TREKIS-3:
Time Resolved Electron Kinetics in SHI-irradiated Solids

Current version: 3.0.8 (update from 17.05.2023)

A transport Monte Carlo code of event-by-event simulation of swift heavy ion penetration in matter, secondary electrons, holes and photons cascades, and energy transfer to the lattice

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I. Disclaimer, how to cite

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The use of the code is at your own risk. Should you choose to use it, appropriate citations are mandatory:

1) N. A. Medvedev, R. A. Rymzhanov, A. E. Volkov, *J. Phys. D. Appl. Phys.* **2015**, *48*, 355303

2) R. A. Rymzhanov, N. A. Medvedev, A. E. Volkov, *Nucl. Instrum. Methods B* **2016**, *388*, 41

Should you use this code to create initial conditions for further molecular dynamics simulations of atomic response to the electronic excitation by a swift heavy ion (e.g. with LAMMPS), the following citation is required:

3) R. Rymzhanov, N. A. Medvedev, A. E. Volkov, *J. Phys. D. Appl. Phys.* **2017**, *50*, 475301

In a publication, we recommend that at least the following parameters should be mentioned for reproducibility of the results: material, its structure, density, speed of sound, the used CDF coefficients, which processes were included (active) in the simulation, ion type, its energy, the model for SHI charge, number of MC iterations.

II. Brief introduction into the model

TREKIS-3 (Time-Resolved Electron Kinetics in SHI-Irradiated Solids, version 3) is the transport Monte Carlo code using event-by-event (analog) simulation of effects of swift heavy ion (SHI) impacts on matter, induced secondary electron and hole cascades, and energy transfer to the lattice/atomic system [1,2]. A swift heavy ion is typically defined as an ion with energy E >1 MeV/amu. Electronic energy losses by such ions constitute over 95% of the energy deposition, whereas energy transfer to target atoms is almost negligible along the entire SHI path (except near the end of the range). Depending on the target, the ion energy and mass, the electronic stopping power may reach 5-50 keV/nm along the ion trajectory. For a review of typical effects of SHI on matter, the reader may have a look at the review [3]; for a review of modeling of SHI effects with help of TREKIS-3 see [4].

TREKIS-3 is capable of modelling ions from hydrogen (proton) to super-heavy elements, however, for protons, only energy above the Bragg-peak are calculated reliably. SHI energies are limited to the regime of nonrelativistic electronic energy losses (from ~1 MeV/amu up to ~100 GeV/amu).

The used scattering cross sections are based on the formalism of the dynamic structure factor proposed by L. van Hove [5], or, equivalently, the loss function (the inverse imaginary part of the complex dielectric function, CDF) in the linear response theory developed by Fano [6]. Ref.[1] contains CDF parameters for a number of materials, extracted from optical data following the Ritchie-Howie formalism [7], and provided as input files together with the code (see below). The procedure of reconstruction of the CDF is described in detail in Refs. [1,2,7].

Based on these cross sections, TREKIS-3 models the following processes: (a) penetration of a swift heavy projectile resulting in ionization of a target and appearance of primary electrons (δ-electrons) and holes; (b) scattering of δ-electrons on lattice atoms and target electrons as well as the kinetics of all secondary

generations of electrons; (c) Auger decays of core holes, also resulting in production of secondary electrons; (d) radiative decays of core holes, following photon transport and photoabsorption exciting new electrons and holes; (e) valence holes transport and their interaction with target atoms. All details of the numerics used and corresponding cross sections for different processes can be found in Refs. [1,2].

III. Files of the code

The code consists of a few modules, using the following internal conventions:
1) All global variables start with "g_", e.g. g_numpar, and all defined in the module "Variables"
2) All modular variable names are defined starting as "m_", e.g. "m_number"
3) Subroutines and functions should be provided with a comment specifying in which module it can be found

1. Source files

Analytical_IMFPs.f90 – The module contains subroutines for calculations and saving of cross sections, mean free paths, and ranges for all particles (SHI, electron, hole, photon)
Cross_sections.f90 – The module contains subroutines for evaluation of cross sections
Dealing_with_EADL.f90 – The module contains subroutines for accessing EPICS2017[†] databases EADL and EPDL, containing atomic parameters (Auger and radiative decay times, ionization potentials, kinetic energies of atomic shells)
Gnuplotting_subs.f90 – The module contains subroutines for creating gnuplot scripts (unfinished and unused)
Monte_Carlo.f90 – The module contains all subroutines for Monte Carlo modelling of particles transport
Objects.f90 – The module contains definitions of all objects and some subroutines to deal with them
Reading_files_and_parameters.f90 – The module contains subroutines for reading input files
Sorting_output_data.f90 – The module contains subroutines for creating output files
Universal_Constants.f90 – The module contains all universal constants as global variables
Universal_MC_for_SHI_MAIN.f90 – This is the main file of the TREKIS-3, assembling the calculations, reading input and creating output files
Variables.f90 – The module contains all global variables

2. Input data

The main input file, where the user sets the material and SHI parameters, is the following:
INPUT_PARAMETERS.txt – the file containing the parameters of the calculations: material, ion, numerical parameters, etc., see an example in Figure 1.
It must contain the following lines, exactly in this order and format:

1) Material name, which must match the name with the file [*material*].cdf with materials parameters, described below
2) Swift heavy ion (SHI) atomic number according to the Periodic Table
3) SHI energy in [MeV]
4) Mass of the SHI in atomic units. Positive number sets the mass, negative number sets the mass according to the most abundant isotope. These masses are taken from the input file INPUT_atomic_data.dat in the directory INPUT_EADL, see below.
5) Total time of the analysis in [fs], setting when the simulation stops.

