Technology Offer

A MONTE-CARLO CODE FOR CALCULATING COLLISION PHENOMENA IN RANDOMIZED TARGETS

Ref.-No.: 1801-6323-WT

The invention relates to a Monte-Carlo program implemented in Fortran 90. It treats the bombardment of incident ions on different target structures such as mono-atomic targets, layer structures or composition target structures. The two general cases considered in the code are the static case, where the target composition is fixed during the simulation, and the dynamic case, where modifications of the target caused by the ion bombardment are taken into account.
A further development of the program also for rough surfaces are SDTrimSP-2D and SDTrimSP-3D. These programs are a 2D and a 3D extension of SDTrimSP.
The changes of the rough surface due to bombardment can be calculated. It uses a 2D/3D mesh of cuboids and cubes (voxels) to represent the surface morphology. The composition and atomic density of each voxel can be chosen independently, which also allows the representation of internal voids. Depending on the surface morphologies reductions of the effective sputter yields to less than 25% have been observed in the simulation results.

Advantages

- More detailed information such as depth or energy distributions
- Can deal with amorphous targets
- Time dependencies of collision cascades can be chosen
- All possible output facilities
- Static or dynamic
- More flexible output, higher portability
- Runs on all sequential and parallel platforms with a Fortran90 compiler

Applications

Collisional calculations of:

- Implantations
- Backscattering
- Transmission
- Sputtering
- Composition changes by ion bombardment

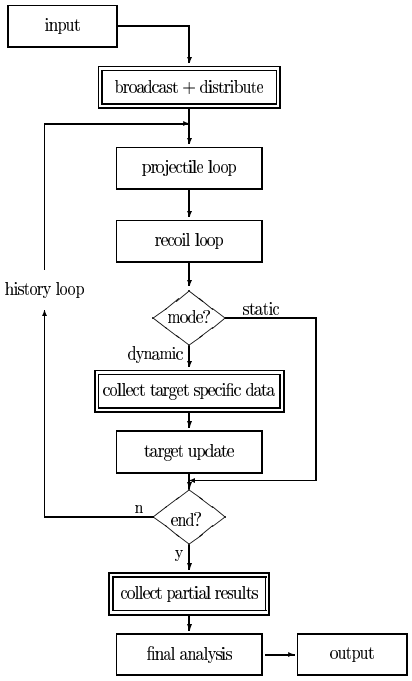

Fig. 1

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Background

In the last 40 years, many computer simulation programs have been developed to describe the interactions of ions bombarding solid, liquid and gaseous targets.
Many of these programs were based on a binary-collision approximation dealing with crystalline and amorphous targets, such as the static Monte-Carlo program TRIM and the corresponding dynamic version TRIDYN. The description of collision effects in solids and the approach to specific physical problems with these programs were of such a success, that the idea to combine both programs into SDTrimSP (where S stands for static and D for dynamic) seemed natural.

Technology

Remarkably, the new program has all possible output facilities used in the past such as sputtering, backscattering or transmission, but still provides a new modular structure achieving a more flexible output.
SDTrimSP is a program, which assumes an amorphous target structure at zero temperature and infinite lateral size. The binary collision approximation is used to handle the atomic collisions. This means, that the change in flight direction due to the collision is given by the asymptotes of the real trajectory. For this evaluation an interaction potential has to be chosen so that the scattering angle of the moving atom can be determined and the energy gain of the recoil can be calculated. In addition, a moving atom looses energy to target electrons, which can also be considered by the program as simultaneous weak collisions. Both incident ions and recoil atoms are treated as a series of subsequent collisions. For each traced atom the important physical quantities such as energy, spatial coordinates or direction of motion are recorded along its path using general data structures. In order to save memory, there are some quantities integrated over all projectiles.
Most data needed for the calculation is taken from a database in form of tables, such as atomic numbers and masses of elements, densities of solid and liquid elements or surface binding energies. The structure of the program is depicted in Fig. 1. In the projectile loop, groups of projectiles are followed and the recoils generated along the trajectories of the incident ions are collected and treated in a separate recoil loop. In case of the dynamic mode, the target is updated after finishing the calculations of the projectiles and the generated recoils, which is not necessary in the static case. Afterwards it can be continued with the next group of projectiles and so forth until finally, the output section is entered. The general output gives the reflection and sputtering coefficients, atomic fractions and densities as a function of depth and the yield versus the generation. In the dynamic case, the change of target thickness and atomic fractions and densities as a function of fluence is given. This minimal output has a size of some kBytes only. Optionally, the output may concern trajectory information, particle information or matrices with frequency distributions.

License

Campus License for 5 and more users SDTrimSP 1D (Version 7.0):	2.000 EUR
Campus License for 5 and more users SDTrimSP 2D (Version 3.00):	2.000 EUR
Campus License for 5 and more users SDTrimSP 3D (Version 1.22):	2.000 EUR
Campus License for Package SDTrimSP 1D + 2D or 3D:	3.000 EUR
Campus License for Package SDTrimSP 1D + 2D + 3D:	4.000 EUR

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Literature

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Reportnr.: IPP 2024-06
doi:10.17617/2.3577532.
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Reportnr.: IPP 12/11
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