T_d = E_i^T - E_T^I$

(2) D_2: $T_d = E_i^0 - E_i^I - E_T^I - E_i^P$

(3) D_3: $T_d = E_T^P - E_i^P$

However, assuming $E_i^0 = E_{total}$, the original definition of the damage energy is given by $T_d = E_i^0 - E_i^I - E_T^I$, and the energy balance equation $E_{total} = E_i^I + E_T^I + E_i^B + E_T^B + E_i^P + E_T^P$ yields the variants of D_2 and D_3 as:

(4) D_2^*: $T_d = E_{total} - E_i^I - E_T^I$

(5) D_3^*: $T_d = E_i^B + E_T^B + E_i^P + E_T^P$

However, we observed that $E_i^0 \neq E_{total}$. Specifically, $E_i^0 \cong E_{total} - E_i^B - E_i^P$ and $E_i^0 \cong E_{total} - E_i^P$ for F-C and Q-C option, respectively. Therefore, D_2 and D_3 can be further adjusted as follows:

(6) D_2^{**}: $T_d = E_i^0 - E_i^I - E_T^I$

(7) D_3^{**}: $T_d = E_T^B + E_T^P$ (for the F-C option)

(8) D_3^{***}: $T_d = E_i^B + E_T^B + E_T^P$ (for the Q-C option)

As for the D_1 method, we found that $E_i^T - E_T^I < E_i^0 - E_i^I - E_T^I$, showing a missing amount of energy that makes the calculated number of vacancies using D_1 lower that the others. By analyzing the numbers from the output files, we were able to get good agreement for D_1^* (modified D_1), D_2**, and D_3** using the following equation:

(9) D_1^*: $T_d = E_i^T - E_T^I + E_i^P$

Using the calculated damage energies, we calculated the total number of vacancies (v) by applying the formula $v = (0.8 \times T_d)/(2 \times E_d)$, which is summarized in Tables A.4-A.8. Note that the expression $v = (0.8 \times T_d)/(2 \times E_d)$ to convert damage energy to vacancies should give a slight underestimate of the vacancy production since the NRT defect production equation at damage energies below $2.5E_d$ (Eqs. A-2a and A-2b) is slightly more than this linear expression. The parentheses in the tables indicate the total vacancy ratio, obtained by dividing the calculated vacancy number by the number of vacancies calculated by the D_2^{**} method using the F-C method with default E_f = 1 eV.

Based on the calculation results of the total number of vacancies using different damage energy methods, our findings include:

1. The calculated damage energies for all investigated methods/equations (D_1-D_3 and their variants) increase between the E_f=1 eV cases and the E_f=E_d cases. This phenomenon appears to defy any physics explanation. If the calculation is prematurely stopped at any energy higher than zero, one would generally expect an equal or lower damage energy compared to the E_f=0 case. Equal damage energies would generally be anticipated if the respective E_f values are below the displacement threshold. However, this equality might not be true for D_2 calculations since some recoil ionization associated with subthreshold recoil atoms would not be subtracted from the incident ion energy for the case of E_f=E_d.
2. It is puzzling that the damage energy for any of the D_1-D_3 variant methods consistently decreases when the E_b and E_s terms are reduced to zero. One would expect that setting these parasitic terms to zero would result in more energy available for nuclear collisions.
3. Taking into account the energy balance equation, it is observed that the damage energy method D_2* precisely equals D_3*, while D_2** approximately equals D_3**. It will be useful to conduct a thorough investigation into how SRIM defines and calculates the six energy loss terms. This examination serves two purposes: first, to accurately determine the damage energy; and second, to identify any potential coding errors that may exist within the SRIM code.
4. If the binding energy (E_b) is not set to zero, it may be necessary to consider the energies lost to lattice binding (E_i^B and E_T^B) when calculating the damage energy involving the phonon energy terms (E_i^P and E_T^P). This consideration was not taken into account in Ref. [9], where binding energies were not set to zero.
5. For all the investigated cases, the calculated damage energies and total number of vacancies using D_1 are lower than those obtained with D_2 and its variants. Note that this statement is

applicable only to D_1 and not its variant D_1^* which is numerically equivalent to D_2^{**}. However, in theory, $E_i^0 - E_i^I$ should be equal to E_i^T, suggesting that D_1 and D_2 (or one of the variants) should yield the same result. This discrepancy indicates that $E_i^0 - E_i^I - E_T^I > E_i^T - E_T^I$, implying that there is missing energy in E_i^T. By analyzing the numbers from the output files, we suspect that $E_T^0 \cong E_i^0 - E_i^I - E_i^B - E_i^P$ in SRIM F-C.

