

EINLADUNG

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HABILITATIONSVORTRAG

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"Analytical validation of variational models for epitaxially-strained thin films"

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<u>Abstract:</u> The focus of the talk is the introduction and validation of some variational models for epitaxy, i.e., the deposition and growth of crystalline films on substrates. During the epitaxial growth of supported nanostructures, multi-scale phenomena take place and the microscopic morphology strongly impacts the material macroscopic properties. Special emphasis is given to the situation of heteroepitaxy, namely when the film and the substrate consist of different materials whose optimal lattices at equilibrium present a mismatch. Such lattice mismatch induces large stresses in the thin film with the consequence of generating corrugations and instabilities on the film profile that have a cost in terms of the surface energy.

The models under investigation take into account the competing mechanisms responsible for the film shape by displaying both a regularizing surface energy and an elastic energy with a roughening effect on the film profile. We begin by deriving the models by relaxation and Gamma-convergence from literature models, and by means of a rigorous discrete-to-continuum passage starting from newly introduced atomistic models. The regularity of energy-minimal films is then studied by establishing the internal-ball condition and by proving geometrical rules for the wetting angle formed by film profiles when touching the substrate. In particular, the Young-Dupré law holds for rigid substrates, yielding what appears to be the first analytical validation of such law in the context of continuum mechanics.

Finally, we discuss the generalization to the setting of Stress-Driven Rearrangement Instabilities (SDRI) in order to move away from graph-like assumptions on the film profiles and to include in the analysis the possibility of delamination and debonding at the film/substrate interface.

> Donnerstag, 28. November 2019 10:30 Uhr – 11:15 Uhr

> > Fakultät für Mathematik Oskar-Morgenstern-Platz 1 SR 06, 1 OG.

Michael Kunzinger Christian Krattenthaler