[†] https://www-nds.iaea.org/epics/ This database is public domain and is freely distributed by its author at http://redcullen1.net/HOMEPAGE.NEW/

Note: Typically, electron cascades are finished within ~100 fs.

6) Two numbers: a) Time step in [fs], how often the data are printed out; b) what kind of the time-grid to use for output printing: 0=linear grid; 1=logarithmic grid.
   Note: too fine grid results in too long calculation times and/or memory overload. Logarithmic grid is recommended, or printing out only the final time instant of the simulation.
7) Cut off energy for stopping of electrons in [eV]. Electrons and valence holes with energies below this value are stopped in the simulation. To exclude this artificial stopping, set any negative number
8) Thickness of the materials to be simulated in [Å]. SHI penetration is modelled within this layer, while all secondary cascades assume periodic boundaries along the ion penetration.
   Note: too large thickness results in too large numbers of secondary particles created, too long calculation times and/or memory overload. The recommended value is 10 Å.
9) Target temperature in [K]. The temperature is set in the temperature factor of the cross section, but not in the CDF itself, for details see [2].
10) Two numbers: a) which model for SHI effective charge to be used [1]: 0=Barkas; 1=Bohr; 2=Nikolaev-Dmitriev; 3=Schiwietz-Grande, 4=fixed Zeff; b) If the fixed value of the SHI charge is used (case=4), the second number set the charge in the units of electron charge.
    Note: it is recommended to use option 0 (Barkas charge), or a specific fixed charge if known from experiments.
11) Index of the model of the SHI charge spatial distribution: 0=point-like charge; 1=Brandt-Kitagawa ion.
    Note: option 0 is recommended as a faster one, whereas option 1 produces only a minor improvement around the Bragg-peak, see [8].
12) Two numbers:
    i) Index of the model of electron and valence hole elastic scattering: -1=disable elastic scattering; 0=Mott, 1=optical phonons CDF [1].
    ii) Index of which effective target charge to use: 0=Barkas-like see [9], 1= fixed charge = 1 (used in all old calculations). It is only used for optical phonon CDF, not other cross section models.
13) Two numbers setting inelastic scattering cross section: a) the first one sets the kind of target dispersion relation: 1=free electron, 2=plasmon-pole, 3=Ritchie [1,2]; b) effective mass of valence hole used in CDF scattering cross-section calculations: 0=from DOS of VB within effective one-band approximation [2]; -1=free-electron; positive number sets a fixed value in free-electron masses.
    Note: the following options are recommended: a) 1; b) 0.
14) Index, setting whether to include plasmon integration limit in the inelastic scattering cross section or not: 0=no, 1=yes [2].
    Note: option 0 is recommended.
15) Effective valence hole mass in units of free-electron mass, used for transport of valence holes.
16) Index, whether to include radiative decay of deep holes or not: 0=no, 1=yes.
    Note: option to exclude is only used for testing, however including radiative decays and ensuing photon transport does not significantly affect the results for nonrelativistic particles.
17) Three numbers setting a model for electron emission from the surface. If on, periodic boundaries are switched off in the simulation, and electrons are allowed to be emitted. The three numbers set: a) Work function in [eV] (if negative number is set, <=0, no emission is used, and periodic boundaries are used instead for bulk simulation); b) surface barrier length in [Å]; c) barrier height for electron emission in [eV]. For details of the model, see [10].
18) Number of MC iterations to be performed.
    Note: at least 1000 iterations is recommended for reliable statistics.

19) Number of threads for parallel calculations with OpenMP (1 if nonparrelelized).

After the line #19, one may set optional flags:

- verbose – makes TREKIS-3 printout additional information on the screen, along the execution of the program (for example, timestamps after execution of various subroutines and during MC), which is useful for testing, code developing and debugging.
- very-verbose – prints out time of each collision of each particle (which is A LOT of output, useful only for debugging, but not any productive calculations).
- info – prints out additional basic information about the code, including citations.

```
SiC          ! material name
83           ! SHI atomic number
710.0        ! [MeV] total SHI energy
-1           ! [proton mass] if mass of the SHI is NONSTANDARD isotop; if standard, put any NEGATIVE number
100.0       ! [fs] total time analyzed
10.0d0 1    ! [fs] timestep, how often the data are saved; kind of time-grid: 0=linear, 1=logarithmic
0.0d0        ! [eV] Cut-off energy (electrons with lower energies are excluded from calculation)
10.0         ! [A] thickness of the layer analyzed
1000.0       ! [K] temperature of the target
0   1.0      ! 0=Barkas; 1=Bohr; 2=Nikolaev-Dmitriev; 3=Schiwietz-Grande, 4=fixed Zeff; Fixed value (only for case=4)
0            ! 0=point-like charge; 1=Brandt-Kitagawa ion
1    0       ! elastic cross sections:-1=disable; 0=Mott, 1=optical CDF; Target Zeff (0=Barkas-like; 1=1 fixed)
1   -1       ! target dispersion (1=free el., 2=plasmon-pole, 3=Ritchie); m_eff [me] (0=effective mass from DOS of VB; -1=free-electron)
0            ! Include plasmon integration limit
-1.0d30»     ! [me] effective valence hole mass in units of electron mass
0            ! include radiative decay of deep holes? (0=no, 1=yes)
0.0 10.0d0  6.18d0  ! [eV] Work function (<=0 - no emission); [A] surface barrier length; [eV] barrier height for electron emission
4            ! number of MC iterations to be performed
4            ! number of threads for parallel calculations with OpenMP (1 if nonparrelelized)

!verbose            ! To printout time of reaching each time-grid point

!very-verbose       ! To printout time of each collision (really A LOT of printout!)

!info       ! printout some basic info about the code
```