6. When $E_b \neq 0$, the two columns in the E2recoil file (representing the beam energy lost to target atoms (E_T^0) and the beam energy absorbed by target atoms (E_i^T)) are not equivalent. Upon analyzing the numbers from the output files, we suspect that $E_i^T \cong E_T^I + E_T^B + E_T^P - E_i^P$. According to the energy balance equation, and considering $E_T^0 \cong E_i^0 - E_i^I - E_i^B - E_i^P$, the difference between E_i^T and E_T^0 is equivalent to E_i^B. Thus, when E_b is set to zero, the values in the two columns of the E2recoil file become exactly the same, i.e., $E_T^0 = E_i^T$. This is apparently another idiosyncrasy of SRIM. In general, the absorbed energy should never be larger than the energy transferred from the ions, but the SRIM F-C E2recoil file consistently calculates $E_i^T > E_T^0$ for $E_b > 0$.
7. The "vacancy.txt" file summarizes the total number of vacancies differently for Q-C and F-C. For Q-C, it is calculated by integrating the values in the 1st and 2nd columns in the "vacancy.txt" file, whereas for F-C (after E_f=E_d correction), only the sum of the values in the 2nd column is included in the calculation. This indicates a coding error in the SRIM-F-C option, or an error in the description of the SRIM F-C results.

Table A.4. Summary of SRIM-calculated total vacancy numbers for 10 MeV Fe into Fe (E_d=40 eV, E_b=5.7 eV, E_s=4.3 eV). Parentheses in the tables show the total vacancy ratio obtained by dividing the calculated vacancy number by the D_2^{**} method's vacancies calculated using the F-C option with E_f=1 eV.

Methods	Damage energy	F-C (E_f=1eV)	F-C (E_f=E_d)	Q-C
D_1	$E_i^T - E_T^I$	10058.84 (0.99)	10369.26 (1.02)	8872.06 (0.87)
D_2	$E_i^0 - E_i^I - E_T^I - E_i^P$	10058.83 (0.99)	10369.29 (1.02)	8872.07 (0.87)
D_3	$E_T^P - E_i^P$	9144.74 (0.90)	9761.86 (0.96)	8353.23 (0.82)
D_1*	$E_i^T - E_T^I + E_i^P$	10208.58 (1.00)	10519.24 (1.03)	8997.49 (0.88)
D_2*	$E_{total} - E_i^I - E_T^I$	10482.78 (1.03)	10712.30 (1.05)	9122.92 (0.89)
D_3*	$E_i^B + E_T^B + E_i^P + E_T^P$	10482.78 (1.03)	10712.30 (1.05)	9122.92 (0.89)
D_2**	$E_i^0 - E_i^I - E_T^I$	10208.57 (1.00)	10519.26 (1.03)	8997.50 (0.88)
D_3**	$E_T^B + E_T^P$	10300.48 (1.01)	10529.74 (1.03)	8966.65 (0.88)
D_3***	$E_i^B + E_T^B + E_T^P$	10333.03 (1.01)	10562.32 (1.03)	8997.49 (0.88)
Summary in vacancy.txt	--	17325.00 (1.70)	10665.00 (1.04)	8945.00 (0.88)
Integration of vacancy.txt (col1+col2)	--	17906.14 (1.75)	11215.18 (1.10)	8945.23 (0.88)
Integration of vacancy.txt (col2)	--	17344.86 (1.70)	10653.42 (1.04)	8413.50 (0.82)

Table A.5. Summary of SRIM-calculated total vacancy numbers for 10 MeV Fe into Fe (E_d=40 eV, E_b=0 eV, E_s=0 eV). Parentheses in the tables show the total vacancy ratio obtained by dividing the calculated vacancy number by the D_2^{**} method's vacancies calculated using the F-C option with E_f=1 eV.

Methods	Damage energy	F-C (E_f=1eV)	F-C (E_f=E_d)	Q-C
D_1	$E_i^T - E_T^I$	9930.35 (0.99)	10243.82 (1.02)	8872.06 (0.88)
D_2	$E_i^0 - E_i^I - E_T^I - E_i^P$	9930.34 (0.99)	10243.86 (1.02)	8872.07 (0.88)
D_3	$E_T^P - E_i^P$	10029.28 (0.99)	10257.09 (1.02)	8872.05 (0.88)
D_1*	$E_i^T - E_T^I + E_i^P$	10080.09 (1.00)	10393.80 (1.03)	8997.49 (0.89)
D_2*	$E_{total} - E_i^I - E_T^I$	10328.76 (1.02)	10557.04 (1.05)	9122.91 (0.91)
D_3*	$E_i^B + E_T^B + E_i^P + E_T^P$	10328.76 (1.02)	10557.04 (1.05)	9122.91 (0.91)
D_2**	$E_i^0 - E_i^I - E_T^I$	10080.08 (1.00)	10393.84 (1.03)	8997.50 (0.89)
D_3**	$E_T^B + E_T^P$	10179.02 (1.01)	10407.07 (1.03)	8997.48 (0.89)
D_3***	$E_T^B + E_i^P + E_T^P$	10179.02 (1.01)	10407.07 (1.03)	8997.48 (0.89)
Summary in vacancy.txt	--	18815.00 (1.87)	12247.00 (1.21)	8945.00 (0.89)
Integration of vacancy.txt (col1+col2)	--	19410.26 (1.93)	12793.58 (1.27)	8945.23 (0.89)
Integration of vacancy.txt (col2)	--	18848.98 (1.87)	12231.82 (1.21)	8413.50 (0.83)

Table A.6. Summary of SRIM-calculated total vacancy numbers for 10 MeV Au into Au (E_d=40 eV, E_b=3.8 eV, E_s=3.8 eV). Parentheses in the tables show the total vacancy ratio obtained by dividing the calculated vacancy number by the D_2^{**} method's vacancies calculated using the F-C option with E_f=1 eV.

Methods	Damage energy	F-C (E_f=1eV)	F-C (E_f=E_d)	Q-C
D_1	$E_i^T - E_T^I$	39478.95 (1.00)	42155.63 (1.07)	43214.52 (1.09)
D_2	$E_i^0 - E_i^I - E_T^I - E_i^P$	39482.30 (1.00)	42159.76 (1.07)	43214.52 (1.09)
D_3	$E_T^P - E_i^P$	37095.48 (0.94)	40453.91 (1.02)	41570.67 (1.05)
D_1*	$E_i^T - E_T^I + E_i^P$	39553.35 (1.00)	42230.41 (1.07)	43282.21 (1.09)
D_2*	$E_{total} - E_i^I - E_T^I$	40550.51 (1.03)	42506.66 (1.07)	43349.89 (1.10)
D_3*	$E_i^B + E_T^B + E_i^P + E_T^P$	40550.51 (1.03)	42506.66 (1.07)	43349.89 (1.10)
D_2**	$E_i^0 - E_i^I - E_T^I$	39556.70 (1.00)	42234.53 (1.07)	43282.21 (1.09)
D_3**	$E_T^B + E_T^P$	40457.87 (1.02)	42413.57 (1.07)	43264.41 (1.09)
D_3***	$E_i^B + E_T^B + E_T^P$	40476.12 (1.02)	42431.89 (1.07)	43282.20 (1.09)
Summary in vacancy.txt	--	86672 (2.19)	49013.00 (1.24)	43259.00 (1.09)
Integration of vacancy.txt (col1+col2)	--	87006.56 (2.20)	50084.54 (1.27)	43259.00 (1.09)
Integration of vacancy.txt (col2)	--	86526.40 (2.19)	49602.29 (1.25)	42790.88 (1.08)

Table A.7. Summary of SRIM-calculated total vacancy numbers for 10 MeV Au into Li (E_d=25 eV, E_b=1.1 eV, E_s=1.6 eV). Parentheses in the tables show the total vacancy ratio obtained by dividing the calculated vacancy number by the D_2^{**} method's vacancies calculated using the F-C option with E_f=1 eV.

