

IOTA-2017: a code for the simulation of ion transport in materials

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Abstract

The report describes a new version of the IOTA code elaborated to study primary radiation defects in composite materials irradiated with ions.

The code is used for the calculation of the total number of primary defects created in materials, displacement cross-sections, and spatial defect distributions. The calculations apply analytical expressions for the differential cross-section for the transfer of the kinetic energy from the moving ion to a lattice atom and tabulated stopping power data. The simulation is based on the binary collision approximation and the Monte Carlo method.

Using the results of molecular dynamics calculations or the arc-dpa model, the IOTA code is applied for joint BCA-MD or BCA-arc-dpa simulations.

The code can be downloaded on <https://goo.gl/DXFqMn> or https://bwsyncandshare.kit.edu/dl/fiVD4QCZgWtqzFacULdvJ6MN/iota_2017.zip .

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1. Introduction

The IOTA code is designed to study primary radiation defects in composite materials irradiated with ions.

The code calculates the total number of primary defects created in materials, the displacement cross-section, and the spatial defect distribution. The calculations are performed using analytical expressions for the differential cross-section for the transfer of the kinetic energy from the moving ion to a lattice atom and tabulated stopping power data. The simulation is based on the binary collision approximation and the Monte Carlo method. Using the results of molecular dynamics calculations or the arc-dpa model, the IOTA code can be applied for joint BCA-MD or BCA-arc-dpa simulations.

The first version of the code [1] was released in 2004.

In recent years, a number of positive ideas and critical comments have accumulated that would make the code more effective. The implementation of recently proposed arc-dpa model [2,3] with parameters obtained in Ref.[4] extends the range of code application and the accuracy of calculations.

The following changes and improvements have been made to 2004 version of the code:

- the SL_LNS4A service code [1] was integrated in the IOTA code
- a faster method of simulation was implemented in the code
- arc-dpa [2,3] calculations with parameters from Ref.[4] are supported for materials from Li to U
- input data file was optimized
- output information was extended
- many minor improvements were made, detected bugs were removed.

Next sections briefly describe the changes, the new input data file and output improvements.

2. Method of calculation

The method of simulation is discussed in details in Ref.[1].

When a new option "arc-dpa" is selected in the input file the number of stable defects produced in the material by the ion with the kinetic energy T below the "critical" value [1] is calculated according to Refs.[2,3]

$$N_d(T_{dam}) = \begin{cases} 0 & \text{when } T_{dam} < E_d \\ 1 & \text{when } E_d < T_{dam} < 2E_d / 0.8 \\ \frac{0.8}{2E_d} \xi_{arc dpa} (T_{dam}) T_{dam} & \text{when } 2E_d / 0.8 < T_{dam} \end{cases}, \quad (1)$$

where E_d is the averaged displacement threshold energy, T_{dam} is the “damage energy” calculated using the Robinson formula [5,6]

$$T_{dam}(T) = \frac{T}{1 + kg(\epsilon)} \quad (\text{keV}), \quad (2)$$

where k and $g(\epsilon)$ are calculated as described in Refs.[5,6].

The defect generation efficiency [2,3] in Eq.(1) is equal to

$$\xi_{arc dpa} (T_{dam}) = \frac{1 - c_{arc dpa}}{(2E_d / 0.8)^{b_{arc dpa}}} T_{dam}^{b_{arc dpa}} + c_{arc dpa} \quad (3)$$

It is supposed that the energies T , T_{dam} , and E_d in Eqs.(1)-(3) are taken in keV.

The $b_{arc dpa}$ and $c_{arc dpa}$ parameters are taken from Ref. [2-4,7]. Instead of the global value of $b_{arc dpa}$ equal to -1 discussed in Ref. [4], the improved value [8] -0.82 is applied.

The BCA calculations are performed above "critical" energy T_{crit} , which default value for all materials is equal to 40 keV. The T_{crit} value can be changed in the input file.

3. Input data file

The input cards are described below.

Any line in the file starting with "*", "c", "C" or "!" symbols and any information after the sign "!" in any line is ignored when the code is executed. There are no restrictions on the format of input variables and the number of spaces between the entries.

Card 1. IDSDT, PAR_ST1, PAR_ST2, IEVEPRINT, KEYTPKA

Note: If the line is empty, all parameters are set equal to 0.

The parameter **IDSDT** defines the method of the $f(t^{1/2})$ function calculation. See details in Ref.[1], Eq.(4), Table1. If **IDSDT** is left blank, the value is set to zero.

Parameters **PAR_ST1** concerns the accuracy of calculations relating to the adopted division of the free path length (*Subroutine Model*). If **PAR_ST1** is equal to 0.0 or is not entered (left blank), the default value 0.1 is applied as in IOTA-2004 [1]. The smaller the parameter, the more precise are results and the longer is the time of calculations.

PAR_ST2 relates to the accuracy of calculations (see Subroutine Model). If **PAR_ST2** is equal to 0.0 or is not entered (left blank), the default value 0.05 is used as in Ref. [1]. The smaller the parameter, the more precise are results and the longer are calculations.

IEVEPRINT defines the output of detailed information in a special file (can be huge). If **IEVEPRINT** is zero, the information is not printed. If results of molecular dynamics (MD) simulation or the arc-dpa model are used for the modelling, the information is not printed. If **IEVEPRINT** is not entered, zero value is taken by default.

KEYTPKA defines the method of the simulation. If it is equal to 0 or 1 or not entered (left blank) the new fast method is applied, the value -1 selects the old method applied in IOTA-2004 [1].

Examples

- A. <blank line> ! (*means the same as the Example B.*)
- B. 0 0 0 0 0
- C. 1 ! (*PAR_ST1, PAR_ST2, IEVEPRINT, and KEYTPKA = 0*)
- D. 3 0.05 0.01 ! (*IEVEPRINT and KEYTPKA are taken =0*)

Card 2. Z1, A1, <SRIM output file>

Z1 and **A1** are the atomic number and the atomic weight (amu) of the projectile. If **A1** is zero the atomic weight is taken for the natural mixture of isotopes for this element (**Z1**) from internal code tables.

<SRIM output file> is the name or the path to the output file of the SRIM code [9] with electronic and nuclear losses for **Z1,A1** projectile + target interaction. The recommended energy range is from 1.1 eV to 5.2 GeV. If **<SRIM output file>** is not entered (left blank), the stopping power will be calculated using the SPAR routine [10,11], see Ref.[1].

Examples

- A. 29 0 Sdata\Cu_Cu.Zie ! (SRIM data file is located in the subdirectory Sdata)
- B. 26 56 ! (SPAR is applied for stopping power calculations)

Card 3. RO, NK, <Keyword for MD/arc-dpa results>, ECRIT, PARTMD

The density of the target (**RO**) is introduced in g/cm^3 . If **RO** is zero, the density is taken from the internal table for this material.

The parameter **NK** is the number of the components of the composite target. It is equal to the number of unique nuclides of the target. For example, for Li_2O the **NK** value is equal to 2, and for $\text{Al}_2(\text{SO}_4)_3$ equal to 3, if only one isotope of each element is involved in calculations. For the mixture of the isotopes the **NK** value should include their amount. If the lithium from the Li_2O compound is considered as a mixture of ^6Li and ^7Li isotopes, and the oxygen consists of ^{16}O , ^{17}O , and ^{18}O , the **NK** value is equal to 5. The maximal number of **NK** is 21 (see parameter MAXC in the code).

The next three entries on the Card 3 are used for BCA-MD or BCA-arc-dpa calculations only.

<Keyword for MD/arc-dpa results> identifies the set of data obtained outside of the IOTA code by MD modelling and parameterized as described in *Subroutine Mdparam* and Ref.[1]. The list of keywords is given in Table 1 and in *Subroutine Mdparam*. The keyword "arc" or "arc-dpa" selects the arc-dpa model.

The parameter **ECRIT** corresponds to the "critical" damage energy (or E_{MD} energy) (keV), which is equal to the value of the E_{MD} energy in Eq.(9), Ref.[1]. Below this energy the MD results for defect production relating to **<Keyword for MD/arc-dpa results>** are used instead of the BCA calculations (Section 2.4 of Ref.[1]). The corresponding critical kinetic energy T_{crit} of the atom is calculated in the code. If **ECRIT** is zero or not entered, the critical energy E_{MD} from *Subroutine Mdparam* or *Arc_parameters* is applied.

