Optimal Device Design

Explore the frontier of device engineering by applying optimization to nanoscience and device design. This cutting-edge work shows how robust, manufacturable designs that meet previously unobtainable system specifications can be created using a combination of modern computer power, adaptive algorithms, and realistic multi-physics models. Applying this method to nanoscience is a path to creating new devices with new functionality, and it could be the key design element contributing to transitioning nanoscience to a practical technology. Basic introductory examples along with MATLAB code are included, through to more formal and sophisticated approaches, and specific applications and designs are examined. Essential reading for researchers and engineers in electronic devices, nanoscience, materials science, applied mathematics, and applied physics.

A.F.J. Levi is Professor of Electrical Engineering and of Physics and Astronomy at the University of Southern California. He joined USC after working for 10 years at AT&T Bell Laboratories, New Jersey. Professor Levi is the author of the book *Applied Quantum Mechanics*, Second Edition (Cambridge University Press, 2006).

Stephan Haas is Professor of Theoretical Condensed Matter Physics at the University of Southern California.

Optimal Device Design

Edited by
A.F.J. LEVI and S. HAAS

CAMBRIDGE
UNIVERSITY PRESS

CAMBRIDGE
UNIVERSITY PRESS

University Printing House, Cambridge CB2 8BS, United Kingdom

One Liberty Plaza, 20th Floor, New York, NY 10006, USA

477 Williamstown Road, Port Melbourne, VIC 3207, Australia

314-321, 3rd Floor, Plot 3, Splendor Forum, Jasola District Centre, New Delhi - 110025, India

103 Penang Road, #05-06/07, Visioncrest Commercial, Singapore 238467

Cambridge University Press is part of the University of Cambridge.

It furthers the University's mission by disseminating knowledge in the pursuit of education, learning and research at the highest international levels of excellence.

www.cambridge.org
Information on this title: www.cambridge.org/9780521116602

First published 2010

A catalogue record for this publication is available from the British Library

Library of Congress Cataloging in Publication data
Optimal device design / edited by A.F.J. Levi, Stephan Haas.
p. cm.
ISBN 978-0-521-11660-2 (hardback)
1. Industrial design. 2. New products. 3. