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EINLADUNG zum IFP-SEMINAR

Design of structural evolution in sputtered multicomponent layers using interactive ray tracing software

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Termin: Mittwoch, 25. Jänner 2023, 16:00 Uhr

Ort: Institut für Festkörperphysik, TU Wien
Wiedner Hauptstraße 8-10, 1040 Wien
Seminarraum DC rot 07 (roter Bereich, 7. OG)

Abstract:

Structure and crystallographic properties of multi-material thin films can be described with an interactive ray tracing software that simulates film deposition in arbitrary sputtering geometries, the so-called Virtual Machine (VM). Although based on a line-of-sight model, the VM also takes into account the decay of the flux density of the particles due to gas phase scattering. To further enhance the prediction capabilities of the VM a microstructure simulation package, based on rate equations and on the Potts Modell, was built.

At the machine level the VM recreates a real combinatorial DC-sputter plant from 3D models including the static arrangement of multiple targets, the substrate and eventual obstacles, as well as dynamics like e. g. rotating substrate holders. For the deposition process, individual sample points can be defined on the substrate to which the line-of-sight model is applied, taking kinematics into account. The resulting thickness and sequence of the layers is used to visualize the thickness-resolved composition. Post-processing the time dependent thickness and temperature data the crystallographic phases with their associated XRD patterns are calculated from a library of binary phase diagrams for the simulated film.

Applying the rate-equation model to a generated layer architecture the microstructure can be calculated. First it is decided whether Frank-van-der-Merwe (continuous layer) or Volmer-Weber growth (island layer) occurs. The distribution of islands follows a thermodynamic equilibrium approach, which considers the process of island formation while minimizing the free energy of the island surface. The crystallite structure of the matrix material surrounding the islands is calculated by a spatially scaled Potts Modell. The Monte Carlo simulator is initialized with a crystallite structure generated using the Voronoi construction of the crystallite density determined from empirical data using rate equations. Since volume diffusion is not yet considered, only immiscible multilayer systems can be investigated at present. On the basis of examples, the above-mentioned comparisons are presented.

Acknowledgments

This project has received funding from the Clean Sky 2 Joint Undertaking under the European Union's Horizon 2020 research and innovation program under Grant No 785414