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On the use of SRIM for computing radiation damage exposure

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ABSTRACT

The SRIM (formerly TRIM) Monte Carlo simulation code is widely used to compute a number of parameters relevant to ion beam implantation and ion beam processing of materials. It also has the capability to compute a common radiation damage exposure unit known as atomic displacements per atom (dpa). Since dpa is a standard measure of primary radiation damage production, most researchers who employ ion beams as a tool for inducing radiation damage in materials use SRIM to determine the dpa associated with their irradiations. The use of SRIM for this purpose has been evaluated and comparisons have been made with an internationally-recognized standard definition of dpa, as well as more detailed atomistic simulations of atomic displacement cascades. Differences between the standard and SRIM-based dpa are discussed and recommendations for future usage of SRIM in radiation damage studies are made. In particular, it is recommended that when direct comparisons between ion and neutron data are intended, the Kinchin–Pease option of SRIM should be selected.

1. Introduction

The Monte Carlo simulation code named Stopping and Range of Ions in Materials, or SRIM (formerly TRIM) was written to permit the calculation of ion deposition profiles in materials exposed to energetic beams of ions [1–4]. Researchers involved in ion beam modification of materials and ion beam implantation were initially the primary users of the code, and a review of the relevant literature (e.g. see almost any issue of *Nuclear Instruments and Methods* or the *Journal of Nuclear Materials*) will reveal that it has found broad application because of its relative power and ease of use. A primary component of the code involves determining the partitioning of the ion beam energy between electronic and nuclear stopping, and most significant modifications during its years of use have been related to improved electronic stopping powers [4]. Ion beams are also used by a large community of scientists to investigate the damage formation and evolution induced by high energy particles in materials in an attempt to study the effects of exposure to high energy neutrons [5]. It is not the purpose of this paper to establish the relevance of this "simulation". Rather, the topic is related to a particular issue that immediately arises when one wishes to compare ion and neutron irradiation, *viz.* that of determining a measure of radiation exposure equivalence.

For many years after the effect of neutron irradiation on material properties was first discovered, it was common practice to correlate radiation-induced property changes with a measure of the neutron fluence (units of neutrons per unit area). Depending on the property of interest and the portion of the neutron energy spectrum that was believed to be responsible for the change, several parameters were used. These included: total neutron fluence, thermal (energy less than about ~0.5 eV) fluence, or fast (energy greater than some specified threshold energy) fluence. In the case of dimensional and mechanical property changes in metals and alloys, the most common measure was neutron fluence above 1.0 MeV because neutrons in this energy range were thought to be primarily responsible for the atomic displacements that created the damage observed.

Based on the initial conceptual work of Seitz [6], a number of models were developed to calculate, at least approximately, the number of atoms displaced by an energetic particle [7–10]. The paper by Snyder and Neufeld [7] is recommended to those who are interested in the first detailed mathematical development of the concepts that were later followed. Since that time, the most widely cited model has been that of Kinchin and Pease [8], which assumed that between specified threshold energy and an upper energy cut-off, there was a linear relationship between the number of Frenkel pair produced and the initial energy of a primary knock-on atom (PKA). Below the threshold, no new displacements would be produced, while the energy above the high energy cut-off was treated as being dissipated in electronic excitation and ionization. Later, Lindhard and co-workers developed a detailed theory for energy partitioning that could be used to compute the fraction of the PKA energy that was dissipated in the nuclear system in elastic col-

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lisions and in electronic losses [11]. By the early 1970s there were several modifications of the Kinchin and Pease model in use; these included the Nelson and half-Nelson models from the United Kingdom and the French model as discussed in Refs. [10,12–14]. The number of displacements predicted by these models was about one-half that obtained from the original Kinchin–Pease model, but the variation among them was about 30%. In 1974, Robinson and Torrens [15] developed the MARLOWE binary collision code to enable detailed computational simulations of high-energy displacement cascades. As a result of their work, Norgett, Robinson, and Torrens (NRT) developed a secondary displacement model for computing the number of displacements per atom (dpa) for a PKA with a given energy [12]. This NRT model was broadly adopted by the international radiation effects community and continues to be the internationally-recognized standard method for computing atomic displacement rates [16–18].