PARTMD defines the part of MD or arc-dpa events at the kinetic energy of ion equal to critical energy T_{crit} in percent. If **PARTMD** is not entered, the default value 3.0 % is used. If **PARTMD** is zero, the sharp transition to BCA calculations above $T > T_{crit}$ is applied, as in IOTA-2004 [1].

Note. To perform pure BCA calculations, only **RO** und **NK** should be entered on the Card 3.

Examples

- A. 3.21 2 ! (density for SiC, no MD results are used)
- B. 0 1 Stoller ! (MD-data from Refs.[17,18], ECRIT is taken from Subroutine Mdparam, part of MD events at $T=T_{crit}$ is equal to 3.0 %)
- C. 0 1 Voertler 40. ! (MD-data from Ref.[16], ECRIT =40 keV)
- D. 0 1 arc-dpa 30. ! (arc-dpa model below ECRIT < 30 keV)
- E. 0 1 arc 0. 0. ! (arc-dpa model below ECRIT from Subroutine arc_parameters, no smoothing)

Table 1. The list of keywords <Keyword for MD/arc-dpa results>

Material	Keyword	Reference
Al	Bacon	[12-14]
Ti	Bacon	[14]
V	Bjorkas	[15]
Cr	Voertler	[16]
Fe	Voertler	[16]
Fe	Stoller	[17,18]
Ni	Bacon	[14]
Cu	Caturla	[19]
Zr ¹	Gao	[20,21]
W	Caturla	[19]
Li to U	arc-dpa	[2-4,7,8]

¹ Temperature is equal to 600 K

Card 4(1), 4(2) ... 4(NK). Z_i , A_i , **ATOMIC_FRACTION_i**, **ED_i**, **<SRIM output file>_i**

Cards describe the components of the target.

Z_i and A_i are the atomic number and the atomic weight (amu) of the i -th component of the target. If A_i is zero the atomic weight is taken for the natural mixture of isotopes for this element (Z_i) from internal code tables.

The parameter **ATOMIC_FRACTION_i** defines the atomic concentration of i -th components: It can be entered in the normalized or the un-normalized form. For example, in the description of the oxygen from Li_2O compound both values 0.333333 or 1 are correct².

The parameter **ED_i** is the averaged threshold displacement energy E_d (eV) for i -th component of the target. If **ED_i** is zero 0 the value is taken by default. For pure BCA calculations, the default **ED_i** value is equal to 40 eV. For combined BCA-MD or BCA-arc-dpa calculations the default values is taken from *Subroutine Mdparam* (MD) or *Arc_parameters* (arc-dpa). For combined calculations, it is recommended to set **ED_i**=0.

<SRIM output file>_i is the name or the path to the output file of the SRIM code with electronic and nuclear losses for Z_i, A_i ion + target interaction. The recommended energy range is from 1.1 eV to 5.2 GeV. If the **<SRIM output file>_i** is not entered (left blank) the stopping power will be calculated using the SPAR routine [1,10,11].

Examples

```
A.  14 28 0.5000 40.0  Si_SiC.Zie    ! (Si from SiC)
     6 12 0.5000 20.0   C_SiC.Zie    ! (C from SiC)

B.  29. 0  1.  0.   cu_cu.SRIM
```

Note. Data for the density and masses of elements are taken from the SRIM code [9].

Card 5. **<NAME1>**, **<NAME2>**, **<NAME3>**

Card contains names of output data files. If some names or the complete line is left blank, the output files get default names.

² if only one isotope of oxygen, for example ^{16}O , is involved in calculations. For the mixture of isotopes the **ATOMIC_FRACTION_i** value must correctly take into account the contribution of each isotope.

Examples

- A. <blank line> ! (Default names are assigned for all output files)
- B. Result.dat ! (Default names are assigned to 2nd and 3rd output files)
- C. Out1.dat Data_in_two.column.format efficiencies_and_more.tmp

Note. Running the code produces three main output files, "inform.txt" and several auxiliary files.

Card 6(1), 6(2) ... 6(N). EN_i , $NHIST_i$, X_i , Y_i , Z_i , $COSX_i$, $COSY_i$, $COSZ_i$

Cards contain kinetic energies of primary ion (EN_i) in the LS (MeV), number of Monte Carlo events ($NHIST_i$), and, optionally, the position and direction of motion of primary ion.

