IM3D_GUI Manual

Introduction

IM3D is a 3D Monte Carlo simulation code designed to run efficiently on serial or parallel computers, which can simulate the transportation/tracing of ions and subsequent radiation damages in arbitrary complex 3D nanostructured materials. It is based on fast indexing of scattering integrals and the SRIM stopping power database, and allows the user a choice of Constructive Solid Geometry (CSG) or Finite Element Triangle Mesh (FETM) method for constructing 3D shapes and microstructures. For 2D films and multilayers, IM3D perfectly reproduces SRIM results, and can be about 102 times faster in serial execution and > 104 times faster using parallel computation. For 3D problems, it provides a fast approach for analyzing the spatial distributions of primary displacements and defect generation under ion irradiation.

IM3D was sponsored by Prof. Ju Li and Prof. Zhi Zeng, and mainly devel- oped by Dr. Yonggang Li during his visiting to MIT in 2014. The supporting of CSG/FETM geometric algorithms form Prof. Zejun Ding as well as useful contributions and discussions from Dr. Machal Short and Yang Yang are very appreciate.

If you have any questions, please contact to Dr. Yonggang Li, who can be emailed at ygli@theory.issp.ac.cn. The IM3D Websites at ISSP and MIT have more infor- mation about the code and its uses.

Installation of IM3D_GUI

IM3D_GUI - Installation in PC with existing IM3D directory

IM3D_GUI can be installed in a separate directory, and it will not interfere with running the old copy of IM3D.

* Make a new directory called IM3D_GUI.

* Download the new IM3D_GUI file from the official website of IM3D (http://theory.issp.ac.cn: 7777). Then, complete the registration and download the compression package of IM3D on the website and put it into this directory.

The user should be build the running environment (ms-mpi) before installing IM3D,

Which can be downloaded via the website (https://docs.microsoft.com/en-us/message-pass-interface/microsoft-mpi).

After the successful installation of the ms-mpi, user can use IM3D by clicking on the IM3D icon in the unzipped file.

* Find the file IM3D.exe. This is the IM3D start-up file. If you already have IM3D working on your computer, this new version should work without any problem.

IM3D_GUI Setup Window

Simulation Module

<<Path>>

The output file path. The path "./output/" is selected in default. For example: ./output

<<Format>>

The output file format. Here "dat","cfg","msh" and "vtk" can be chosen. For example: dat

<<Normalize>>

Whether normalize output results or not. If choose "Y", normalize it; choose "N", do not normalize it. For example: Y

<<Display>>

The displaying interval. The number should range from 1 to "max no ions" in "Ion Beam Parameter" setup. For example: 100

<<Storage>>

The storaging interval, range from 1 to "max no ions". For example: 1000

<<Transmitted ions>>

Whether store transmitted ions or not. Choose "Y", store them; choose "N", do not store them. For example: Y

<<Recoil cascades>>

Whether store the exact recoil cascades or not. Choose "Y", store them; choose "N", do not store them. For example: Y

<<Energy deposit>>

Whether the arrays with deposited energy are created and stored. Choose "Y", create and store them; choose "N", do not create and store them. For example: Y

<<Damage>>

Whether store irritation damages or not. Choose "Y", store them; choose "N", do not store them. For example:Y

<<Exiting recoils>>

Whether store exiting recoils or not. Choose "Y", store them; choose "N", do not store them.

if choose "Y", please make some settings about "Exiting limit"; if choose "N", "Exiting limit" is not displayed. For example: Y

<<Exiting limit>>

The maximum number of exiting recoils to be stored. For example: 100

<<Ion paths>>

Whether store the exact ion paths or not. Choose "Y", store them; choose "N", do not store them.

Notice: "Y" is only for the serial version.

if choose "N", "Path limit" is not displayed,

if choose "Y", please make some settings about "Path limit".for example:Y

<<Path limit>>

The maximum number of stored ion paths, it is recommended that the number ranges from 1 to 1000. For example: 100

Control Module

<<Transport type>>

Two transport types are optional. "S" means "full and accurate projectile transport", while "M" means "fast projectile transport", if choose "S", "Multiple collisions" is not displayed; if choose "M", please make some settings about "Multiple collisions". For example: S

<<Multiple collisions>>

The maximum number of multiple collisions.For example: 1

<<Flight length type>>

Two parameters are optional. "P" means "Random Poisson distribution", while "C" means it is constant. if choose "P", "Flight length C" is not displayed; if choose "C", please make some settings about "Flight length C". For example: C

<<Flight length C>>

It means flight length constant. It should be approximately lattice constant. For example: 0.3

<<Scattering calc>>

the scattering calculation type, "D" means using "SRIM-Corteo database"; "M" means using "MAGIC approximation". For example: D

