Numerical Simulation of Nanostructured Layered Materials Using IM3D and SRIM

Nimphy Sarkar, Nitin Kumar Puri

Department of Applied Physics, Delhi Technological University, Delhi-110042, India

Abstract: The understanding of fundamental ion interaction processes is relevant for radiation detectors, ion implantation, ion beam etching, irradiation induced degradation of materials, nanostructure formation, ion-induced mass redistribution, sputter yield amplification etc. Thus, simulation of radiation damage and displacement is essential for research and many industrial applications. In this paper, simulations were performed by using SRIM and IM3D to compare and discuss the effect of ion irradiation in different nanostructured materials. Additionally, We have studied the Ion beam sputtering induced bending in tungsten wire using Finite Element Triangle Mesh (FETM) method in 3D geometry in IM3D code using full cascades (FC) option and discussed the results. The study showed good agreement between computations and simulations of results of IM3D and SRIM. The aim of the paper is to demonstrate the performance and accuracy of SRIM and IM3D codes on a variety of problems.

Keywords: Ion Irradiation, Radiation damage, SRIM code, IM3D code

1. Introduction

Ion irradiation inevitably produces a significant concentration of defects and lattice disorder in solids resulting in the degradation[3-7] of key material properties by numerous mechanisms, such as amorphization, phase and blister formation, void swelling, irradiation-induced creep, and radiation enhanced corrosion. The effects of irradiation on materials properties and performance are disadvantageous to safety and reliability of reactor operations[3], efficiency, production of nuclear waste and acceptable used nuclear fuel disposition. In fusion reactors, irradiation effects cause irradiation creep, radiation induced swelling, loss of fracture toughness and possibly irradiation assisted stress corrosion cracking. However, ion irradiation has applications[4] in doping of bulk and ion beam nitriding of steels, synthesize nanowires and change their morphology in a controllable manner and tailor their mechanical, electronic, magnetic properties and widely applied to study high-DPA radiation effects in structural materials. There is growing scientific and commercial interest in research and manufacture of nuclear nanostructured materials that can survive in severe irradiation environment and mitigate radiation-induced damage[8-10] for the uses in advance reactors due to their high volume fraction of buried interfaces and efficiency in the trapping and recombination of radiation-induced defects[11]. With growing increase in theoretical and experimental research of different kinds of nanostructured nuclear materials[12-47], there is a need for studying ion irradiation induced in complex three-dimensional (3D) geometries for the better understanding of these materials. Research on ion irradiation and its application was accompanied by the development of computer simulation codes mainly based on binary collision Monte Carlo simulation programs. However, recent advancement in research and development has led to the need of user-friendly specialized codes aimed at enabling high-fidelity, precise analysis, simulations and modeling in 3D geometric structures to provide the better understanding of theoretical and experimental data.

SRIM (Stopping and Range of Ions in Matter) has been the de facto standard tool for stopping power calculations for more than 30 years[1]. SRIM uses a simplified “beam” model for Monte Carlo simulations and also calculates the 3D distribution of the ions and kinetic phenomena associated with the ion’s energy loss such as target damage, sputtering, ionization and phonon production. The simplified model of the SRIM code is that it assumes that the target material layers as homogenous and static with no feedback from the replaced ions. In SRIM manual [1], threshold energy is sharply set as displacement energy. Assuming the temperature \( t = 0 \text{ K} \), imagine ion trajectories knock off atoms from its original positions in the target material. If the kinetic energy of ‘knocked off atoms’ is greater than displacement energy, heat is generated which is dissipated to the surroundings. After the dissipation of energy, the material falls back to \( t = 0 \text{ K} \). If target material is monoatomic, isotropic or homogenous, counting the number of Frenkel pairs gives DPA (displacement per atom) estimation. However, if the target material is complex, isotropically or chemically variant, DPA has the limitation with completely characterize of radiation damage. Furthermore, due to dynamic processing, a number of point defects anneal out and an absolute accurate damage profile cannot be obtained. This model of using displacement energy as threshold cut-off in SRIM leads to the inaccurate estimation of replacement fractions in total displacement events. Replacement process should occur only when the energy of the trajectory atom after replacement is lower than the binding energy in bulk. Else, the trajectory atom after replacement leaves the lattice site. It migrates to other position, which generates a pair of interstitial and vacancy. IM3D uses binding energy instead of the displacement energy as the threshold cut-off energy for replacements and produces the more accurate ion-depth profiles with the same absolute values.