Note: If X_i , Y_i , Z_i , $COSX_i$, $COSY_i$, and $COSZ_i$ are omitted, the default values are $X_i=Y_i=Z_i = 0$, and $COSX_i = COSY_i = 0$, $COSZ_i = 1$. If X_i , Y_i , Z_i , $COSX_i$, $COSY_i$, and $COSZ_i$ are specified, EN_i , and $NHIST_i$ must be entered explicitly, without default instructions discussed below.

If $NHIST_i$ is not entered, the value is determined by default (*Subroutine NHIST_default*).

Parameters EN_i and $NHIST_i$ can be replaced by keywords, which are described below.

The keyword **all** can be used instead of the EN_i to perform calculations at energies from E_d to 5000 MeV. In this case, the default list of energies is defined in the code (*Subroutine E0_definition*).

Instead of EN_i , the minimal and maximal energies, separated by symbols “..” (two or more consecutive points) can be specified to define the energy range of primary particles. If the lower energy is not entered, it is taken by default equal to E_d . The energies between the specified range limits are defined in the code.

Instead of $NHIST_i$, “**x M**” or “*** M**” can be entered, where “**M**” is a value that is multiplied by the $NHIST_i$ value, defined by default.

Examples

- A. all ! (the energy range of primary ions and NHIST values are defined in the code)
- B. all x1.5 ! (the energy range of primary ions and NHIST are defined in the code, default NHIST values will be multiplied on 1.5)
- C. all 1000 ! (the energy range of primary ions is defined in the code. The NHIST-value equal to 1000 is applied for each energy of primary ion.)
- D. 0.1 1500. ! (the list of energies between 0.1 MeV and 1500 MeV
2000. x 10 ! is defined in the code, the default NHIST value is
3000 700 ! used for each energy from the list. For the
primary energy 2000 MeV the default NHIST
value is multiplied by 10. For 3000 MeV the
NHIST is taken equal to 700)
- E. ... 100 1200 ! (calculations are performed for the energy range
1201000 x 2 ! from E_d to 100 MeV with NHIST= 1200 and for
the energy range from 120 MeV to 1000 MeV with
default NHIST-values multiplied by 2)
- F. 5.e-5 1000 ! (the calculation for the primary energy 50 eV is
1.e-4 800 ! performed with NHIST=1000, for 100 eV and
1.e-3 800 ! 1 keV with NHIST=800, and for 10 keV with NHIST
1.e-2 500 ! equal to 500. For the energy 0.15 and 0.2 MeV
0.15 ! the default NHIST-values are applied. In the energy
0.2 ! range between 0.5 MeV and 5000 MeV the list of
0.5..5000 ! primary energies and NHIST values are defined
by default)

Note. Up to 50,000 different energies can be entered in one job. The reading stops at end-of-file. The default energies and **NHIST**-values are printed in the output file "inform.txt".

Examples of the input file are shown below.

Example 1

The input file for W+W interactions for joint BCA-arc-dpa calculations

```
* IOTA code input
0
*
* projectile
74 0 d:\Srim_outputs\W_W.ZIE
*
0 1 arc
*
* material
74. 0. 1.0000 0.00 d:\Srim_outputs\W_W.ZIE
*
* Output
W.dat
*
* energies
...5000 ! from Ed to 5 GeV
```

Example 2

The input file for Si+SiC interactions

```
* IOTA code input
0
* Z, A of the projectile ion and the SRIM file with dE/dx data
14 28 si_siC.Zie
* media description: density (g/cm3), the number of components
3.21 2
*
* description of the components for compound
* Z, A, atomic fraction, Ed displacement energy (eV), file with
dE/dx
14 28 0.5000 40.0 si_siC.Zie
6 12 0.5000 20.0 C_siC.Zie
*
*output file names
res1.dat res2.dat res3.dat
*
* energy of projectile (MeV) and number of Monte Carlo events
1.00000E-04 500
1.00000E-03 500
1.00000E-02 500
1.00000E-01 500
1.0000 500
5.0000 500
10. 500
100.0000 50
```

4. Preparation of the file with stopping power data using the SRIM code

To use the SRIM code one should download it from Ref.[9] and install it on PC.