Methods	Damage energy	F-C (E_f=1eV)	F-C (E_f=E_d)	Q-C
D_1	$E_i^T - E_T^I$	20340.24 (0.98)	20717.47 (1.00)	17581.29 (0.85)
D_2	$E_i^0 - E_i^I - E_T^I - E_i^P$	20340.24 (0.98)	20717.50 (1.00)	17581.29 (0.85)
D_3	$E_T^P - E_i^P$	19563.94 (0.94)	20388.24 (0.98)	17267.49 (0.83)
D_1*	$E_i^T - E_T^I + E_i^P$	20791.57 (1.00)	21168.56 (1.02)	17955.75 (0.86)
D_2*	$E_{total} - E_i^I - E_T^I$	20905.39 (1.01)	21650.91 (1.04)	18330.20 (0.88)
D_3*	$E_i^B + E_T^B + E_i^P + E_T^P$	20905.39 (1.01)	21650.91 (1.04)	18330.20 (0.88)
D_2**	$E_i^0 - E_i^I - E_T^I$	20791.58 (1.00)	21168.59 (1.02)	17955.75 (0.86)
D_3**	$E_T^B + E_T^P$	20415.35 (0.98)	21161.14 (1.02)	17919.74 (0.86)
D_3***	$E_i^B + E_T^B + E_T^P$	20454.06 (0.98)	21199.82 (1.02)	17955.74 (0.86)
Summary in vacancy.txt	--	22733.00 (1.09)	18285.00 (0.88)	17829.00 (0.86)
Integration of vacancy.txt (col1+col2)	--	24931.44 (1.20)	20482.56 (0.99)	17828.72 (0.86)
Integration of vacancy.txt (col2)	--	22731.94 (1.09)	18284.67 (0.88)	15783.54 (0.76)

Table A.8. Summary of SRIM-calculated total vacancy numbers for 1 MeV H into Au (E_d=40 eV, E_b=3.8 eV, E_s=3.8 eV). Parentheses in the tables show the total vacancy ratio obtained by dividing the calculated vacancy number by the D_2^{**} method's vacancies calculated using the F-C option with E_f=1 eV.

Methods	Damage energy	F-C (E_f=1eV)	F-C (E_f=E_d)	Q-C
D_1	$E_i^T - E_T^I$	8.12 (0.53)	10.03 (0.66)	10.02 (0.66)
D_2	$E_i^0 - E_i^I - E_T^I - E_i^P$	8.53 (0.56)	13.10 (0.86)	12.87 (0.84)
D_3	$E_T^P - E_i^P$	7.07 (0.46)	9.21 (0.60)	9.56 (0.63)
D_1*	$E_i^T - E_T^I + E_i^P$	14.83 (0.97)	17.12 (1.12)	15.81 (1.04)
D_2*	$E_{total} - E_i^I - E_T^I$	21.58 (1.42)	24.17 (1.59)	21.58 (1.42)
D_3*	$E_i^B + E_T^B + E_i^P + E_T^P$	21.58 (1.42)	24.17 (1.59)	21.58 (1.42)
D_2**	$E_i^0 - E_i^I - E_T^I$	15.24 (1.00)	20.19 (1.32)	18.66 (1.22)
D_3**	$E_T^B + E_T^P$	14.60 (0.96)	16.82 (1.10)	15.56 (1.02)
D_3***	$E_i^B + E_T^B + E_T^P$	14.87 (0.98)	17.08 (1.12)	15.80 (1.04)
Summary in vacancy.txt	--	21.00 (1.38)	14.00 (0.92)	12.00 (0.79)
Integration of vacancy.txt (col1+col2)	--	28.38 (1.86)	20.71 (1.36)	11.79 (0.77)
Integration of vacancy.txt (col2)	--	21.36 (1.40)	13.73 (0.90)	5.445 (0.36)

Table A.9. Summary of SRIM-calculated total vacancy numbers for 1 MeV H into Au (E_d=40 eV, E_b=0 eV, E_s=0 eV). Parentheses in the tables show the total vacancy ratio obtained by dividing the calculated vacancy number by the D_2^{**} method's vacancies calculated using the F-C option with E_f=1 eV.