In both SRIM and IM3D codes, user is provided with the choice of ‘Quick kinchpin (QKP)’ and ‘Full cascades (FC)’ options[1, 52]. The ‘Quick Kinchin-Plase’ option in both SRIM and IM3D codes provides faster, efficient, and more accurate estimation of DPA. In serial execution, IM3D is \( \sim 10^7 \) times faster than SRIM. FC option is slower. It tends to give a wrong answer [52] because of DPA estimation at the wrong temperature. SRIM FC provides an overestimated DPA by a factor of around two compared to

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the QKP option [52]. In contrast to SRIM, the open-source nature of IM3D leaves room for further modifications and improvements for both FC and QKP options.

SRIM code uses the MAGIC algorithm [1] while IM3D code uses fast database indexing technique or the MAGIC approximation formula. Thus, IM3D exhibit a significant speed gain by several orders of magnitude compared to SRIM with no loss in terms of accuracy and efficiency. IM3D can run on a single processor or in parallel with distributed-memory message-passing parallelism (MPI) [2]. While SRIM is limited to be used on Windows operating system, IM3D can be used on multiple platforms. It can run on only single or multiprocessors desktop/laptop machines including parallel computers.

SRIM/TRIM code has limitations in describing geometrically complex structures for modeling radiation displacements and damage [49] in nanostructured materials. For complex targets, SRIM code simulates complex geometric structures as bulk or as a finite stack of two-dimensional homogeneous layered targets. In case of nano-structured materials, which are of the same size as the ion range or the damage cascade, SRIM codes cannot account for effects occurring in irradiation of nanostructured materials. There are several other advanced codes [53-60] for 3D simulation of Ion irradiations. However, these codes are not widely available, have limited applications or low computational efficiency. IM3D code can model arbitrary complex targets constructed by the 3D geometric algorithms of CSG/FETM methods, with complex materials including single elements (atomic numbers from 1–92), alloys and compounds.

In this paper, ions depth – distributions of argon ions into silicon, helium ions into nickel and Au ions into ZrO2/Si samples are determined and compared using SRIM and IM3D with Quick Kinchin-Pease option. We have discussed the benefits and limitations of using SRIM and IM3D. We have also studied gallium ion irradiation in tungsten wire using Finite Element Triangle Mesh (FETM) method in 3D geometry in IM3D code using full cascades (FC) option and discussed the results.

2. IM3D

IM3D [2, 68-69] (Irradiated Microstructures in 3D) is a freely available, accurate, efficient and universal 3D structural MC model developed based on the standard SRIM databases, the fast database indexing technique [78] and MPI parallel algorithm as well as the 3D structural algorithms of Constructive Solid Geometry (CSG) [61-62] and Finite Element Triangulated Mesh (FETM) methods [63-67]. IM3D can rapidly simulate the transportation of ions and the production of defects in nanostructured materials. It can model arbitrarily complex 3D targets made of different geometric elements, each composed of different materials. IM3D can be used to calculate and model both the 3D distribution of ions and ion’s energy loss, such as displacement, sputtering, damage, ionization, and phonon production. IM3D is open source and can be modified at will. In IM3D manual, it is mentioned that IM3D can run on single or multi-processor laptops/Desktop computers as well as parallel computers. IM3D takes single input script or four separate input files in config format. For visualization of output files, we have used AtomEye [70]. There are other options for output visualizations tools like Gmsh [71], paraview [72] etc.

IM3D mainly includes three components, i.e. the accurate physical models, the universal 3D structural models, and the efficient calculation algorithms.

Physical Model: Collision physics IM3D are similar to well-established SRIM-like codes which basically introduced the random phase approximation (RPA), the binary collision approximation (BCA) and the central potential approximation (CPA) [1, 53, 78]. The flowchart (Fig. 1) describes the ions tracing and defects generation in a target. The detailed physical background can also be found elsewhere [1].

MAGIC approximation [1] or fast indexing technique [78] is used in IM3D for sampling in terms of accuracy and efficiency. IM3D uses a screened repulsive Coulomb potential described by a dimensionless screening function, such as the Thomas-Fermi potential [79], the Lenz-Jensen potential [80], the Moliere potential [81], the Bohr potential [82] and the universal Ziggler-Biersack-Littmark (ZBL) potential [1] to describe the interaction potential between two atoms. Also, the recoil energy of a target atom (due to elastic nuclear collisions) can be evaluated by the BCA between two charged particles involved in one scattering process.
figure 1: IM3D program flowchart showing ion tracking and defect generation methods, source: Li, Y.G. et al. IM3D: A parallel Monte Carlo code for efficient simulations of primary radiation displacements and damage in 3D geometry. Sci. Rep. 5, 18130; doi: 10.1038/srep18130 (2015).