<<Tracing recoil>>

The way of tracing the exact recoils cascades. "KP" means "Quick Kinchin-Pease"and IM3D will trace only the main cascasdes; While "FC" means "Full Cascades" and IM3D will trace full cascade. Note: "FC" can only be calculated by Serial version. For example: KP

<<Detailed sputtering>>

Whether calculate the detailed sputtering or not. Choose "Y", calculate it, choose "N", do not calculate it. if choose "N", "Sputter yields" is not displayed; if choose "Y", please make some settings about "Sputter yields". For example: Y

<<Sputter yields>>

#Whether store sputtering yields for single ions or not. choosing "Y" means storing sputtering yields for single ions and "N" means not storing. For example: Y

<<Straggling model>>

The optional straggling model types. Here "No straggling", "Bohr", "Chu" and "Chu+ Yang" are available. For example: Chu+Yang

<<Min energy>>

The minimum energy below which all projectiles are stopped, it can range from 0 to "Ion E0" in "Ion Beam". For example: 5

Ion Beam Module

<<source type>>

The selection of source file. "0" means the source is ions, "0" means the source is PKA and "2" means the source is PKA cumulative distribution.

if choose "1" or "2", please import the source file - "source.in" some settings about "Sputter yields".For example: 1

<<Max no ions>>

The number of ions in a simulation. It can range from 1 to 100000000. For example: 50000

<<Ion Z>>

The atomic number (the mass in atomic mass unit) of the ion. It can range from 1 to 92. For example: 14

<<Ion M>>

The atomic mass of the ion. For example: 28.0

<<Ion E>>

The primary incident energy of the ion in unit of eV/amu. Range from 10eV to 2GeV. For example: 50000

Incident Direction

<<Ion vx; Ion vy; Ion vz>>

The the incident direction (vx, vy, vz) of the ion; range of (0, 1) and $vx^2+vy^2+vz^2=1$. For example: 0; 0; 1

<<Ion distribution>>

The distribution type of the incident ion beam on x-y plane of the target. There are five parameters available: "random" means random distribution, "centered" means centered distribution, "defined position" means choose incident position by yourself, "random square" means random square distribution around predefined position, "Gaussian beam" means gaussian distribution around predefined position with sigma. "Circular" means Circular distribution around predefined position.

if choose "random", you needn’t choose anything in the end;

if choose "centered", "defined position" and "random square", "Gaussian" and "Circular", please make some settings about "Incident position";

if choose "Gaussian", please make some settings about "Beam spread".for example: Centered

If choose "Circular", please make some settings about "Enter x; Enter y; Enter z" and "Beam spread"

Incident position:

<<Enter x; Enter y; Enter z>>

The enter position (x; y; z) of ions. When "random" is not chosen, z must be higher than the target, when "Circular" is chosen, which represent the coordinates of the center of the circle. For example: 20; 20; -10

<<Beam spread>>

The spread of the beam in xy-space for Gaussian beam. when "Circular" is chosen, which represent the radius of circular. For example: 1.5

Material Module

<<Material name>>

The name of the material to be calculated. For example: GaAs

<<Material count>>

The number of the material to be calculated. For example: 2

<<Element name>>

The name of the element for current material.

<<PT>>

Import the element via the periodic table of the elements.

<<Element count>>

The number of element types. For example: 2

<<Density>>

The atomic density of the material in unit of atom/cm3. For example: 4.43e22

<<Z>>

The atomic numbers of elements in the current material. For example: 31, 33

<<M>>

The atomic weights of elements in the current material. For example: 69.72, 74.92

<<Concentration>>

The atomic number of atoms in the current material. For example: 0.5, 0.5

<<Displacement energy>>

The displacement energies of atoms in the current material. For example: 20.0, 25.0

<<Lattice energy>>

The bulk lattice energies of atoms in the current material. For example: 3.0, 3.0

<<Surface energy>>

The surface lattice energies of atoms in the current material. For example: 2.0, 1.2

<<Ion surface energy>>

The surface lattice energies of the ion in the current material. For example: 2.0

Target Module

<<Geometry model>>

the geometry model of the target # the geometry type : BULK: LAYER: CSG: Constructive Solid Geometry FETM: Finite Element Triangle Mesh CSG

<<BULK>>

Target object is Bulk. And if choose "BULK", "No substrate" and "Gen shape" are not displayed

"Semi-infinite bulk target" is no action.

<<LAYER>>

Target object is layers.And if choose "LAYER", "Gen shape" is not displayed.

<<CSG>>

Target object is arbitrary complex geometric structure constructed by Constructive Solid Geometry.And if choose "CSG", "Gen shape" is not displayed. And select an existing CSG file from your files

<<FETM>>

Target object is arbitrary complex geometric structure constructed by Finite Element Triangle Mesh. And Select an existing FETM file

<<No Substrate>>

Whether exist the substrate under the target or not. "Y" means existing, and "N" means not existing.