The NRT displacement model gives the total number of stable Frenkel pair produced by a PKA with kinetic energy E_{PKA} as:

$$\nu_{NRT} = 0.8T_{dam}(E_{PKA})/2E_d \quad (1)$$

where the parameter T_{dam} is called the damage energy and represents the portion of the PKA energy that is dissipated in elastic collisions with atoms in the lattice. As indicated in Eq. (1), the damage energy is a function of the PKA energy, and the ratio T_{dam}/E_{PKA} decreases as the PKA energy increases due to the increasing importance of electronic stopping at higher energies [11,12,14,16]. The energy required to create a stable Frenkel pair is referred to as the displacement threshold energy and is denoted by E_d in Eq. (1). The displacement threshold energy is strongly dependent on the crystallographic direction and an appropriate mean value should be used in Eq. (1). This requires averaging over many crystallographic directions [14,19]; recommended values for a number of metals can be found in Ref. [17].

The adoption of the NRT model, which was built on the basis of the earlier displacement models [6–9], provided a standardized exposure parameter and eliminated the ambiguity associated with the proliferation of displacement models. Moreover, the NRT dpa has a number of benefits relative to the various particle fluence parameters mentioned above. Since it explicitly accounts for the total energy used to create atomic displacements, it provides a common basis of comparison for data obtained in different types of irradiation sources, e.g. different neutron energy spectra, ion irradiation, or electron irradiation [14,20,21–23]. The neutron energy spectrum can vary significantly from one reactor to another depending on the reactor coolant and/or moderator (water, heavy water, sodium, graphite), which leads to differences in the PKA energy spectrum. This can confound attempts to correlate irradiation effects data on the basis of neutron fluence parameters. More importantly, it is impossible to directly compare any given neutron fluence with a charged particle fluence. However, in any of these cases, the PKA energy spectrum and corresponding damage energies can be calculated, and the total number of displacements obtained using Eq. (1) in an integral calculation. Thus, the NRT dpa provides an environment-independent radiation exposure parameter that in many cases can be successfully used as a radiation damage correlation parameter. Of course, other aspects of primary damage production such as transmutation products, notably He, are not accounted for in any displacement model. In addition, it should be mentioned that parameters other than dpa may be more appropriate for correlating certain types of radiation-induced phenomena. For example, dpa does not account for the number of atomic replacements, collisions in which one atom replaces another on the same lattice site. Knowing the number of atomic replacements is significant to understanding the behavior of ordered alloys and ion beam mixing [5,24].

In addition to other parameters relevant to ion beam implantation and ion beam processing of materials, SRIM has the capability to compute the dpa. Since the calculation is relatively easy, most researchers who employ ion beams as a tool for inducing radiation damage in materials use SRIM to determine the dpa associated with their irradiations. However, there are multiple ways to obtain the number of atomic displacements or dpa from SRIM. The purpose of this short paper is to provide a comparison of what the different options provide, and to recommend an approach which is most consistent with the internationally-recognized standard NRT dpa. The authors do not assert that the number of displaced atoms calculated in this way is accurate in any absolute sense, but rather that the result will provide the most appropriate value for comparison with the dpa reported for neutron irradiation experiments since the standard codes employed by the commercial nuclear and research communities implement the NRT model for computing dpa [16,18,25,26]. A representative set of SRIM calculations for iron and nickel are presented which illustrate the motivation for this short paper. These include both heavy and light ions with energies that provide a wide range in the relative fractions of electronic and nuclear stopping power.