Figure 1. An example of the file Input_Parameters.txt

Directory INPUT_CDF contains files [*material*].cdf with material parameters. Files with extension cdf (they are just text files) contain the description of material parameters and complex dielectric function (CDF), see an example in Figure 2. File names [*material*] in this directory must exactly coincide with the name given above in the file Input_Parameters.txt. Or, the other way around, only materials, whose parameters are set in this directory, can be simulated.

To create a new material, a cdf-file must be set according to the format described below. All lines must be exactly in the described format and order.

```
Lithium fluoride
2              ! how many elements are in this molecule of solid
9       1      ! atomic number, contribution of 1st element into compound
3       1      ! atomic number, contribution of 2d element into compound
2.635   4200.0  7.3     ! density [g/cm^3], speed of sound [m/s], fermi energy [eV]
2              ! number of shells of the first element: F
1       1       689.1e0 2       3.6e0   ! number of CDF functions, shell-designator, ionization potential, number of electrons, Auger-time
400     350     450     ! E0, A, Gamma coefficients
7       63      14.6e0  8       1.0e23  ! number of CDF functions, shell-designator, ionization potential, number of electrons, Auger-time
13.5    4.3     0.45    ! E0, A, Gamma coefficients
15.5    8.5     1.3
18.0    4.9     1.2
24.5    99.0    1.5
26.0    43.0    3.0
29.0    15.0    1.5
37.0    500.0   40.0
1              ! number of shells of the second element: Li
2       1       61.0e0  2       1.0e23  ! number of CDF functions, shell-designator, ionization potential, number of electrons, Auger-time
85.0    120.0   20.0    ! E0, A, Gamma coefficients
85.0    120.0   40.0
2              ! phonon peaks:
0.083   0.0022  0.0035  ! E0, A, Gamma coefficients
0.0635  0.00009 0.01
```

Figure 2. An example of file LiF.cdf

The cdf format is defined as follows:

Line 1: Material name. May be arbitrary name within 100 symbols length.

Line 2: Number of atoms in a molecule of the target (integer). E.g. For LiF, it must be 2; for $MgFeSiO_4$ it is 4, etc. This number defines the number of following lines, since each atom type must be set in a separate line.

Line 3: Sets two numbers:

1) Atomic number of the first kind of atoms of the compound according to the Periodic Table (integer)
2) Stoichiometric contribution of this element into the molecule of the target (real)

Note: elements must be sorted according to their atomic number in descending order. E.g., for LiF, the first line must define F, the second line Li, not the other way around.

E.g., for LiF, the first line must be:

9 1 – element 9, one per molecule.

For Si_3N_4, the line looks like:

14 3 - First element is 14 (Si), 3 of them per molecule (Si_3N_4)

Line 4: In case of a compound, the line type is identical to the previous one, setting the parameters of the second element. In LiF, it is

3 1 - Element 3 (Li), contribution 1

In case of Si_3N_4, that is

7 4 - element 7 (N), contribution 4 in a molecule (Si_3N_4).

Line 5 (or another number, depending on the number of elements in the compound): Three numbers:

1) Material density in [g/cm^3]
2) Speed of sound [m/s]
3) Fermi energy in [eV]

Line 6: Number of atomic shells in the first element of the compound

Note: valence band is set only among the shells of the first element of the target; for all other elements, valent energy levels, contributing into the valence band, must be omitted to exclude double counting.

For example, in LiF, this line contains 2, corresponding to two shells: K-shell and the valence band.

Note: all shells must be sorted according to ionization potential in descending order.

Line 7: This line sets the parameters of the first atomic shell (in case of LiF, K-shell of F):

It contains 5 numbers (see Figure 2):

1 1 689.1e0 2 3.6e0

1) Number of oscillator functions in the CDF for this shell (integer)
2) Shell designator, according to the EPDL convention[‡] (see example in Table below, Figure 3).

Note: for the valence band, the number 63 must be used; this addition to the EPDL convention allows TREKIS to identify the valence band.

Note 2: setting here a negative number will force TREKIS to use atomic BEB cross-sections [11], instead of CDF, for electrons and holes (whereas for SHI only CDF model is available).

3) Ionization potential of the shell in [eV] (real).
   Note: setting here a negative number, a default value from EADL database will be used. To find a correct value in the EPICS2017 database, it requires a correct setting of the shell designator.
4) Number of electrons in this atomic shell (per atom) or in the valence band (per molecule) (real).
   Note: setting here a negative number, a default value from EADL database will be used. It cannot be used for the valence band, since it is an atomic database.
5) Auger decay time of this shell in [fs] (real). If decay is not possible, an “infinite” number must be set here (e.g. 1e20).

[‡] http://www-nds.iaea.org/epdl97/

Note: setting here a negative number, a default value from EADL database will be used. It cannot be used for the valence band, since it is an atomic database.

Line 8: This and following lines (number of lines is set by the first number in the previous line) sets the CDF oscillators coefficients according to the Ritchie-Howie formalism [7,12]: E0, A, Gamma (real)

For example, for K-shell of F, we set 1 CDF oscillator, so there will be only one line with the CDF coefficients.

Line 9: The same 5 numbers setting the next atomic shell parameters (see Figure 2):

7 63 14.6e0 8 1.0e23

In this case, the valence band (note designator 63) has 7 CDF oscillators coefficients. This indicates that the next 7 lines define the CDF coefficients of the valence band in LiF, in the same order as described below: E0, A, Gamma.

Line 17: Sets the number of shells for the next element in the compound. In case of LiF, it sets Li parameters, which has only 1 shell: K-shell; valence band was already set when the first element (F) was defined.

Line 18: Sets 5 numbers, defining the shell parameters in the same way as line 9 above, for K-shell of Li:

2 1 61.0e0 2 1.0e23

Lines 19-20: Sets the CDF coefficients for this shell: E0, A, Gamma.

After defining all elements in the compound, it is optional to define phonon-CDF for elastic scattering, following the Kuhr-Fitting method (analogous to Ritchie-Howie formalism for inelastic scattering) [13].

Line №21: Number of CDF-oscillators for phonon peaks (in case of LiF, it is 2).

Lines №22-23: CDF coefficients E0, A, Gamma for phonon peaks.

Note: if phonon CDF is absent, the elastic scattering cross sections for electron and valence hole scattering, TREKIS will use Mott's cross section with Molier screening parameter [14].

Table VI. Atomic Subshell Designators

Desig-nator	Subshell	Desig-nator	Subshell	Desig-nator	Subshell
1.	K (1s1/2)	21.	N4 (4d3/2)	41.	Pl (6s1/2)
2.	L (2)	22.	N5 (4d5/2)	42.	P23 (6p)
3.	Ll (2s1/2)	23.	N67 (4f)	43.	P2 (6p1/2)
4.	L23 (2p)	24.	N6 (4f5/2)	44.	P3 (6p3/2)
5.	L2 (2p1/2)	25.	N7 (4f7/2)	45.	P45 (6d)
6.	L3 (2p3/2)	26.	O (5)	46.	P4 (6d3/2)
7.	M (3)	27.	O1 (5s1/2)	47.	P5 (6d5/2)
8.	Ml (3s1/2)	28.	O23 (5p)	48.	P67 (6f)
9.	M23 (3p)	29.	O2 (5p1/2)	49.	P6 (6f5/2)
10.	M2 (3p1/2)	30.	O3 (5p3/2)	50.	P7 (6f7/2)
11.	M3 (3p3/2)	31.	O45 (5d)	51.	P89 (6g)
12.	M45 (3d)	32.	O4 (5d3/2)	52.	P8 (6g7/2)
13.	M4 (3d3/2)	33.	O5 (5d5/2)	53.	P9 (6g9/2)
14.	M5 (3d5/2)	34.	O67 (5f)	54.	P1011 (6h)
15.	N (4)	35.	O6 (5f5/2)	55.	P10 (6h9/2)
16.	Nl (4s1/2)	36.	O7 (5f7/2)	56.	P11 (6h11/2)
17.	N23 (4p)	37.	O89 (5g)	57.	Q (7)
18.	N2 (4p1/2)	38.	O8 (5g7/2)	58.	Ql (7s1/2)
19.	N3 (4p3/2)	39.	O9 (5g9/2)	59.	Q23 (7p)
20.	N45 (4d)	40.	P (6)	60.	Q2 (7p1/2)
				61.	Q3 (7p3/2)

Figure 3 EPDL atomic subshell designators

Directory INPUT_DOS contains files [*material*].dos with the density of states of the valence band of the material. The name of the material must coincide with the name provided in the file INPUT_PARAMETERS.txt. Files with extension dos are just text files, containing two columns: energy in [eV], and electronic DOS in arbitrary units (DOS is renormalized in TREKIS to match the number of valence electrons).
Note: the energy scale must start from the bottom of the valence band, and end at the top of the valence band, *strictly* in the ascending order: non-monotonously increasing energy grid may produce errors in TREKIS calculations.

Directory INPUT_EADL contains files three files with the databases of atomic parameters:
INPUT_atomic_data.dat – Parameters of the Periodic Table
epdl97.all – EPDL parameters from EPIS2017 database, containing photon parameters for scattering on atoms
eadl.all – EADL parameters from EPIS2017 database, containing atomic parameters

!READ_ME_TREKIS_3.doc or !READ_ME_TREKIS_3.pdf – this very manual.