In IM3D code, the physical parameters such as electronic energy loss and straggling are based on the standard SRIM databases[1], and Bragg’s rule[86] is used to estimate the stopping power of a compound by the linear combination of the stopping powers of its individual elements. For energy straggling, either the Bohr[83], Chu[84], or Yang[85] formulas can be selected. IM3D provides user with the options of the analytical modified Kinchin-Pease (KP)[87] model or the computationally full cascade (FC) simulation for defect generation processes. The FC option allows one to follow all target atom cascades in detail.

3D geometric models: In IM3D, 3D nanostructured samples can be generated by graphical softwares beforehand and traced by the sophisticated 3D structural algorithms based on the CSG/FETM [61,62, 63, 67] methods. Based on CSG (Constructive Solid Geometry) geometric model, nine basic shapes such as sphere, tetrahedron, cuboid, ellipsoid, taper, column, polyhedron, paraboloid, hyperboloid and their assemblies can be constructed at present to model many regular targets with different materials. The user is given the choice to use different types of spatial distributions (i.e., specified point, center point, uniform or Gaussian random distributions and so on) for sampling ion beams with different atomic numbers and incident directions. CSG[61,62] method can be used to model a complex geometric structure with some basic and simple 3D bodies as elements and can be analytically detailed with limited parameters.
In case of FETM (Finite Element Triangulated Mesh) method in IM3D, different graphical softwares (such as Gmsh software[71]) can be used to outline the 3D geometric structure using different algorithms to construct a 3D geometric structure. This method can be used for simulating many complex targets with less consuming time. FETM[63-67] method uses a finite element triangle mesh to construct a sample surface, and furthermore, by using the space subdivision method to accelerate the calculation. This method can be used to construct an arbitrary-complex geometric structure with smooth or roughness surface.

Efficient calculation algorithms: IM3D utilizes the fast database indexing technique proposed in Corteo[78] to sample the scattering and azimuthal angles as well as a linear speed-up MPI parallel algorithm or a multi-threading parallel algorithm with improved accuracy, efficiency, and memory usage.

3. Results and discussion

For comparisons, three benchmark cases including the ion/damage depth- distributions in bulk/multi-layer targets are performed in IM3D and compared with that of TRIM code. For each case, simulations are done using the total of $10^5$ ions. In Fig. 3, Ar ions implantation into bulk silicon with a flat surface and with ion energies 10 KeV and 100 KeV was simulated using IM3D and TRIM. The resulting Gaussian type profiles of ion depth-distributions are in good agreement with that of TRIM code. The ion-depth profiles IM3D are obtained much faster computationally compared to TRIM code.

For multi-layer, Au ions depth-distribution in ZrO$_2$/Si sample, under Au ion irradiation with the energy of 2.0 MeV and normal incidence at the center point of the sample for 305.1 nm thickness are calculated. A nearly perfect agreement is obtained from TRIM code and IM3D code as shown in Fig. 5.
The results from SRIM and IM3D codes are in good agreement, but some discrepancy is found in the results. IM3D underestimates the straggling a few percent compared to TRIM at low energies. This discrepancy is due to the difference the replacement fractions because a small fraction of the displacements does not lead to vacancies but to replacement fraction. The simplified model of SRIM code cannot be expected to give accurate results because the threshold energy is set as displacement energy in SRIM manuals. Using the displacement energy as a sharp cut-off to calculate the replacement fraction leads to inaccurate results. IM3D takes binding energy as threshold energy for displacemnt events and accurate ion-depth profiles are obtained. Also, It is found in many studies that the range of ion depth-distributions calculated by SRIM code are usually shallower than that of experiments comparatively[1, 49, 52]. This leads to an overestimation of the electronic stopping powers used in SRIM, especially for low-energy heavy ions. SRIM is not open source software. The working of its algorithm for defect generation is not clearly described in both SRIM’s manual and published papers[1]. IM3D is open source distribution with high portable C. IM3D can be modified. As IM3D uses fast database indexing technique [78] or the MAGIC approximation formula [1]for sampling in terms of accuracy and efficiency, it is faster than SRIM by two or three orders of magnitude, depending on the simulation parameters.

