SIMTRA: simulate your deposition profile

Abstract

The software package SIMTRA is a test particle Monte Carlo code that simulates the transport of metal atoms during magnetron sputter deposition by calculating the trajectories of sputtered particles from source to substrate. The package includes a graphical user interface which is used to create a (simplified) 3D representation of an experimental setup using predefined surface shapes and set other input parameters such as custom racetracks, initial energy and angular distributions, sputter gas, pressure, temperature and an interaction potential. Output data consists of, but is not limited to, the number of particles deposited on each surface, their deposition energy and direction of incidence.

Simulating deposition rates

A Ti target is mounted on a vertically placed lab scale rotatable magnetron. Five samples are placed horizontally in front of the target at a distance of 6 cm. The deposition rate can be calculated from SIMTRA simulations using the following formula:

\[ \text{deposition rate} = \frac{I_d \cdot e \cdot (1 + \gamma)}{r \cdot \text{flux} \cdot \text{area}} \]

Fraction of particles arriving per surface area as calculated by SIMTRA

Verification of the substrate metal flux

The angular distribution of Cu atoms arriving on a substrate was verified using a metal flux monitor (MFM) [1]. The MFM is a pinhole camera which converts the angular distribution of the arriving flux into a thickness profile on the substrate. Experiments and simulations were performed at different target - substrate distances.

Misalignment of a rotatable magnetron

The misalignment of a small lab scale rotatable was implemented by a precession of the target around the central axis of the magnetron [1]. The opening angle of the cone was 1°. During the deposition the target was rotating at 1 RPM while a substrate was moving 7 cm below the target at 0.5 m/min.

The resulting deposition profile, which is a compilation of 50 simulations corresponding to the different positions of target and substrate, shows a strong modulation of the relative thickness across the substrate.

Concusion

SIMTRA has been validated by several case studies and it is shown how the software can help with optimization of deposition setups or the prediction of film composition when multiple sources are used. This combined with an intuitive graphical user interface, the ability to construct custom setups, low computation times and free access at the DRAFT website, make SIMTRA a valuable tool for anyone active in the field of sputter deposition.

User interface

Each input file consists of 3 parts: a vacuum chamber, a magnetron object and any number of 'dummy' objects. The position and orientation of these objects can be set in the main window together with the gas element, pressure and temperature. Objects are created in the designer window and consist of predefined surfaces. Each surface is defined by its surface parameters, position and orientation with respect to the object reference frame.

A magnetron object requires additional input parameters which are set in the Target and Transport subwindow:

- Racerack specifications
- Angular distribution: custom or SRIM [1]
- Energy distribution: Thompson or SRIM
- In- or exclude gas motion and diffusion
- Interaction potential

Conclusion

Mission statement: At DRAFT we want to become the recognized leader in the understanding of thin film growth by reactive magnetron sputtering and enjoy research by experiments and simulations.