3. Compiling, executing

- Makefile – make-file for compilation of the TREKIS-3 code under Unix system with help of make[§] program. Requires ifort2011 or a later version (change the compiler name in the file accordingly) and OpenMP installed, or modify to match an existing Fortran compiler and OpenMP settings on your computer. Calling make creates the executable TREKIS.x.
- Make.bat – cmd-file for compilation for TREKIS-3 code under Windows system, where direct calls of ifort.exe and /Qopenmp are made. All paths must be written in the system variables to be found from your command line. The easiest way to use, is to install Microsoft Visual Studio Community[**], and oneAPI HPC Toolkit[††] containing freely distributed Intel Fortran compiler and OpenMP (and other) libraries. Calling make (or Make.bat) in the Intel oneAPI command prompt creates the executable TREKIS.exe that can be run in the same command line. Compilation with debug options (currently only available for Windows) is make db or make DEBUGOMP. Compiling with this option creates the executable TREKIS_DEBUG_OMP.exe.
- To run the code, call TREKIS.exe (or ./TREKIS.x in Linux). The code also accepts additional options in the command line: ‘verbose’, ‘very-verbose’, and ‘info’ described above (on page 6) – for that, call the code, e.g., as TREKIS.exe verbose info.

IV. OUTPUT DATA

TREKIS creates a directory with output files named OUTPUT_[*material*], containing a number of output files, produced in simulation runs using this material target.

1) Error log file

File with errors that TREKIS can identify will be named [*SHI*]_in_[*material*]_error_log.txt. If there were any errors that TREKIS identifies, it will save their description in the file, and save the file after the

[§] https://en.wikipedia.org/wiki/Make_(software)
[**] https://visualstudio.microsoft.com/vs/community/
[††] https://www.intel.com/content/www/us/en/developer/tools/oneapi/hpc-toolkit-download.html

simulation. Otherwise, an empty file will be deleted at the end of simulation. So, if the file is present after the simulation ends, it makes sense to check what's in the file.

2) Files with mean free paths

If files with calculated mean free paths (of electrons, valence holes, and photons) do not exists (e.g., it is the first run of the code with the given SHI), or if the file with the material parameters (cdf-file described above) was modified later than the MFP-files, TREKIS will create (overwrite) files with the mean free paths in this material, to reuse them in all future runs without recalculating them. Electrons and valence holes elastic and inelastic mean free paths are saved in the following files: OUTPUT_[*particle*]_[*type*]_[*CS*].dat where:
[*particle*] is either Electron or Hole
[*type*] is either IMPS (inelastic mean free path) or EMFP (elastic)
[*CS*] is the model of the cross section, such as CDF or BEB, at what temperature of the target, etc.
Those files contain a few columns: particle energy in [eV], mean free paths in [Å]. Number of columns with mean free paths depends on the particular material: for each shell of each element, as set in the cdf-file (described in the input files), and the las column is the total mean free path according to the Matthiessen rule.

3) Files with ranges

Electron and valence holes ranges, calculated within the continuous slowing down approximation, are saved in files OUTPUT_[*particle*]_Range_[*CS*].dat where
[*particle*] is either Electron or Hole
[*CS*] is the model of the cross section, such as CDF or BEB, at what temperature of the target, etc.
Those files contain 3 columns:
Column 1 is energy of electron or hole in [eV]
Column 2 is energy loss in [eV/Å]
Column 3 is the residual range of the particle in [Å]

4) File with density of states

File OUTPUT_[*material*]_DOS_analysis.dat contains the data with the DOS, as used in the TREKIS (after renormalization and extracted parameters required in the code). It contains 5 columns:

Column 1 is energy of the valence band counted down from the Fermi energy (top of the valence band) in [eV]

Column 2 is the corresponding wave-vector within the effective one-band approximation [2] in [1/m]

Column 3 is the valence DOS, interpolated on the grid used by TREKIS

Column 4 is the integral of the DOS

Column 5 is the effective valence hole mass, according to the effective one-band approximation in [free electron mass units]

5) Valence holes self-diffusion coefficient

In case if the valence holes transport is allowed, file Hole_selfdiffusion_coeff_in_[*material*].txt will contain a self-diffusion coefficients of valence holes, calculated via its mean free path and velocity.

6) SHI mean free paths, energy losses, and ranges

If the file with SHI mean free path does not exist, or the cdf-file with material parameters was modified later than the MFP-file, TREKIS will calculate the inelastic MFP of the given SHI and save it in

the file. SHI mean free paths, energy losses, and ranges, are saved in the files analogous to those for electrons and holes (see above). They will be saved in an ion-specific directory.

Files OUTPUT_[*SHI*]_[*charge*]_[*charge_model*]_[*output*].dat where

[*SHI*] is the SHI elements name

[*charge*] is the marker of the model of the effective ion charge used:

1) Barkas [15]
2) Bohr [16]
3) ND stands for Nikolaev-Dmitriev approximation [17]
4) SG stands for Schiwietz-Grande approximation [18]
5) Fixed marks the user-defined constant charge

[*charge_model*] identifies the model of the shape of the SHI:

1) P stands for point-like charge
2) BK stands for the Brandt-Kitagawa approximation [19]

[*output*] marks what exactly is in the file:

1) IMFP is for the mean free path
2) dEdx is for the energy loss of SHI
3) Range is for the SHI residual range
4) effective_charges stands for the effective charge

In those files, the first column is always the ion energy in [MeV], the second one is Mean free path in [Å]; or energy loss in [eV/Å]; or residual range in [Å]; or calculated effective charge in [units of electron charge].