<<Gen shape>>

Generate fetm shape from ply2 file by IM3D (1) or pregenerated fetm shape by triangle.f90 code (0)

<<Pbc>>

Periodic boundary conditions in x and y directions or not

<<Layer count>>

The number of layer

<<Current Layer>>

The current use of this layer

<<Layer material>>

The material composition of this layer

<<Layer thick>>

The thick of this layer

<<Select a FETM file>>

Select an existing FETM file

<<Materials file name>>

Materials File Name = Materials.in # the filename that defines the materials in the target, in default

<<Target structure file name>>

Target structure File Name = Structure.in # the filename that define the structure of the target, in default

<<Cell count x y z>>

The numbers of cells along (x; y; z)-axis respectively. The total number of cells should be less than the eighth power of 10, or leading to memory overflow. The recommendation is in the order of 100 * 100 * 100. For example: 60，60，20

<<Cell size x y z>>

The intervals of cells along (x; y; z)-axis respectively. This is a size on the order of nm, this size and the size of the cell count should be within the bulk or as large as the

bulk. For example: 10，10，5

<<Sub surf z>>

The z-position of the substrate surface. For example: 101

<<Incidence surf z>>

The projection z-plane for oblique incident ions. For example: 100.0

<<Composition file name>>

The file name defines the composition in the target in default.

Computing Module

<<Serial>>

In order to further increase the efficiency of the code, We introduce the fast database indexing technique for fast Monte Carlo sampling and two numerical acceleration techniques (MPI parallel and multi-threading) to implement parallel computing on a Beowulf cluster or a multi-core computer.

<<Parallel>>

In order to further enhance the computational efficiency, the MPI parallel and multi-threading methods have been integrated in IM3D code.

<<Number of threads>>

Number of threads for this system

<<Random seeds>>

Random numbers in a simulation

<<Parameters Preview>>

Preview the parameters which have been set

Running Module

<<Save>>

Save this calculation as a file

<<Load>>

Select an existing calculation file

Select you want to load

<<BULK Demo (Si)>>

A demo example of bulk material (Si)

<<LAYER Demo (ZrO2-Si)>>

A demo example of layer material (ZrO2-Si)

<<CSG Demo (Fe-Y2O3)>>

A demo example of CSG (Constructive Solid Geometry) material (Fe-Y2O3)

<<FETM Demo (Ga-W)>>

A demo example of FETM (Finite Element Triangle Mesh) material (GaW)

<<Load an existing computing>>

<<Start>>

Start calculating

Analysis Module

Output files and analysis results

<<aiv.xyz.cfg>>

aiv.xyz.cfg is an output file of the detailed position of ions and defects generated in 3D, which contains 7 columns, that is, x, y, z, defect type, defect belong to which ion, material and element. It is in the format of .cfg at present and can be viewed by AtomEye software directly

<<azimuth angle dist.dat>>

azimuth angle dist.dat is an output file of the azimuth-angle distribution of outgoing/exiting particles (ions and atoms). which contains 7 columns, that is, azimuth angle (0-359 degree), number of outgoing/exiting ions, energy of outgoing/exiting ions (eV), number of outgoing atoms, energy of outgoing/exiting atoms, total number of outgoing/exiting particles and total energy of outgoing/exiting particles.

<<Cascades>>

cascades is an output file of detailed trajectory of each cascade, which contains 4 columns, that is, x (nm), y (nm), z (nm) and energy (eV). Different cascades are divided by a blank line.

<<depth dist functions.dat>>

depth dist functions.dat is an output file of the depth distribution of ions, energies and defects in materials, which contains 9 columns, that is, z, implanted ions, replacing ions, electron energy deposition, phonon energy deposition, interstitials, replacements, vacancies and displacements.

<<disp.mat∗.cfg/.msh/.vtk>>

disp.mat ∗ .cfg/.msh/.vtk is an output file of the space distribution of displacements in 3D, which contains at least 5 columns, that is, x (nm), y (nm), z(nm), total displacement in material * (number), displacements of element 1 in material * (number), ...

<<energy.deposit.cfg/.msh/.vtk>>

energy.deposit.cfg/.msh/.vtk is an output file of the space distribution of electron and phonon energy deposition in 3D, which contains 5 columns, that is, x (nm), y (nm), z(nm), electron energy deposition (eV), phonon energy deposition (eV).

<<exiting energy dist.dat>>

existing energy dist.dat is an output file of the energy distribution of outgoing/existing particles (ions and atoms), which contains 4 columns, that is, energy (eV), number of outgoing/existing ions, number of outgoing/existing atoms, total number of outgoing/exiting particles.