If the SRIM code is installed, the instruction to prepare the file with the stopping power data, suitable for the IOTA code calculation, is the following

1. Select "Stopping/Range Tables" in the main SRIM menu (general panel).
2. Select the appropriate projectile and the target material. In the case of the compound one should introduce the correct density of the compound. It is the same value as **RO** in the *Card 3* of the input file of the IOTA code (see Section 3).
3. Set the minimal energy of the projectile to 0,001 keV and the maximal energy to 5200000 keV, i.e. the energy range between 1 eV and 5,2 GeV (the maximal energy allowable in the IOTA code). *Note: commas should be entered instead of points*
4. Select the units for the stopping power equal to MeV/(mg/cm²) (default in the main SRIM menu).
5. Perform the operation "Calculate table" and specify the same name for the output file that will be used in the input file for the IOTA code (Section 3). The file name must not have spaces.
6. Repeat this procedure for all atoms of the compound, considered as a projectile.

Note. If the calculations are performed for the same material and the various projectiles with the equal atomic number and the different atomic weights it is not necessary to prepare the SRIM stopping power data for each isotope.

If the SRIM data are prepared for the ion with Z and A and the actual projectile in the task is Z and A', the electronic stopping power will be correctly recalculated. See details in Ref.[1], pages 17,18. New data for the stopping power are written in the output file RENORM.STO.

The example of the menu of the SRIM code and the output file for Fe+Fe interaction is given below (Example 4 and 5).

Example 4

The SRIM code window with the information for Fe+Fe interactions to be used in the IOTA code



Example 5

The SRIM code output for the Fe+Fe interaction

```

=====
SRIM version ---> SRIM-2013.00
Calc. date ---> Oktober 13, 2017
=====

Disk File Name = SRIM Outputs\Iron in Iron.txt

Ion = Iron [26] , Mass = 55,935 amu

Target Density = 7,8658E+00 g/cm3 = 8,4817E+22 atoms/cm3
===== Target Composition =====
Atom   Atom   Atomic   Mass
Name   Numb   Percent  Percent
-----
Fe     26    100,00   100,00
=====
Bragg Correction = 0,00%
Stopping Units = MeV / (mg/cm2)
See bottom of Table for other Stopping units

      Ion      dE/dx      dE/dx      Projected   Longitudinal   Lateral
      Energy   Elec.      Nuclear    Range      Stragglng     Stragglng
-----
      1,1 eV   1,520E-03  1,695E-02    1 A        1 A           A
      1,2 eV   1,520E-03  1,800E-02    1 A        1 A           A
      1,3 eV   1,582E-03  1,902E-02    1 A        1 A           A
      1,4 eV   1,642E-03  2,002E-02    1 A        1 A           A
      <lines skipped>
      5,00 GeV  3,601E+00  1,334E-03    1,05 mm    41,96 um     7,50 um
      5,20 GeV  3,506E+00  1,288E-03    1,12 mm    43,18 um     7,97 um
      <lines skipped>
      1,3574E-01      L.S.S. reduced units
=====
(C) 1984,1989,1992,1998,2008 by J.P. Biersack and J.F. Ziegler

```

5. Output information

The code produces three main output files and a number of auxiliary files. Main files are briefly described below. The order of files corresponds to the sequence of their names in the input file.

1. File with detailed information about results obtained. The output information is described in Ref.[1], pages 20-25. Important values are provided with numbers in brackets "()". In addition to the IOTA-2004 output [1], the code prints the damage energy T_{dam} , Eq.(2), value "(8)", and for the joint BCA-arc-dpa calculations the number of displacements calculated using Eq.(1), value "(9)".

2. File with results in column format. File contains values provided with brackets "()" in the file 1 for each energy of the projectile. Depending on the task, the values from "(1)" to "(9)" are printed.

3. File with efficiencies and other information. The output information contains defect generation efficiencies, i.e. the ratios of the calculated numbers of defects to the numbers obtained using the NRT model [5], and the relevant values. The record "(i)/(1)" means the ratio of the value "(i)" printed in the first file to the value "(1)" calculated with NRT.

5. Running the code

There are two ways to run the code: with arbitrary name of the input data file and with the input data file "input", as in IOTA-2004 [1].