2. Damage calculations in SRIM

Most users who wish to use SRIM to compute ion-induced displacement damage parameters employ one of two basic options: (1) "Ion Distribution and Quick Calculation of Damage," and (2) "Detailed Calculation with full Damage Cascades." There is a third option called "Monolayer collition steps" which was not assessed in detail for this paper. However, two sample calculations were done for this case and the results relevant to the discussion presented below appear to be consistent with those of option (2). One advantage of the latter option is that it provides a complete listing of the energy for all the knock-on atoms produced by the incident ions. For either of these two options, the user must designate the nature and energy of the incident ion, the nature of the target, and both the displacement threshold energy and the lattice binding energy. Since this paper does not address sputtering, the surface binding energy and related output files will not be addressed. In both cases SRIM produces a number of output files; those relevant to this discussion are described in Table 1. These files each contain a table of values as a function of distance from the surface where the ions enter, with units as shown in the table. For purposes of calculating the damage depth profile, SRIM divides the thickness of the target layer specified by the user into 100 equal-width bins. For the first three entries in Table 1, an integral over the path of the ions for all ions will yield an energy, and a similar integral for the vacancy.txt file will yield the total number of vacancies. In each file, the first column is relevant to the incoming ion and the second column to the target atoms. In the case of the file e2recoil.txt, values in both columns are nominally identical

Table 1
SRIM output files relevant to displacement damage calculations.

File name	Contents	Units
e2recoils.txt	Energy transferred from incident ions to target atoms and energy absorbed by target atoms	eV/angstrom/ion
Ioniz.txt	Energy absorbed in electronic stopping by target atoms from incident ions and recoil atoms	eV/angstrom/ion
Vacancy.txt	Vacancies created	Vacancies/angstrom/ion
Collison.txt	Table of all ion/target atom collisions which lead to target damage	

Table 2
Definition of symbols used.

E_i^o	Incident ion or beam energy	SRIM input parameter
E_d	Displacement threshold energy	SRIM input parameter
E_B	Lattice binding energy	SRIM input parameter
E_i^T	Beam energy lost to target atoms	"*Energy from ions*" in e2recoil.txt
E_i^I	Beam energy lost to ionization	$E_i^B = E_B.v_i$
E_i^P	Beam energy lost to phonons	"*Energy absorbed by target*" in e2recoil.txt
v_i	Vacancies created by ions	
E_i^B	Beam energy lost to lattice binding energy	
E_T^o	Beam energy absorbed by target atoms	
E_T^I	Target atom energy lost to ionization	$E_T^B = E_B.v_T$
E_T^P	Target atom energy lost to phonons	
v_T	Vacancies created by target atoms	
E_T^B	Target atom energy lost to lattice binding energy	

since they refer to energy transfer between the ion and the target in each bin. The nomenclature and symbols used in the following discussion are defined in Table 2.Based on the definitions contained in Table 2, and assuming that each of the parameters has been integrated over target layer thickness, the following relationships should hold (again sputtering is neglected):

$$E_i^o = E_i^T + E_i^I + E_i^P + E_i^B \tag{2}$$

$$E_T^o = E_T^I + E_T^P + E_T^B + E_i^B \tag{3}$$

$$E_i^T = E_T^o - E_i^B = E_T^I + E_T^P + E_T^B \tag{4}$$

In the language of SRIM, the incident ion energy is ultimately distributed into electronic excitation (superscript I), lattice phonons (superscript P), and lattice binding energy (superscript B). The last term is the product of the input lattice binding energy and the number of vacancies created. The source may be one of the incident ions (subscript i) or one of the recoiling target atoms (subscript T). The total lattice binding energy, which is the product of input lattice binding energy sum and the number of vacancies created is also assumed to be dispersed in lattice phonons. Sums such as those in Eqs. (2)–(4) are accurate to within the limits of the finite binning scheme used to prepare the output data. To obtain a value for the damage energy from SRIM which is essentially consistent with the definition of the NRT damage energy in Eq. (1), either of the two sums in Eq. (5a) can be used:

$$T_{\mathrm{dam}} = E_i^o - E_i^I - E_T^I = E_i^P + E_i^B + E_T^P + E_T^B \tag{5a}$$

$$T_{\mathrm{dam}} = E_i^o - E_i^I - E_T^I = E_i^P + E_T^P \tag{5b}$$

To be fully consistent with the NRT model, the lattice binding energy should be set to zero (see discussion in Ref. [14]), leading to Eq. (5b). In this case, the damage energy is simply the energy that goes into SRIM "phonons" which is also the initial ion energy minus the energy dissipated in ionization. Quantitative assessments of the different possible methods of computing atomic displacement in SRIM will be discussed below. Here we point out that if the SRIM "Quick" Kinchin and Pease damage calculation is selected and Eq. (5b) is used to compute T_{dam}, the number of displacements obtained using Eq. (1) is almost the same as the number of vacancies obtained from a sum of v_i and v_T. The difference may due to small errors arising from the discrete binning of the energy tables in the SRIM output, or some deficiency of the SRIM model for computing the number of vacancies created. This question is examined further below.

3. Radiation-induced displacement production: comparison with the NRT model

Primary radiation damage production is a complex process, involving a range of phenomena and mechanisms [14,19] which could never be adequately accounted for by a secondary displacement model as simple as the NRT. What the NRT model dose is provide a method for converting a calculable parameter, the damage energy, into a number of stable atomic displacements. It is not the "right" number of displacements in any absolute sense; its importance lies in its broad adoption as a standard reference value. As such, the NRT displacements provide a basis for evaluating the results obtained from SRIM using the different possible options. Molecular dynamics (MD) cascade simulations provide a more computational intensive method of obtaining the number of displaced atoms created by a PKA of a given energy. MD simulations comprise a more realistic picture of cascade damage production and provide results which are generally consistent with relevant experimental data [19,27,28]. Notably, MD results provide information on the time dependence of atomic displacement cascades, can account for the effects of lattice temperature, and provide

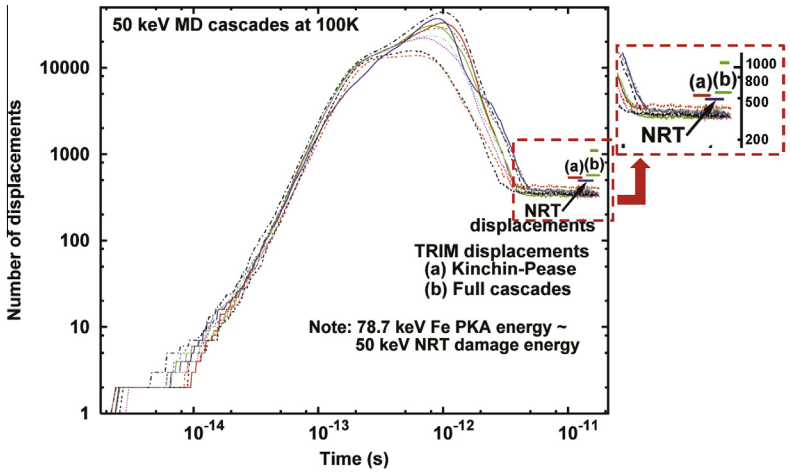

Fig. 1. Comparison of displacement production in iron predicted using various approaches; range of values for (b) reflects two methods of calculating the number of displacements for SRIM Full Cascade model (see text).

Table 3
Displacements obtained for 78.7 keV PKA (~50 keV damage energy) in iron.

