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Quantifying athermal recombination corrected radiation damage in ion-irradiated Fe and W utilizing the SRIM code

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Abstract Athermal recombination corrected displacements per atom (arc-dpa) is a recently proposed correction to the standard Norgett-Robinson-Torrens (NRT) model employed for radiation damage calculations, which takes into account intra-cascade recombination. The correction is not yet implemented in any of the widely used ion transport codes, and special data handling is required to obtain arc-dpa damage parameters in ion irradiations. In the current work, the widely used code SRIM was employed to calculate arc-dpa parameters in two metals of key interest for fusion materials research, Fe and W. For this, an interpolation was devised for the ion energy deposited to target damage, which was then used for post-processing of SRIM output. The NRT- and arc-dpa results obtained with this method are in general agreement with previous studies.

Keywords radiation damage, SRIM, athermal recombination corrected dpa (arc-dpa), F, W, displacement per atom (dpa)

INTRODUCTION

In radiation damage studies, the unit of displacements-per-atom (dpa) is typically used as a measure of radiation exposure, mainly due to its conceptual simplicity and the ability to compare results obtained under different irradiation conditions. Currently, dpa calculations are performed according to the Norgett-Robinson-Torrens (NRT) model [1]. Regarding ion irradiation, this model is embedded into one of the most widely used software tools for ion transport calculations: SRIM [2]. Apart from its friendly user interface, SRIM employs an extensive database of ion stopping powers. In SRIM’s “Full-Cascade” (F-C) simulation mode, these detailed stopping powers are used not only for the projectile but also for the secondary ion recoils. Thus, this mode gives the most accurate estimation of energy deposition in the target. Alternatively, the much faster “Quick Calculation” (Q-C) mode, employs Lindhard’s approximation for the energy partition of secondary recoils. Many studies have discussed in detail the differences in NRT-dpa obtained with the two different simulation modes [3, 4, 5, 6].

Recently, a correction to the standard NRT-dpa exposure calculation has been proposed. It is termed athermal recombination corrected dpa (arc-dpa) and takes into account intra-cascade recombination, which becomes significant at high cascade energies and leads to substantially lower defect numbers compared to NRT [7]. The arc-dpa correction is not yet implemented in any of the widely used ion transport codes, including SRIM. However, different methods have been proposed for obtaining arc-dpa damage parameters by post-processing SRIM output [8, 9].

In the current contribution, the arc-dpa damage parameters were calculated using SRIM in two elemental metals with great interest for fusion materials research: Fe and W. For this, both the Q-C mode, as described in [9] and the F-C mode, as previously proposed by Nordlund et al. [8] were employed. The differences in the damage parameters obtained with the two simulation modes are discussed and the present results are compared to previous studies.

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ESTIMATION OF RADIATION DAMAGE WITH SRIM

Damage models (both NRT- and arc-dpa) give the number of displaced atoms, v , created by a primary knock-on atom (PKA) as a function of the damage energy T_{dam} , i.e., the part of the PKA recoil energy that is available for atomic displacements. Key parameters in both NRT- and arc-dpa are the displacement threshold energy, E_d , and the cascade multiplication threshold, $L = 2.5E_d$. The models are described by the following equations:

- Norget-Robinson-Torres (NRT-dpa):

$$v_{NRT}(T_{dam}) = \begin{cases} 0, & 0 < T_{dam} \leq E_d \\ 1, & E_d < T_{dam} \leq L \\ T_{dam}/L, & L < T_{dam} \end{cases} \quad (1)$$

- Athermal Recombination Corrected (arc-dpa):

$$v_{arc}(T_{dam}) = \begin{cases} 0, & 0 < T_{dam} \leq E_d \\ 1, & E_d < T_{dam} \leq L \\ v_{NRT}(T_{dam}) \cdot \xi(T_{dam}), & L < T_{dam} \end{cases} \quad (2)$$

where $\xi(T_{dam}) = (1 - c)(T_{dam}/L)^b + c$ is the cascade efficiency factor defined in the arc-dpa model and b, c are material specific constants [7].