7) Directory with results of MC simulations

A directory with all results of the Monte Carlo simulations is created with the name
[*SHI*]_E_[*Energy*]_MeV_[*simulation_time*]_fs

For example, for a gold ion with energy of 2187 MeV and total simulation time of 100 fs, the directory will be called Au_E_2187.00_MeV_10.0_fs.

In case identical parameters were used in previous simulations, the new directory will have a number at the end, e.g., Au_E_2187.00_MeV_10.0_fs_1, and then Au_E_2187.00_MeV_10.0_fs_2 etc. TREKIS will not overwrite existing results.

The following files are created in this directory:

8) File !Parameters.txt

This file contains the information about the used input parameters, and parameters extracted from the EPICS2017 database, such as atomic energy levels, decay times etc.

9) Total numbers and energy

The total numbers of excited electrons and their energy are saved in the file
Total_numbers.txt where
Column 1 in time in [fs],
Column 2 is the total number of electrons
Column 3 is the total energy in [eV]
The total energy should conserve in simulations without electron emission after the SHI passage.
The file Total_energies.txt contains the total energies of the electrons, holes, and atoms.

10) Files with radial distribution of electrons and their energy

Radial distributions of electron density and energy density are printed in the files:
Radial_electron_density[1_cm^-3].txt and
Radial_electron_energy[eV_A^-3].txt, respectively.
The units are shown in the file names: electron density is in [1/cm^3], and energy density is in [eV/Å^3].
In each file, the first line is a comment declaring the columns. The first column is always radius in [Å], counted from the SHI trajectory. Next columns are the electron density or energy density at different time instants defined by the user.
Energy is also printed out in terms of average kinetic temperature in the classical limit (T=2/3E) in the file:
Radial_electron_temperature[K].txt

11) Files with radial distribution of photon and their energy

Analogously to the electronic radial distributions, photons distributions are printed out in the files
Radial_photon_energy[eV_A^-3].txt and
Radial_photon_density[1_cm^-3].txt,
only if the radiative decays, producing photons, are included in the code.

12) Files with holes radial distributions and their energy

Analogously to electrons radial distributions, distributions of holes densities and energy densities are saved in a number of files
Radial_Valence_holes_density[1_A^-3].txt,
Radial_Valence_holes_pot_energy[eV_A^-3].txt and
Radial_Valence_holes_kin_energy[eV_A^-3].txt
For the number of valence holes, and their kinetic and potential energies. The valence energy is counted from the top of the valence band. The potential energy is the band gap of the material, counted for each valence hole.
For atomic deep shells (core shells), analogous files are created, but without the kinetic energy, with their potential energy only. Files are marked by the element and shell names, e.g., Radial_Li_K-shell_holes_density[1_cm^-3].txt stands for the K-shell of Li atoms in our example of LiF.
Energy is also printed out in terms of average kinetic temperature in the classical limit (T=2/3E) in the file:
Radial_Valence_holes_temperature[K].txt

13) File with radial distribution of the energy transferred to lattice

Energy transferred to the lattice in elastic scattering of electrons and valence holes is printed in the file Radial_Lattice_energy[eV_A^-3].txt. Energy is also printed out in terms of average kinetic temperature in the classical limit (T=2/3E) in the file: Radial_Lattice_temperature[K].txt

14) File with radial distribution of the total energy transferred to lattice

Total energy transferred to the lattice (via elastic scattering of electrons and valence holes summed with potential and kinetic energy of valence holes) is printed in the file Radial_Track_energy[eV_A^-3].txt. This file may be used for setting initial conditions for MD simulations, as discussed below in Section V.

15) Files with electron and VB holes spectra

File Electron_distribution_vs_E[1_eV].txt contains electronic distribution in energy space (electronic spectrum). The distribution is normalized to the total number of electrons. Each column is printed for the chosen time instant.

File VB_holes_distribution_vs_E[1_eV].txt is the same but for valence-band electrons.

16) File with electron velocity distribution by azimuth angle (theta)

File Electron_theta_distribution.txt contains distribution of electron velocities by the azimuth angle theta, allowing to trace how electron transport loses preferential direction. The first column is the angle from 0 to 180 degrees. Others are electron distributions at different time instants.

17) File with valence-band holes velocity distribution by azimuth angle (theta)

File VB_holes_theta_distribution.txt contains distribution of VB holes velocities by the azimuth angle theta, allowing to trace how holes transport loses preferential direction. The first column is the angle from 0 to 180 degrees. Others are VB holes distributions at different time instants.

18) File with self-diffusion coefficient of valence holes

File Hole_mean_diffusion_coefficient.txt contains valence holes self-diffusion coefficient, averaged over all holes. The first column is time in [fs], the second column is the diffusion coefficient in [cm^2/s].

V. Combining TREKIS-3 with MD via output-input

Following the methodology developed in [20], one can model formation of the track after an SHI impact with atomic resolution using classical molecular dynamics (MD) simulations, such as, e.g., LAMMPS [21]. The electronic kinetics, providing energy to the atomic system of the target, may be calculated with TREKIS-3. It is important to take into account that there are three distinct channels of energy transfer from excited electrons to atoms of the target:

- electron elastic scattering,
- valence holes elastic scattering,
- nonthermal modification of the interatomic potential [22].