NRT model	Eq. (1) with T_{dam} = 50 keV	500
SRIM-2008 Kinchin–Pease quick calculation, 5000 ions	Eq. (1) with T_{dam} from Eq. (5b)	540
SRIM-2008 Kinchin–Pease Quick calculation, 5000 ions	Sum of v_i and v_T from vacancy.txt file	530
SRIM-2008 Full Cascade calculation, 5000 ions	Eq. (1) with T_{dam} from Eq. (5b)	572
SRIM-2008 Full Cascade calculation, 5000 ions	Sum of v_i and v_T from vacancy.txt file	1099
Molecular dynamics, 50 keV, 100 K, 9 simulations at ~15 ps	n/a	168+/−4.04 (Standard error)

information on damage production parameters beyond the total number of displacements produced. For example, they can reveal the effects of atomic mixing mentioned above and demonstrate that a significant fraction of the cascade-produced point defects are in clusters. Overall, MD results provide the best benchmark for estimating the actual number of stable atomic displacements created in a displacement cascade.

A single energy point comparison of the NRT model, SRIM, and MD simulations is shown in Fig. 1 and summarized in Table 3. Using the approximation from Ref. [12], the calculated NRT damage energy for a 78.7 keV PKA in iron is 50 keV. Using 50 keV for the damage energy and the recommended 40 eV displacement threshold in Eq. (1), 500 NRT displacements are predicted. SRIM calculations were carried out using the 2008 version for a 78.7 keV PKA energy and 40 eV displacement threshold energy with the lattice binding energy set to zero. Using these parameters, SRIM code calculations were carried out using both the Kinchin–Pease (K–P) and "Full Cascade" (F–C) options. The number of displacements predicted by SRIM was determined in two ways: (1) obtaining T_{dam} from Eq. (5b) and solving Eq. (1) and, (2) simply summing v_i and v_T from the vacancy.txt file. Since the MD simulations do not account for electronic stopping, all of the input cascade energy is absorbed in elastic collisions. This is the equivalent of the NRT damage energy. Therefore, a cascade energy of 50 keV was employed in simulations at 100 K. This involves some approximation since the energy associated with electronic losses is effectively subtracted at time zero rather being lost continuously during the cascade. The results of nine MD simulations are shown in Fig. 1, along with the NRT value and the SRIM results. The large number of transient defects obtained in MD simulations is clearly visible in Fig. 1, along with the statistical variation between cascades. Only the stable number of defects predicted by the MD simulations, i.e. those which remain after ~10–20 ps, should be compared to the value obtained from either SRIM or the NRT model. The mean value from the nine MD simulations was 168 net displacements.

Several conclusions may be drawn from the comparison of NRT, MD, and SRIM values shown in Table 3. The first is that both cascade models in SRIM predict somewhat more defects than the NRT model, and the disparity is greater for the F–C than for the K–P calculation. The most unexpected result is the very high number of predicted displacements obtained from the vacancy.txt file when using the F–C calculation. The ratio of displacements obtained from the damage energies in the F–C to K–P calculations is 572/540 = 1.06, while the ratio from the vacancy.txt files is 1099/530 = 2.07. As discussed further below, the inconsistency between results based on the damage energy and the vacancy.txt for the F–C model provides a strong argument for using the damage energy obtained from the SRIM K–P calculation to determine the number of displacements. The number of stable defects produced in the MD simulations is about one-third of the NRT value, 168 compared to 500. The discrepancy with the MD results is greater for any of the values obtained from SRIM. The difference between the MD and NRT values is reasonably attributed to in-cascade close-pair recombination which is not accounted for in the NRT model. When the damage energy approach is used, part of the difference between the NRT and SRIM results is likely due to the more modern electronic stopping model in SRIM compared to the model used in Refs. [11,12]. However, the discrepancy between the damage energy results and the vacancy.txt file raise questions about the model used within SRIM to calculate the number of vacancies (displacements).