SRIM cannot treat heterogeneities structures, such as nanostructures and roughness. effects called nano-size effect and geometric effect observed in nano-objects. TRIM code uses bulk/multi-layer options which is not useful to understand complex nanostructured materials with different shapes and components as errors are introduced when TRIM is used [33-35]. Furthermore, In case of nano-structured materials, the ion range or dimension of the collision cascades becomes comparable to the size of the nano-object itself. Due to the high surface-volume ratio of nanostructured materials, there are two special effects called nano-size effect and geometric effect observed in nano-objects. When geometric and nano-size effects are taken into consideration, more precise information could be obtained to determine primary radiation damage and distributions. Nano-geometric effect can influence the trajectory of an ion when it moves through the target. Nano-geometric effect can also affect the processes such as sputtering, and shading[34] etc. The geometric effect can significantly affect the behaviors of ion irradiation. It cannot be neglected. Thus, 3D structured geometry is needed to understand the complex nano-structured materials precisely. For this, arbitrary 3-dimensional structures are needed to study these effects. IM3D can use a set of modified parameters to account for the nano-energetic effects. IM3D can simulate arbitrary complex targets constructed by the 3D geometric algorithms of CSG/FETM methods, with complex materials including single elements (1–92), alloys and compounds.

In experiment[73], nanowires have been observed to bend under ion beam irradiation with high fluencies. The direction of the bending can be controlled by the ion species and energy, and this effect can even be used to align nanowires. To demonstrate the 3D distribution of defects, we have studied the bending of tungsten nano-wires induced by gallium ion beam irradiation using FETM method. Using IM3D, we calculated the damage distributions for sputtering W nanowire under the irradiation of Ga ions with the incident direction of 40 degrees angle and the energy of 150 keV in FC option.

![Figure 5: Comparison of IM3D results with TRIM predictions for Au ion depth - distribution in ZrO2/Si sample, under Au ion irradiation with the energy of 2.0 MeV energy.](image)
figure 6 (a) Using FETM geometric method, vacancy spatial distribution for a bent W nanowire under randomly distributed Ga ion sputter with energy of 150 keV, (b) remaining excess vacancies for a bent W nanowire under randomly distributed Ga ion sputtering with an energy of 150 keV.

Under high fluences[73–77] of ion irradiation, the tungsten nanowires have been observed to bend towards and finally align with the ion beam. Excess vacancies should remain on the side facing the ion beam while the excess interstitials remain at the back side, causing the inhomogeneous distribution of defects which in turn leads to an inhomogeneous expansion of the material. Under the irradiation of Gallium ions at finite temperature, most of the ion beam induced defects anneal out immediately, diffuse to the other side or deposit directly. Assuming annihilation of defects in each simulation cell, we computed the remaining damage using the difference value of interstitials minus vacancies in tungsten nanowire. In order to consider the final remaining damage in W nanowire, we use the difference between produced vacancies and interstitials by assuming that annihilation of defects only occurs in each cell. Under inner stress due to an inhomogeneous expansion of the nanowire, a bending momentum towards the ion beam in induced, as observed in the experiment[73]. This causes the shading of the ions on their incident path by a particle leads to a decrease of damage behind the particle also known shading/shadowing effect. This effect is seen in Fig. 6 (b). Thus, IM3D can be used to observe the bending of nanowire under ion irradiation and other cases where 3D modeling is needed.

4. Conclusions

IM3D is the most universal, robust, computationally efficient and massively parallel 3D MC code for simulating the spatial distributions of primary radiation damage and displacement in nanostructured materials under ion irradiation. Comparisons were done for bulk/multilayer simulations and it was found that results calculated using IM3D code were in good agreement with that of SRIM code. IM3D code is considerably faster than SRIM and efficient. In addition, IM3D was successfully used to explain the ion beam induced bending of nanowires. In contrast to SRIM code, IM3D allows general 3D geometric structures and can thus account for ion beam irradiation effects peculiar to nano-sized objects. SRIM has limitations in describing general 3D geometric structures for modeling radiation displacements and damage in nanostructured materials. For 3D structural geometry, IM3D provide the users with the choice of CSG/FETM library as the 3D structural description to simulate new 3D geometry-dependent effects, such as the nano-energetics effect, the nano-geometric effect, the shading effect. Furthermore, IM3D is open source and can be modified and developed further.

References

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