ISNM
International Series of Numerical Mathematics
Vol. 149

Multiscale Modeling in Epitaxial Growth

Edited by
Axel Voigt

Birkhäuser Verlag
Basel · Boston · Berlin

Editor:

Axel Voigt
research center caesar
Crystal Growth Group
Ludwig-Erhard-Allee 2
D-53175 Bonn
Germany

2000 Mathematics Subject Classification 35R35, 80A22, 82B80

A CIP catalogue record for this book is available from the Library of Congress, Washington D.C., USA

Bibliographic information published by Die Deutsche Bibliothek
Die Deutsche Bibliothek lists this publication in the Deutsche Nationalbibliografie; detailed bibliographic data is available in the Internet at http://dnb.ddb.de.

ISBN 3-7643-7208-7 Birkhäuser Verlag, Basel – Boston – Berlin

The cover picture shows the adatom density on a submonolayer, the finite element solution of the Burton-Cabrera-Frank equation.

Part of Springer Science+Business Media
Printed on acid-free paper produced of chlorine-free pulp. TCF ∞
Printed in Germany
ISBN-10: 3-7643-7208-7
ISBN-13: 978-3-7643-7208-8
9 8 7 6 5 4 3 2 1 www.birkhauser.ch

Multiscale Modeling in Epitaxial Growth

Mini-Workshop at Mathematisches
Forschungsinstitut Oberwolfach
January 18–24, 2004

ISNM 149
ISBN 3-7643-7208-7

Edited by

A. Voigt

Editors:

Axel Voigt
Crystal Growth group
research center caesar
Ludwig-Erhard-Allee 2
D-53175 Bonn
Germany

Contents

Preface

Thin film growth by molecular beam epitaxy (MBE) is a modern technology of growing single crystals that inherit atomic structures from substrates. It is technologically relevant, experimentally well explored and a very active area of theoretical research. Modeling of epitaxial growth is a challenging multi-scale problem. Given the fact that the macroscopic evolution of the growing film is directly related to movements of adatoms on surfaces and their various bonding configurations, it is appealing to use atomic scale simulations for a theoretical description of epitaxial growth. However in order to reach the length and time scales of interest for various applications continuum models have to be used. Today a hierarchy of models has been investigated to describe epitaxial growth: From fully atomistic models, via semi-discrete step flow models to continuum models for the height of the growing film. The main challenge in modeling epitaxial growth is to bridge the gap between these different models and to describe growth process on a continuous scale by incorporating atomistic effects. With the advent of powerful numerical techniques for the solution of such models combined with a deep understanding of the physical and chemical phenomena during the growth process this goal might be achieved in the near future.

The goal of the book is to summarize recent developments in modeling epitaxial growth, with emphasis on multi-scale approaches and numerical methods. The book provides a compact overview and can serve as an introduction for applied mathematicians, theoretical physicists and computational materials scientists into this highly active interdisciplinary field of research.

The book results from a workshop held at the *Mathematisches Forschungsinstitut Oberwolfach* on *Multiscale Modeling in Epitaxial Growth* from January 18th to 24th 2004. This volume contains 14 refereed original papers which are subdivided into three parts corresponding to the three classes of models. Each part starts with an introductory review article.

Part 1: *Atomistic models.* The methods discussed range from first-principle methods, which determine energy pathways and barriers to diffusion and other kinetic processes; classical Molecular-Dynamics method, which are applied to study the diffusion on a crystalline surface; kinetic Monte Carlo methods, which are combined with Molecular-Dynamics to study the influence of strain on the morphology of the film and quasi-continuum Monte Carlo methods which coarse grain the atomistic picture and draw a connection to step flow models.

Part 2: *Step flow models.* At sufficiently low temperatures the surface of a crystal consists of atomic steps. These steps provide a basis for the description of the surface morphology on an intermediate mesoscopic scale, between atomistic and continuum scales. The steps are assumed to be continuous curves of zero thickness which serve as free boundaries for the adatom density on the terraces. Sharp interface and phase field methods for this class of free boundary problems are discussed. Simulations show the influence of various anisotropies on the shape of single islands, investigate instabilities in step dynamics and study homoepitaxial Ostwald ripening.

Part 3: *Continuum models.* The surface of the film is described through a partial differential equation for the evolution of the interface between film and vapor. The discrete nature of the steps is coarse grained and a smooth surface is assumed on a macroscopic scale. The derivation of such models makes use of inherent symmetries in the physical process, i.e., mass conservation and crystal symmetry, and results in nonlinear diffusion equations for the height of the growing film. Besides this heuristic derivation a computational approach to derive a continuum model from step flow models is discussed. Furthermore a more thermodynamical approach for the evolution of a surface, which is based on an anisotropic surface energy is considered and numerically solved by a level set method.

I hope that this book will contribute to the exciting ongoing discussion in the field of epitaxial growth and will encourage young researchers to join this area. I express my gratitude to the authors, to the publisher and last but not least to the *Mathematisches Forschungsinstitut Oberwolfach*.

Bonn, July 20th 2004 Axel Voigt

Part 1

Atomistic Models