Several additional calculations were carried out to assess the difference between the K–P and F–C options using SRIM-2008 for a pure iron target using the incident ions and energies listed in Table 4. These ions and energies encompass a range of ionizing to nuclear stopping ratios, with damage energy varying from ~1% to ~68% of the incident ion energy. Several parameters from both displacement options are summarized in Table 4. The number of displacements was obtained from the vacancy.txt file in two ways, the reported sum (column 3) and by integrating the vacancy.txt file (column 4). Column 6 lists the damage energy calculated using Eq. (5b) and the corresponding NRT displacements obtained from Eq. (1) are listed in column 7. The results are consistent with those shown in Table 3, i.e. the number of displacements obtained from the vacancy.txt file for the F–C calculation is more than a factor of two larger than that from the K–P calculation (column 5). However, the values of the damage energy calculated from these two models are almost the same. Since the number of displacements is linearly dependent on the damage energy in the NRT model, the damage energy values obtained from SRIM imply that the information in the vacancy.txt file is not a reliable indicator of dpa. Similar damage energies should lead to similar numbers of displacements. Even if all the energy of the 69 keV Fe ion in Table 4 was converted into displacements (i.e. there was no electronic stopping), the NRT value would predict 690 displacements as an upper bound. Thus, the value of ~950 displacements obtained from the vacancy.txt file for this case is not plausible.

In order to provide a final example of the difference between the K–P and F–C models in SRIM, calculations were carried out

Table 4
Damage calculations for three test cases using SRIM-2008.

Incident ion and nergy (keV)	Calculation option in SRIM	Displacements from vacancy.txt			Displacements from damage energy		
		Summary in vacancy.txt	Integration of vacancy.txt	F–C to K–P displacement ratio	Damage energy, T_{dam} from Eq. (5b) (keV)	ν_{NRT}, Eq. (1)	F–C to K–P displacement ratio
Fe, 69	K–P	469	469	2.06	47.171	472	1.05
Fe, 69	F–C	953	966		50.097	501	
Fe, 5000	K–P	7,893	7,895	2.13	793.255	7,933	1.10
Fe, 5000	F–C	16,333	16,839		875.652	8,757	
Proton, 2000	K–P	14	14	2.43	1.871	19	1.05
Proton, 2000	F–C	27	34		2.025	20	

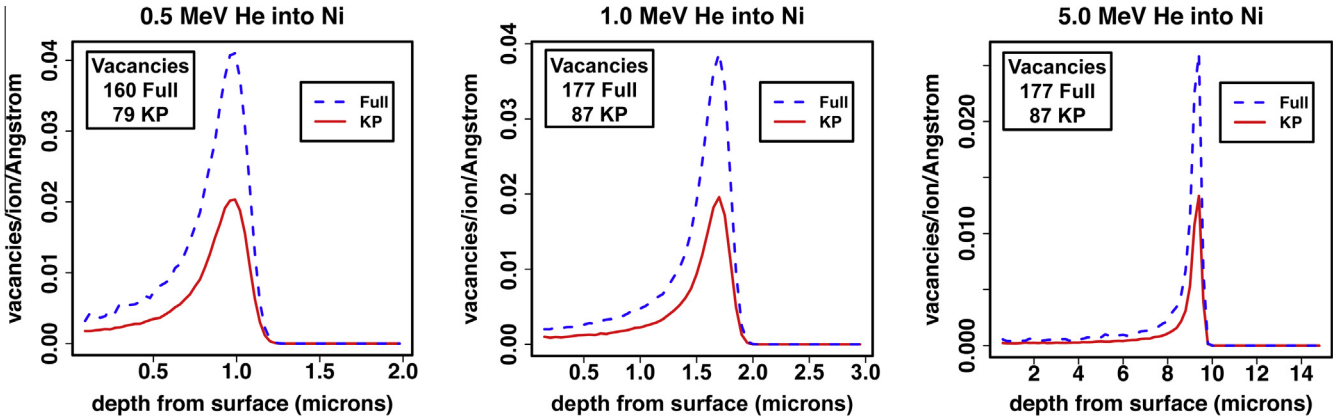

Fig. 2. SRIM calculation of vacancy production due to He implantation in nickel using 0.5, 1, and 5 MeV He ions, results taken from vacancy.txt files.

for He ion implantation into nickel for a range of He ion energies, 0.5, 1.0 and 5.0 MeV. The depth dependence of vacancy production predicted by SRIM for all three energies is shown in Fig. 2, in which the data from the vacancy.txt file has been plotted for both the K–P and F–C models. In this example, the predictions of the F–C model are again about a factor of two greater than the K–P calculation independent of the electronic to nuclear stopping ratio.