Examples

- A. `lota170929.exe input_just_in_case.tmp.dat`
- B. `lota170929.exe`

6. Examples of calculations

Figures 1-3 show the examples of calculations performed using the IOTA code.

For comparison, figures show the result of the calculation using the SRIM/TRIM code [9] and applying the number of defects obtained in MD simulations [17-19]. As in the IOTA code, cascades with the energy of ions below T_{crit} were cut and the number of defects at lower energies was evaluated using results of MD simulations. The calculations apply the output SRIM/TRIM file "COLLISON.txt" [9].

Experimental data are taken from Ref.[22]. The systematics values are based on the data of Fig.3 of the Ref.[22].

7. Conclusion

This report describes briefly new features of the code IOTA code, the input data file and the output. The code can be downloaded on <https://goo.gl/DXFqMn> or https://bwsyncandshare.kit.edu/dl/fiVD4QCZgWtqzFacULdvJ6MN/iota_2017.zip

Please, send any comments and critics to alexander.konobeev@kit.edu

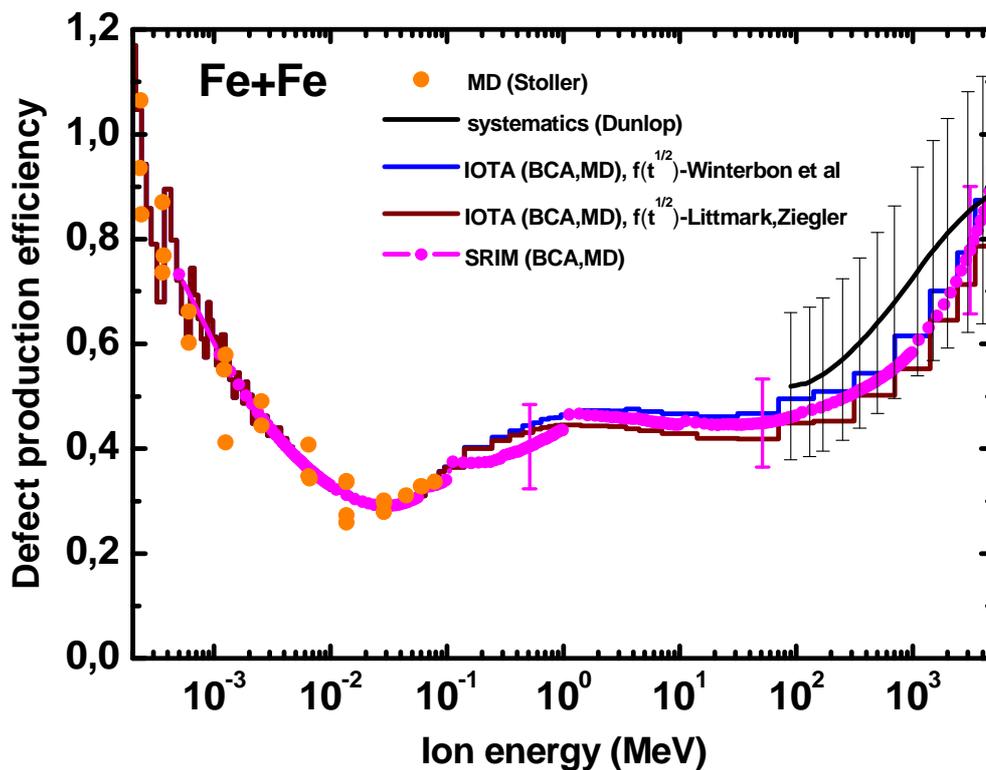


Fig.1 The ratio of the number of defects calculated using the IOTA code and the SRIM/TRIM code to the number predicted by the NRT model for Fe+Fe irradiation.

See explanations in the text.