<<full angle dist.cfg>>

full angle dist.cfg is an output file of angular distribution of outgoing/exiting particles (ions and atoms) in .cfg file format, which contains 9 columns, that is, x (a.u.), y (a.u.), z (a.u.), number of outgoing/exiting ions, energy of outgoing/exiting ions (eV), number of outgoing atoms, energy of outgoing/exiting atoms, total number of outgoing/exiting particles and total energy of outgoing/exiting particles.

<<full angle dist.dat>>

full angle dist.dat is an output file of angular distribution of outgoing/exiting particles (ions and atoms) in .dat file format, which contains 8 columns, that is, polar angle (0-179 degree), azimuth angle (0-359 degree), number of outgoing/exiting ions, energy of outgoing/exiting ions (eV), number of outgoing atoms, energy of outgoing/exiting atoms, total number of outgoing/exiting particles and total energy of

outgoing/exiting particles.

<<int.mat*.cfg/.msh/.vtk>>

*int.mat * .cfg/.msh/.vtk* is an output file of the space distribution of interstitials in 3D, which contains at least 5 columns, that is, x (nm), y (nm), z(nm), total interstitials in material * (number), interstitials of element 1 in material * (number), ...

<<ion paths>>

ion path is an output file of detailed trajectory of each ion, which contains 4 columns, that is, x (nm), y (nm), z (nm) and energy (eV). Different ions are divided by a blank line. The total number of tracing ions is limited by *store path limit*.

<<ions.replacements.cfg/.msh/.vtk>>

ions.replacements.cfg/.msh/.vtk is an output file of the space distribution of replacing ions in 3D, which contains 4 columns, that is, x (nm), y (nm), z(nm), replacing ions (number)

<<ions.total.cfg/.msh/.vtk>>

ions:total.cfg/.msh/.vtk is an output file of the space distribution of implantaed ions in 3D, which contains 4 columns, that is, x (nm), y (nm), z(nm), implanted ions (number).

<<leaving directions.ions>>

leaving directions.ions is an output file of the number of escaping/leaving ions in 8 directions (quadrants) from materials, in the form of (*+x; +y; +z*) *number of leaving ions*.

<<leaving directions.sum>>

leaving directions.sum is an output file of the number of escaping/leaving particles (including ions and atoms) in 8 directions (quadrants) from materials, in the form of (*+x; +y; +z*) *number of leaving particles*.

<<leaving directions.z*1.m*2.mat*3.elem*4>>

*leaving directions.z * 1:m * 2:mat * 3:elem * 4* is an output file of the number of escaping/leaving atoms (element number z*1 with atomic weight of m*2 for element *4 in material *4) in 8 directions (quadrants) from materials, in the form of (*+x; +y; +z*) number of leaving atoms.

<<leaving recoils.z*1.m*2.mat*3.elem*4>>

*leaving recoils.z * 1:m * 2:mat * 3:elem * 4* is an output file of the number of escaping/leaving recoils (element number z*1 with atomic weight of m*2 for element *4 in material *4) in 8 directions (quadrants) from materials, in the form of (*+x; +y; +z*) number of leaving atoms.

<<leaving.mat*.cfg/.msh/.vtk>>

*leaving.mat * :cfg/.msh/.vtk* is an output file of the last positions of sputtered atoms in 3D, which contains at least 5 columns, that is, x (nm), y (nm), z(nm), total sputtered atoms in material * (number), sputtered atoms of element 1 in material * (number), ...

<<polar angle dist.dat>>

polar angle dist.dat is an output file of the polar-angle distribution of outgoing/exiting particles (ions and atoms). which contains 7 columns, that is, polar angle (0-179 degree), number of outgoing/exiting ions, energy of outgoing/exiting ions (eV), number of outgoing atoms, energy of outgoing/exiting atoms, total number of outgoing/exiting particles and total energy of outgoing/exiting particles.

<<radial dist functions.dat>>

radial dist functions.dat is an output file of the radial distribution of ions, energies and defects in materials, which contains 9 columns, that is, z, implanted ions, replacing ions, electron energy deposition, phonon energy deposition, interstitials, replacements, vacancies and displacements.

<<repl.mat*.cfg/.msh/.vtk>>

*repl:mat * .cfg/.msh/.vtk* is an output file of the space distribution of replacements in 3D, which contains at least 5 columns, that is, x (nm), y (nm), z(nm), total replacements in material * (number), replacements of element 1 in material * (number),

<<transmitted.ions>>

transmitted.ions is an output file of the projectiles leaving the simulation volume, which contains 7 columns, that is, x (nm), y (nm), z (nm), vx (*sinθcosφ*), vy (*sinθsinφ*), vz (*cosθ*), energy (eV).

<<vac.mat∗.cfg/.msh/.vtk>>

vac:mat ∗ .cfg/.msh/.vtk is an output file of the space distribution of vacancies in 3D, which contains at least 5 columns, that is, x (nm), y (nm), z(nm), total vacancies in material * (number), vacancies of element 1 in material * (number), ...