Methods	Damage energy	F-C (E_f=1eV)	F-C (E_f=E_d)	Q-C
D_1	$E_i^T - E_T^I$	7.92 (0.53)	10.10 (0.67)	10.02 (0.67)
D_2	$E_i^0 - E_i^I - E_T^I - E_i^P$	8.33 (0.55)	15.11 (1.00)	12.87 (0.86)
D_3	$E_T^P - E_i^P$	7.79 (0.52)	9.79 (0.65)	10.01 (0.67)
D_1*	$E_i^T - E_T^I + E_i^P$	14.63 (0.97)	17.16 (1.14)	15.81 (1.05)
D_2*	$E_{total} - E_i^I - E_T^I$	21.21 (1.41)	23.91 (1.59)	21.58 (1.43)
D_3*	$E_i^B + E_T^B + E_i^P + E_T^P$	21.21 (1.41)	23.91 (1.59)	21.58 (1.43)
D_2**	$E_i^0 - E_i^I - E_T^I$	15.04 (1.00)	22.17 (1.47)	18.66 (1.24)
D_3**	$E_T^B + E_T^P$	14.50 (0.96)	16.85 (1.12)	15.80 (1.05)
D_3***	$E_i^B + E_T^B + E_T^P$	14.50 (0.96)	16.85 (1.12)	15.80 (1.05)
Summary in vacancy.txt	--	23.00 (1.53)	15.00 (1.00)	12.00 (0.80)
Integration of vacancy.txt (col1+col2)	--	29.73 (1.98)	22.28 (1.48)	11.79 (0.78)
Integration of vacancy.txt (col2)	--	22.71 (1.51)	15.24 (1.01)	5.44 (0.36)

Table A.10. Summary of SRIM-calculated total vacancy numbers for 1 MeV H into Li (E_d=25 eV, E_b=1.1 eV, E_s=1.6 eV). Parentheses in the tables show the total vacancy ratio obtained by dividing the calculated vacancy number by the D_2^{**} method's vacancies calculated using the F-C option with E_f=1 eV.

Methods	Damage energy	F-C (E_f=1eV)	F-C (E_f=E_d)	Q-C
D_1	$E_i^T - E_T^I$	8.72 (0.63)	9.00 (0.65)	7.26 (0.53)
D_2	$E_i^0 - E_i^I - E_T^I - E_i^P$	8.72 (0.63)	9.20 (0.67)	7.26 (0.53)
D_3	$E_T^P - E_i^P$	4.33 (0.31)	8.46 (0.61)	7.10 (0.52)
D_1*	$E_i^T - E_T^I + E_i^P$	13.76 (1.00)	14.22 (1.03)	11.42 (0.83)
D_2*	$E_{total} - E_i^I - E_T^I$	14.73 (1.07)	19.16 (1.39)	15.57 (1.13)
D_3*	$E_i^B + E_T^B + E_i^P + E_T^P$	14.73 (1.07)	19.16 (1.39)	15.57 (1.13)
D_2**	$E_i^0 - E_i^I - E_T^I$	13.77 (1.00)	14.42 (1.05)	11.42 (0.83)
D_3**	$E_T^B + E_T^P$	9.58 (0.70)	13.85 (1.01)	11.33 (0.82)
D_3***	$E_i^B + E_T^B + E_T^P$	9.68 (0.70)	13.95 (1.01)	11.41 (0.83)
Summary in vacancy.txt	--	12.00 (0.87)	10.00 (0.73)	9.00 (0.65)
Integration of vacancy.txt (col1+col2)	--	17.41 (1.26)	15.40 (1.12)	8.67 (0.63)
Integration of vacancy.txt (col2)	--	11.94 (0.86)	9.92 (0.72)	3.95 (0.29)

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