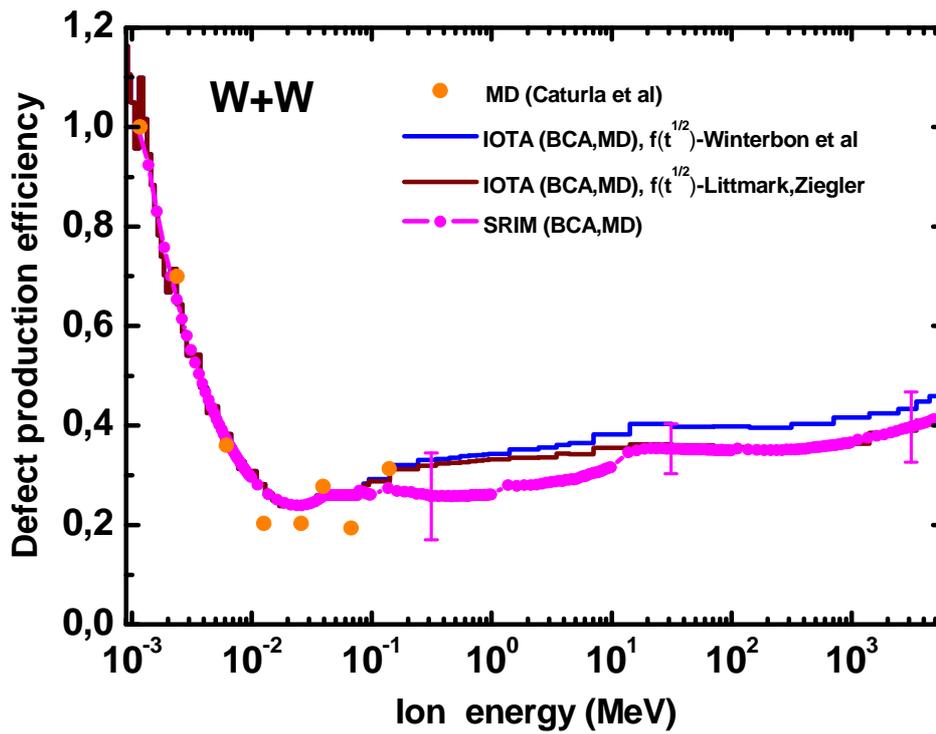


Fig.2 The same as in Fig 1, but for the W+W irradiation.

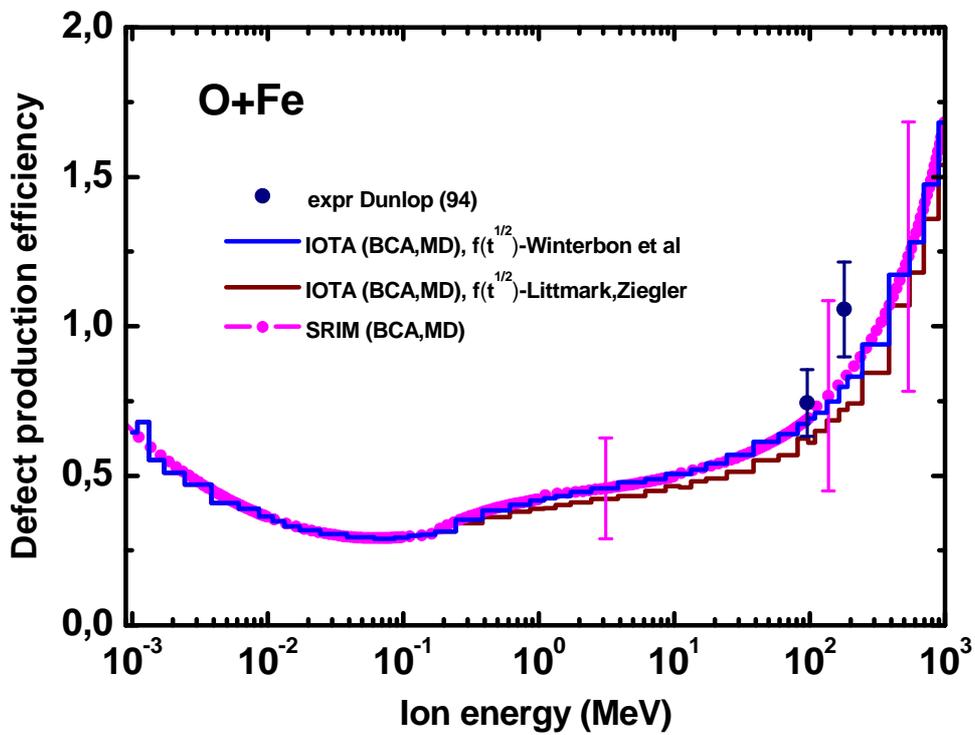


Fig.3 The same as in Fig 1, but for the O+Fe irradiation.

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