The NRT equation is directly employed in the Q-C mode of SRIM for the estimation of target damage. As noted by a number of previous authors [3-6], this mode may be preferable if NRT-compatible results are required for purposes of comparison. However, T_{dam} is only approximately calculated by the Lindhard-Scharff-Schiott (LSS) theory in Q-C [10,11]. This yields good results at medium energies and low ion masses but can lead to significant discrepancies at high energy recoils [5]. Better estimates of T_{dam} can be obtained in the F-C mode, which utilizes more accurate stopping powers for both the primary ion and subsequent ion recoils. The average T_{dam} obtained from a SRIM simulation can then be used with eq. (1) to evaluate the NRT damage. According to a recent study, the difference in NRT-dpa values obtained by the two SRIM simulation modes can be up to 25% in some cases [5].

The application of SRIM for arc-dpa damage calculations requires special handling due to the fact that the model is non-linear with respect to T_{dam} , as can be seen from eq. (2), in contrast to NRT which is linear for $T_{dam} > L$. Thus, the average value of T_{dam} per ion from SRIM is not sufficient for calculating the damage and one has to obtain the T_{dam} of every single recoil to apply eq. (2) and then take the average. As shown in [9], this can be done with the help of the COLLISON.txt output file from SRIM Q-C mode, which contains a list of all PKAs and their recoil energies. Employing LSS theory to convert the PKA recoil energy, E_r , to T_{dam} , one can process this data and obtain the average arc-dpa exposure. A different method, which may potentially give more accurate results, was suggested by Nordlund et al. in their original work introducing the arc-dpa concept [8]. They first performed a series of F-C simulations to evaluate T_{dam} for a number of different E_r values and obtain an interpolation function through this data. The interpolation was then used for post-processing the COLLISON.txt file of a Q-C simulation to finally obtain the arc-dpa values. Nordlund et al. applied this method for the calculation of the arc-dpa parameter in Fe, however, only for a very limited range of recoil energies. To implement their method to a wide range of irradiation conditions, an interpolation of T_{dam} was derived for recoil energies up to 100 MeV in both Fe and W. Then, the NRT- and arc-dpa exposures obtained by SRIM were compared, using either the simple Q-C/LSS method (Method 1) or the potentially more accurate method by Nordlund et al. (Method 2).

INTERPOLATION OF $T_{dam}(E_r)$

A series of SRIM simulations of PKA recoil cascades in Fe and W were performed in F-C mode for a range of recoil energies from 100 eV to 100 MeV. The special SRIM option “Recoil Cascades from neutrons etc. (full cascades) using TRIM.DAT” was used, which enables the direct simulation of cascades within the target volume without incident ions. This, simplifies data handling and avoids some ambiguities regarding the energy partition in SRIM [4, 5]. The specific parameters of each cascade, i.e., PKA energy, position and direction, are defined by the user in the specially prepared input file TRIM.DAT. T_{dam} is obtained from the output file PHONONS.txt, which gives the energy that is deposited to the lattice.

It was found that the data can be well described throughout the energy range by the following interpolation function, which is similar in form to the LSS theory [10,11]:

$$T_{dam}(E_r) = \frac{E_r}{1 + A \cdot k_L \cdot (E_r/E_L) + B \cdot k_L \cdot (E_r/E_L)^{1/6}} \quad (3)$$

The material relevant constants k_L and E_L are defined in the LSS theory, while the free parameters A and B are adjusted in order to fit our results. The values of A, B are obtained by plotting the quantity:

$$Y = \frac{E_L}{k_L \cdot E_r} \cdot \left(\frac{E_r}{T_{dam}} - 1 \right) = A + B \cdot (E_r/E_L)^{-5/6} \quad (4)$$

as a function of (E_r/E_L) and fitting to eq. (4).

Fig. 1 shows Y as a function of (E_r/E_L) for both Fe and W, as obtained from the SRIM F-C simulations (circles), from the fitted function of eq. (4) (dash-dotted line) and from the LSS approximation (dashed line). As seen in the figure, for both Fe and W the chosen interpolating function describes adequately the $T_{dam}(E_r)$ relation. Compared to LSS, the T_{dam} obtained from F-C SRIM is 11% higher in Fe and differs by only 4% in W. The fitted parameters A and B for Fe and W are given in Table 1.