4. Discussion and summary

As stated above, it is not possible to determine the "right" number of displacements generated by a given PKA in any absolute sense. MD simulations provide the most realistic estimate, but MD results are also model (interatomic potential) dependent to some degree. Other approximations are made in both SRIM and most of the MD simulations that have been carried out to investigate primary radiation damage formation. For example, the charge state of the moving ions has not been accounted for in either case. Temperature is known to have a modest impact on point defect production in MD simulations [19] but this is not accounted for in SRIM. On the other hand, until recently MD simulations have not accounted adequately accounted for the effect of continuous electronic losses [29].

For the radiation damage community the importance of the NRT model lies not in it accuracy but in its broad adoption as a standard reference value. When using the popular SRIM code to compute radiation damage production, the users typically choose between the "quick Kinchin–Pease calculation" and the "Full Cascade" options. The nomenclature implies that calculations employing the F–C option will be more accurate; in fact, the guidance provided in the SRIM manual explicitly recommends using the full cascade model. However, we have shown that this is not the case. Two issues have been raised. The first is the discrepancy between the number of displacements obtained from the vacancy.txt file and the damage energy calculated with the two models. In any displacement model, a given amount of damage energy should produce the same number of displacements. The damage energies obtained from the K–P and F–C models are generally similar, but the number of displacements obtained from the vacancy.txt for these two options varies by more than a factor of two. This difference between the two models has also been noted by the authors of SRIM [3]. Secondly, the fact that the F–C model predicts a greater number of displacements than the K–P model indicates there is a fundamental problem in the SRIM model used to calculate the number of vacancies created. As shown in Fig. 1, the number of displacements obtained from SRIM is comparable to the NRT model if it is calculated using the damage energy, i.e. applying the damage energy from Eq. (5b) in Eq. (1), but much higher if it is obtained from the vacancy.txt file in the F–C mode. The large number of vacancies obtained from the F–C vacancy.txt file is inconsistent with both MD simulations and cryogenic neutron irradiation experiments which demonstrate that the number of stable atomic displacements created by a PKA is actually significantly less than the NRT model [19,27,28].

In summary, if a researcher intends to use SRIM to compute dpa from an ion irradiation experiment and wishes to compare the data to the results of neutron or other ion irradiation experiments, it is important that the calculation produce values consistent with the international standard [12,17]. The following recommendations should be complied with:

(1) run SRIM using the "Quick" Kinchin and Pease option,
(2) choose the recommended displacement threshold energy from Ref. [17], which is 40 eV for iron or iron-based alloys,[1]
(3) set the lattice binding energy to zero,
(4) compute the damage energy according to Eq. (5b), and
(5) use the computed value of T_{dam} to calculate the number of displacements according to Eq. (1).

Calculating the number of displacements based on the damage energy is preferred over simply reporting the number of vacancies in the vacancy.txt file even when using the K–P option because the F–C calculations discussed above indicate there is a significant error in SRIM's internal model for calculating the number of vacancies. It is likely that the same error influences the vacancy calculation in the K–P case. Finally, in order to avoid misleading comparisons of data from different experiments, authors should fully describe how they have calculated any dpa values they report and endeavor to determine how the dpa were calculated in any previous experiments to which they compare their own data. Although the NRT model has been broadly used since the mid 1970s, some historical data was reported using the other dpa variants discussed above, and other computer codes such as E-DEP (Energy Deposition) [30] were formerly used to calculate dpa.

[1] If the material of interest is not listed in Ref. [17], it may be appropriate to choose a metal of similar mass and crystal structure. Information on other materials may also be available in the literature [31,32], or MD simulations may be carried out to determine the threshold energy.

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