DS 16: Thermoelectric and Phase Change Materials; Layer Deposition

Time: Thursday 11:30–13:00 Location: SCH A 315

DS 16.1 Thu 11:30 SCH A 315

A Multiscale Simulation Method for Deposition Processes: Micrometer-scale Off-Lattice Film Growth with Atomistic Precision — •Erik E. Lorenz[1] and Jörg Schuster[2,1] — [1]Center for Mikrotechnologies, Chemnitz University of Technology, Chemnitz, Germany — [2]Fraunhofer Institute for Electronic Nano Systems ENAS, Chemnitz, Germany

We present a multiscale method for the simulation of thin film deposition processes such as PVD, CVD and ALD. By combining Kinetic Monte Carlo (KMC) methods for adsorption event sampling and Molecular Dynamics (MD) for adsorption simulation and nanostructure relaxation with a graph-based triangulating bulk-surface representation, fast and efficient highly-parallel surface growth simulations are facilitated.

The enhancement of KMC-MD coupling with a graph-based bulk-surface representation enables efficient subdomain decompositions, bulk KMC event insertions and removals, and the robust and constant-time update of connected subdomain. Using the same graph structure, the effects of further computational improvements such as incident particle ray tracing, surface diffusion and limited KMC time warping are shown.

We demonstrate the growth of atomistic copper seed layers on a Tantalum substrate for micrometer-scale electronic devices in parallelized simulation runs saturating over 1000 CPU cores, and compare it to established methods.

DS 16.2 Thu 11:45 SCH A 315

Characterization and optimization of MgZnO thin films with steep lateral composition gradient — •Laurenz Thyen, Max Kneiss, Holger von Wenckstern, and Marius Grundmann — Universität Leipzig, Felix-Bloch-Institut für Festkörperphysik, Linnéstraße 5, 04103 Leipzig, Germany

The materials magnesium- and zinc-oxide have been widely investigated in the past. Corresponding step graded ternary alloy thin films of $Mg_xZn_{1-x}O$ have been of great interest [1]. Pulsed laser deposition (PLD) has been used to grow laterally and vertically graded thin films [2]. The precise control of chemical composition is of great importance for possible applications. Additionally, in the course of miniaturization of electrical devices like wavelength-selective multi-channel UV photodetectors, a well-defined steep slope of the material gradient will be beneficial [3,4].

In this contribution the properties of $Mg_xZn_{1-x}O$ thin films with lateral compositional gradient grown by pulsed laser deposition will be discussed. In order to obtain information about the material composition of the thin films, energy-dispersed X-ray spectroscopy, spatially resolved ellipsometry and micro-photoluminescence spectroscopy measurements have been conducted. Moreover, steep lateral gradients with a slope of up to 20 % Mg/mm were realised.

[1] Z. Zhang, *et al.* IEEE Journal Quantum Elec, 20.6, 106-111, (2014)
[2] H. v. Wenckstern, *et al.* physica status solidi (b) 257.7 (2020)
[3] M. Grundmann, IEEE Transact. Elec. Dev. 66.1 (2018): 470-477
[4] M. Kneiß, *et al.* ACS Combinatorial Science 20.11 (2018): 643-652.

DS 16.3 Thu 12:00 SCH A 315

Physical properties of $Ni_xCu_{1-x}I$ thin films deposited by magnetron co-sputtering — •Christiane Dethloff, Sofie Vogt, Daniel Splith, Holger von Wenckstern, and Marius Grundmann — Felix-Bloch-Institut, Universität Leipzig, Deutschland

The highly conductive, p-type semiconductor CuI is subject to various doping approaches to tailor optical and electrical properties [1-4]. As recently shown [5], doping CuI with Ni reduces its high hole density of up to 2×10^{19} cm^{-3} [4]. After surpassing a threshold of 15 % Ni content, a carrier conversion, as observed by Annadi *et al.*, turns the $Ni_xCu_{1-x}I$ alloy into an n-type semiconductor, which predestines $Ni_xCu_{1-x}I$ to fabricate p-n-homojunctions.

We present our investigations regarding morphology, electrical and possible ferromagnetic properties of $Ni_xCu_{1-x}I$ thin films with varying Ni contents. The deposition was conducted by reactive magnetron co-sputtering of metallic Cu and Ni in an iodine and argon athmosphere. X-ray and scanning electron microscope as well as Hall-effect and conductivity measurements were used to investigate the thin films. First measurements yielded a low resistivity of 5×10^{-3} Ωm for x=0.035.