The first two channels are accounted for in TREKIS-3, and the energy provided to lattice atoms is printed out in the file #13 (Radial_Lattice_energy[eV_A^-3].txt) described above. The last one is not directly included, however, may be approximately accounted for *via* the approximation of the instantaneous conversion of the potential energy to the kinetic energy of the atoms [23]. In this case, the potential energy associated with the nonthermal modifications of the interatomic potential is approximated as the band gap energy, assigned to each hole [20]. Thus, the energies of holes from the point 12 above, must be added to the atomic energy.

The sum of all these energies is printed out in the file #14 above. It can be used at the time instant when electronic cascades are finished, can then be used to set the initial conditions for further atomic dynamics. The time instant for that is typically ~100 fs [20]. TREKIS-3 output at 100 fs defines the initial atomic energy in cylindrical layers to be used in LAMMPS (or other MD simulations). The kinetic energies of atoms in the corresponding cylindric layers should be set according to the calculated energy transfer in the layer, whereas momentum direction can be sampled randomly.

The justification for it is discussed in Ref. [9]. Validation of the proposed methodology was presented in Ref. [4] and references therein.

VI. Consistency checks and known problems

Prior to productive simulation runs, the following checks must be performed.

1) Make sure that the calculated electron, valence hole, and photon mean free paths are correct. They are printed in the output files #2-3. Electron mean free paths for many materials may be checked against databases such as, e.g., NIST [24], electron ranges may be found, e.g., in X-ray-data booklet [25]. If the agreement is poor, there may be a few reasons for it: model CDF parameters are incorrect and CDF oscillators need an adjustment; other model parameters such as effective masses set in the input file may be incorrect.

2) Make sure that the interpolated DOS in the file #4 looks reasonable. If it has several sub-bands in the valence band, the gaps between them must be exactly zero. Atomic energy levels must not overlap with the DOS of the valence band (if they do, you probably have double-counting, and some atomic levels must be excluded and transferred into the valence band).

3) Make sure that calculated SHI energy loss function S_e printed in the file #6 is correct. It may be compared to known databases such as SRIM[‡‡] [26], IAEA[§§], or NIST[***]. Note, however, that the residual ranges may have a rather large mismatch by the absolute value, but qualitatively the same if shifted to match the Bragg peaks.

4) Make sure that the values of the atomic energy levels and decay time printed out in the file #8 make sense. Those provided by the user in cdf-file may contain errors and would need to be adjusted.

5) Make sure that the total energy in the MC calculations printed in the files #9 is conserved (if electron emission is not allowed in the simulation). If it is not, it may indicate some bug in the code we missed.

6) If the program stops without producing output data, most probably it is due to memory overflow. In such a case, try reducing the number of time grid point in the output – you may try to use temporal log-scale with only a few points to print out. It may also indicate that the thickness of the chosen simulated layer is too large, which results in a too large number of secondary particles created.

VII. References

[1] N.A. Medvedev, R.A. Rymzhanov, A.E. Volkov, Time-resolved electron kinetics in swift heavy ion irradiated solids, J. Phys. D. Appl. Phys. 48 (2015) 355303. https://doi.org/10.1088/0022-3727/48/35/355303.

[2] R.A. Rymzhanov, N.A. Medvedev, A.E. Volkov, Effects of model approximations for electron, hole, and photon transport in swift heavy ion tracks, Nucl. Instruments Methods Phys. Res. Sect. B Beam Interact. with Mater. Atoms. 388 (2016) 41–52. https://doi.org/10.1016/j.nimb.2016.11.002.

[3] M. Lang, F. Djurabekova, N. Medvedev, M. Toulemonde, C. Trautmann, Fundamental phenomena and applications of swift heavy ion irradiations, in: Compr. Nucl. Mater., Elsevier, 2020: pp. 485–516. https://doi.org/10.1016/B978-0-12-803581-8.11644-3.

[4] R.A. Rymzhanov, N. Medvedev, J.H. O'Connell, V.A. Skuratov, A. Janse van Vuuren, S.A. Gorbunov, A.E. Volkov, Insights into different stages of formation of swift heavy ion tracks, Nucl. Instruments Methods Phys. Res. Sect. B Beam Interact. with Mater. Atoms. 473 (2020) 27–42. https://doi.org/10.1016/j.nimb.2020.04.005.

[‡‡] www.srim.org

[§§] https://www.iaea.org/resources/databases/stopping-power

[***] https://www.nist.gov/pml/stopping-power-range-tables-electrons-protons-and-helium-ions

[5] L. Van Hove, Correlations in Space and Time and Born Approximation Scattering in Systems of Interacting Particles, Phys. Rev. 95 (1954) 249–262. https://doi.org/10.1103/PhysRev.95.249.
[6] U. Fano, Penetration of Protons, Alpha Particles, and Mesons, Annu. Rev. Nucl. Sci. 13 (1963) 1–66. https://doi.org/10.1146/annurev.ns.13.120163.000245.
[7] R.H. Ritchie, A. Howie, Electron excitation and the optical potential in electron microscopy, Philos. Mag. 36 (1977) 463–481. https://doi.org/10.1080/14786437708244948.
[8] N.A. Medvedev, R.A. Rymzhanov, A.E. Volkov, Complex dielectric function formalism for description of the electron kinetics in swift heavy ion tracks in LiF and Y2O3, Nucl. Instruments Methods Phys. Res. Sect. B Beam Interact. with Mater. Atoms. 315 (2013) 85–89. https://doi.org/10.1016/j.nimb.2013.04.090.
[9] N. Medvedev, F. Akhmetov, R.A. Rymzhanov, R. Voronkov, A.E. Volkov, Modeling time-resolved kinetics in solids induced by extreme electronic excitation, Adv. Theory Simulations. 5 (2022) 2200091. https://doi.org/10.1002/ADTS.202200091.
[10] R.A. Rymzhanov, N.A. Medvedev, A.E. Volkov, Electron emission from silicon and germanium after swift heavy ion impact, Phys. Status Solidi. 252 (2015) 159–164. https://doi.org/10.1002/pssb.201400130.
[11] Y.-K. Kim, M. Rudd, Binary-encounter-dipole model for electron-impact ionization, Phys. Rev. A. 50 (1994) 3954–3967. https://doi.org/10.1103/PhysRevA.50.3954.
[12] A. Akkerman, T. Boutboul, A. Breskin, R. Chechik, A. Gibrekhterman, Y. Lifshitz, Inelastic Electron Interactions in the Energy Range 50 eV to 10 keV in Insulators: Alkali Halides and Metal Oxides, Phys. Status Solidi. 198 (1996) 769–784. https://doi.org/10.1002/pssb.2221980222.
[13] J.-C. Kuhr, H.-J. Fitting, Monte Carlo simulation of electron emission from solids, J. Electron Spectros. Relat. Phenomena. 105 (1999) 257–273. https://doi.org/10.1016/S0368-2048(99)00082-1.
[14] T.M. Jenkins, W.R. Nelson, A. Rindi, Monte Carlo Transport of Electrons and Photons, Springer US, Boston, MA, 1988. https://doi.org/10.1007/978-1-4613-1059-4.
[15] W.H. Barkas, Nuclear research emulsions., New York, 1963. http://hdl.handle.net/2027/uc1.b3533401 (accessed November 20, 2013).
[16] H.-D. Betz, Charge States and Charge-Changing Cross Sections of Fast Heavy Ions Penetrating Through Gaseous and Solid Media, Rev. Mod. Phys. 44 (1972) 465–539. https://doi.org/10.1103/RevModPhys.44.465.
[17] V.S. Nikolaev, I.S. Dmitriev, On the equilibrium charge distribution in heavy element ion beams, Phys. Lett. 28 (1968) 277–278.
[18] G. Schiwietz, K. Czerski, M. Roth, F. Staufenbiel, P.L. Grande, Femtosecond dynamics – snapshots of the early ion-track evolution, Nucl. Instruments Methods Phys. Res. Sect. B Beam Interact. with Mater. Atoms. 226 (2004) 683–704. https://doi.org/10.1016/j.nimb.2004.05.043.
[19] W. Brandt, M. Kitagawa, Effective stopping-power charges of swift ions in condensed matter, Phys. Rev. B. 25 (1982) 5631–5637. https://doi.org/10.1103/PhysRevB.25.5631.
[20] R. Rymzhanov, N.A. Medvedev, A.E. Volkov, Damage threshold and structure of swift heavy ion tracks in Al2O3, J. Phys. D. Appl. Phys. 50 (2017) 475301. https://doi.org/10.1088/1361-6463/aa8ff5.
[21] A.P. Thompson, H.M. Aktulga, R. Berger, D.S. Bolintineanu, W.M. Brown, P.S. Crozier, P.J. in 't Veld, A. Kohlmeyer, S.G. Moore, T.D. Nguyen, R. Shan, M.J. Stevens, J. Tranchida, C. Trott, S.J. Plimpton, LAMMPS - a flexible simulation tool for particle-based materials modeling at the atomic, meso, and continuum scales, Comput. Phys. Commun. 271 (2022) 108171. https://doi.org/10.1016/J.CPC.2021.108171.
[22] N. Medvedev, A.E. Volkov, Nonthermal acceleration of atoms as a mechanism of fast lattice heating in ion tracks, J. Appl. Phys. 131 (2022) 225903. https://doi.org/10.1063/5.0095724.
[23] N. Medvedev, F. Akhmetov, R.A. Rymzhanov, R. Voronkov, A.E. Volkov, Modeling time-resolved kinetics in solids induced by extreme electronic excitation, 2022. https://arxiv.org/abs/2201.08023v1 (accessed January 31, 2022).
[24] C.J. Powell, A. Jablonsky, NIST Electron Inelastic-Mean-Free-Path Database: Version 1.2, (2014) http://www.nist.gov/srd/nist71.cfm. http://www.nist.gov/srd/nist71.cfm.
[25] A. Thompson, D. Vaughan, J. Kirz, D. Attwood, E. Gullikson, M. Howells, K.-J. Kim, J. Kortright, I. Lindau, P. Pianetta, A. Robinson, J. Underwood, G. Williams, H. Winick, X-Ray Data Booklet,

Center for X-ray Optics and Advanced Light Source, Lawrence Berkeley National Laboratory, Berkeley, CA, USA, 2009. http://xdb.lbl.gov/ (accessed August 26, 2015).
[26] J.F. Littmark, J.P. Ziegler, U. Biersack, The Stopping and Range of Ions in Solids, Pergamon Press, New York, 1985.