Table 1. Parameters of the interpolation function, eq.(3), for obtaining T_{dam} as a function of E_r in Fe and W for $100 \text{ eV} \leq E_r \leq 100 \text{ MeV}$

Target Material	A	B
Fe	0.88 ± 0.03	2.31 ± 0.06
W	0.94 ± 0.10	3.92 ± 0.14

APPLICATION TO ARC-DPA DAMAGE CALCULATIONS

To test the quantification of arc-dpa damage parameters with SRIM using either the Q-C/LSS combination (Method 1) or the method of Nordlund et al. [8] with the interpolation functions obtained in the previous section (Method 2), a number of SRIM simulations of Fe and W irradiation was performed at conditions that are typically anticipated in radiation effects experiments. Projectile ions ranged in atomic mass from Z=1 (H) to 79 (Au) and in energy from 1 to 10 MeV. Target thickness was set appropriately so that all impinging ions stop inside the target. More details can be found in [9]. Both NRT- and arc-dpa damage were estimated for reference. The steps to implement the two methods are as follows:

Method 1 – T_{dam} from LSS approximation

1. Process “COLLISON.txt” file to obtain v_{NRT} of each PKA as calculated by SRIM
2. Use eq. (1) to convert v_{NRT} to T_{dam} (this corresponds to the LSS- T_{dam} evaluated by SRIM)
3. Calculate v_{arc} according to eq. (2)

Method 2 – T_{dam} from interpolation by eq. (3)

1. Process “COLLISON.txt” to obtain the PKA recoil energies (E_r)
2. Calculate T_{dam} from interpolation formula (3)
3. Calculate v_{NRT} and v_{arc} according to formulas (1) and (2) respectively

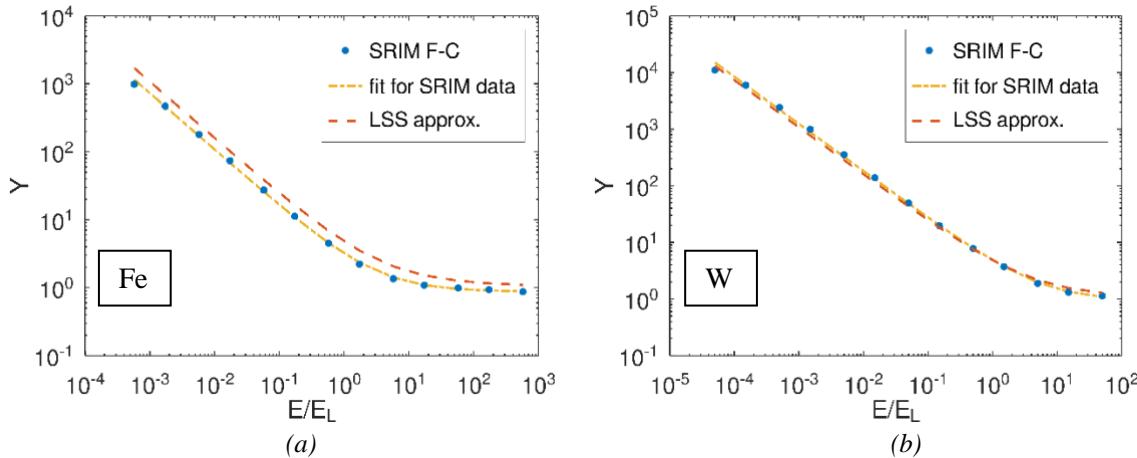


Figure 1. The quantity Y of eq. (4) obtained by SRIM simulations (circles) in (a) Fe and (b) W as a function of scaled recoil energy E_r/E_L . Dash-dotted lines represent the fitted interpolation function and dashed lines depicts the LSS approximation.

