

From Source to Substrate: Monte Carlo Simulation of Particle Transport during Magnetron Sputtering

State of the Art

The DRAFT research group (Department of Solid State Sciences, Ghent University) investigates the growth of thin films by (reactive) magnetron sputtering. Thin-film growth is governed the arrival of material, energy, and momentum at the substrate. The material flux consists of film-forming species, such as sputtered atoms and reactive gas molecules, as well as energetic neutral gas atoms. The arrival rate of each species, along with their energy and incidence angle can strongly influence the resulting film microstructure and texture.

Directly measuring these properties is extremely challenging. Consequently, most researchers rely on simulation tools to obtain detailed information on the transport processes involved. These models describe the trajectories of atoms from the source to the substrate, during which collisions with working gas atoms may occur. An accurate description of these collisions is therefore a key component of such simulations.

To address this challenge, the research group has developed a test-particle Monte Carlo code called **SiMTRA**. The software is widely used within the thin-film research community and is downloaded several times each week. It combines an accurate physical description of particle transport with a user-friendly graphical interface.

Project Goals

The PhD project has two major objectives: (i) extending the code to describe more complex physical phenomena and (ii) further developing the graphical interface and automation capabilities of the software.

• Physics Development

At present, the code is limited to the interaction of energetic atoms with a single type of working gas atom. A first work package will, therefore, focus on implementing and studying transport processes in inert gas mixtures. This work package may subsequently be complemented by experimental validation.

Currently, the code models collisions using spherical interaction potentials. This approach excludes the simulation of reactive gas atmospheres containing molecules such as nitrogen or oxygen. Implementing these interactions is a second package and will require an in-depth study of molecular interaction potentials and their numerical implementation.

A further extension of the code will involve the simulation of multiple magnetron sources. Owing to potential interactions between the sources, this third work package is considerably more complex than simply replicating the existing single-source implementation.

The project is sufficient flexible to adjust its content based on own input of the PhD student.

• Software Development

The current version of the code is based on a combination of Visual Basic and C++. Migrating the software to a more modern framework will be one of the first objectives of the project.

In addition, the functionality for importing energy and angular distribution data from third-party software packages will be further improved. To increase the flexibility and applicability of the code, additional surface definitions will be implemented. Furthermore, a physical description of the target will be incorporated to facilitate simulations that require modelling of target erosion effects.

Candidate Profile

We are looking for a highly motivated Master's student with a background in Physics, Engineering Physics, or a related engineering discipline, and a strong interest in modelling and simulation. You have achieved good to excellent academic results and possess solid programming experience in C++. Experience limited to scripting languages, such as Python, is not sufficient for this project.

You are also willing to contribute, to a limited extent, to the teaching and social activities of the department.

What We Offer

You will receive daily guidance and support and become part of a dynamic research environment with a strong interest in solid-state physics and thin-film science. The position offers opportunities to attend national and international conferences and to collaborate with leading research groups worldwide.

The appointment consists of an initial one-year contract, which can be extended for an additional three years upon positive evaluation. Successful completion of the project will lead to the degree of *Doctor of Science: Physics and Astronomy (PhD)*.

Contact

Interested? Send your application to Diederik.Depla@ugent.be.