[1]T. Jun *et al.*, Advanced materials 2018 30, e1706573
[2]H. Wu *et al.*, Appl. Phys. Lett. 2021 118, 222107
[3]P. Storm *et al.*, Phys. Status Solidi RRL. 2021 15, 2100214
[4]A. Annadi *et al.*, Applied Materials Today. 2020 20, 100703
[5]A. Annadi *et al.*, ACS applied materials & interfaces. 2020 12, 6048

DS 16.4 Thu 12:15 SCH A 315

Self-assembled droplet etching during semiconductor epitaxy for versatile quantum structures — •Christian Heyn, Ahmed Alshaikh, and Robert Blick — Center for Hybrid Nanostructures (CHyN), University of Hamburg

As a fundamental extension of conventional epitaxy, we describe the integration of self-assembled top-down strategies into the bottom-up molecular beam epitaxy (MBE) of semiconductor quantum structures (QS). The samples are fabricated using standard solid-source MBE without any additional equipment. Ga, Al, or In droplets are formed on a GaAs or AlGaAs surface driven by the minimization of surface and interface energies in Volmer-Weber mode. The metal droplets drill self-assembled nanoholes into the semiconductor surface which is called local droplet etching (LDE). Afterwards, the nanoholes are filled with a material different from the substrate for the generation of QS. This presentation discusses the general mechanism of LDE, the influence of the process parameters on the density, size, and shape of the resulting nanoholes, as well as an intermixing with substrate material. For LDE with Ga droplets on AlGaAs, a crystalline wall formed around a nanohole represents a GaAs quantum ring. Further strain-free QS are created by filling of nanoholes drilled using Al droplets in AlGaAs with GaAs. The size and shape of the resulting QS is controlled by the initial nanohole, the amount of deposited material for hole filling, and capillary. Examples are QS that are shaped like the shell of a cone and vertically coupled quantum dot molecules.

DS 16.5 Thu 12:30 SCH A 315

Interplay of Glass Dynamics and Crystallization Kinetics of Photonic Phase Change Materials Sb2S3 & Sb2Se3 — •Felix Hoff[1], Julian Pries[1], Maximilian J. Müller[1], Eric N. Lensker[1], and Matthias Wuttig[1,2,3] — [1]I. Institute of Physics (IA), RWTH Aachen University — [2]Jülich-Aachen Research Alliance (JARA FIT and JARA HPC) — [3]PGI 10 (Green IT), Forschungszentrum Jülich GmbH

Due to their large bandgaps, the chalcogenide phase-change materials (PCM) antimony sulfide Sb2S3 and antimony selenide Sb2Se3 are interesting for photonic applications in the visible and telecommunication wavelength range. They are promising for photonic integrated circuits or tunable metasurfaces. While recent literature focuses on the optical properties and the resulting applications, a systematic quantification of the amorphous glass phase, as well as its influence on the process of crystallization under different conditions, is missing. In this work, both the standard glass transition and fragility of antimony sulfide are presented and discussed. Sb2S3 is found to crystallize from the undercooled liquid phase for all technologically relevant heating rates spanning over six orders of magnitude. In contrast, Sb2Se3 appears to show a glass transition only for higher heating rates. This can be used to explain the unusual temperature dependence of its crystallization mechanism in thin films.

DS 16.6 Thu 12:45 SCH A 315

Seebeck coefficient inversion in highly doped organic semiconductors — •Morteza Shokrani[1], Kai Xu[2], Tero-Petri Ruoko[2], Dorothea Scheunemann[1], Hassan Abdalla[2], Hengda Sun[2], Chi-Yuan Yang[2], Yuttapoom Puttisong[2], Nagesh Kolhe[3], José Silvestre Mendoza Figueroa[2], Jonas Pedersen[2], Thomas Ederth[2], Weimin Chen[2], Magnus Berggren[2], Samson Jenekhe[3], Daniele Fazzi[4], Martijn Kemerink[1,2], and Simone Fabiano[2] — [1]Heidelberg University, Germany — [2]Linköping University, Sweden — [3]University of Washington, USA — [4]University of Cologne, Germany

The investigation of the thermoelectric properties of organic semiconductors (OSC) with the aim of increasing their efficiency as active material in thermoelectric generators has attracted attention for the past years. The maximum efficiency of the energy conversion process in a

thermoelectric material is set by zT, which is proportional to electrical conductivity and Seebeck coefficient (S) squared. A common way of increasing zT is by doping, which typically increases the charge carrier density and electrical conductivity, while decreasing S. The sign of S is often used to determine the polarity of the majority charge carriers in OSC. In recent years, a surprising change in the sign of S has sometimes been observed to occur in highly doped OSC. Here, by combining conductivity and S measurements with kinetic Monte Carlo simulations, it is shown that density of state filling in combination with the opening of a hard Coulomb gap around the Fermi energy is responsible for the sign inversion