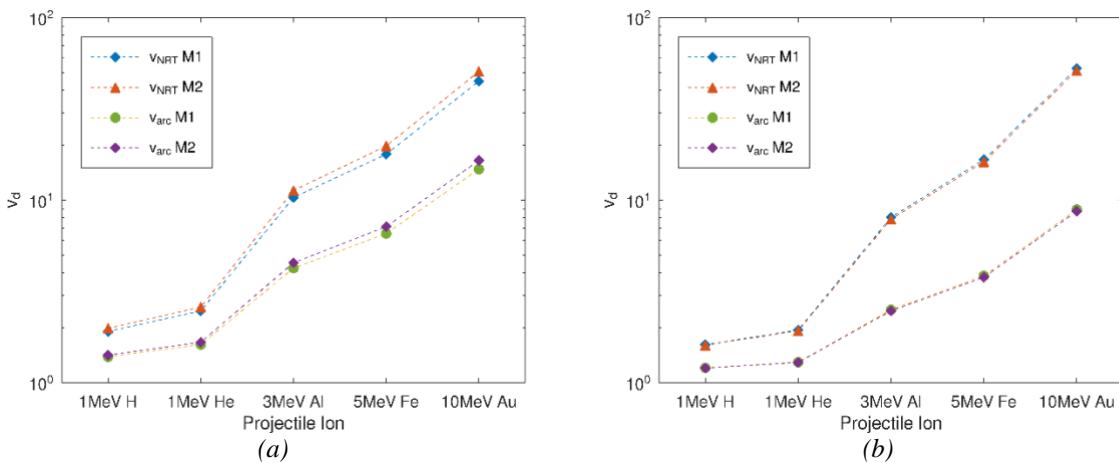


Figure 2. Comparison of NRT- and arc-dpa average displacements per PKA for different projectile energy and mass in (a) Fe and (b) W. The results obtained by methods M1 and M2 are given with different symbols and colors.

The results for the average NRT- and arc-dpa displacements per PKA obtained by the two methods are shown in Fig. 2. The arc-dpa result is always below NRT, as expected, and this becomes more pronounced at higher projectile energy/mass, where high-energy cascades play an important role. Comparing the values obtained by the two methods, it is seen that for both NRT- and arc-dpa there are very small differences between M1 & M2, increasing with ion mass/energy. In Fe, the difference between two methods reaches up to 12%, while for W, both methods give similar results with only about 2% difference. This is due to the fact that LSS theory gives a good description of recoil energy partition in W. A direct comparison of the two methods can be seen in Fig. 3, where the ratio of average

displacements per PKA obtained by M1 and M2, v^{M1}/v^{M2} , is depicted for both Fe and W. The figure clearly shows that in Fe, there is an underestimation of damage by method M1 compared to M2 (up to 12%), while in W, there is a very small overestimation (about 2%).

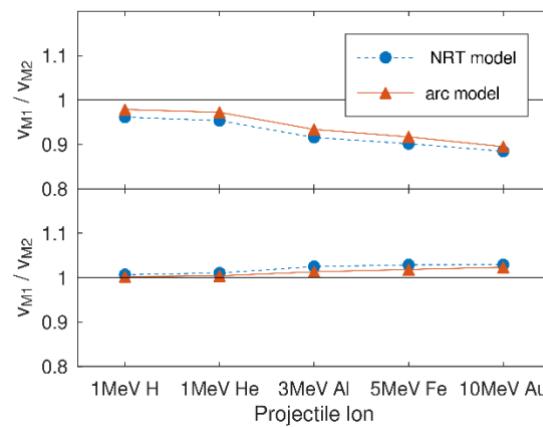


Figure 3. The ratio of displacements per PKA obtained by methods M2 and M1 for both NRT- and arc-dpa models in Fe and W

CONCLUSIONS

The use of SRIM for calculating arc-dpa parameters for Fe and W was demonstrated, based on a method proposed by Nordlubd et al. [7-8], expanding it to a wide range of PKA recoil energies, E_r . The method employs SRIM's accurate stopping powers to obtain an interpolation of the damage energy, T_{dam} , as a function of E_r continuously up to 100 MeV recoil energy. The method was applied in the simulation of typical Fe and W irradiation conditions and damage parameters were obtained by both this newly introduced method (M2) and by another method (M1) previously proposed in [9]. The present results for NRT- and arc-dpa damage estimation indicate that both methods produce similar results, with most significant differences up to 12% observed in Fe and very small discrepancies of only 2% in W. The application of both methods can be extended to all targets for which arc-dpa parameters are available.

DATA AVAILABILITY

All SRIM input and output data for the current study along with post-processing scripts in OCTAVE/MATLAB are freely available in [12].

Acknowledgments

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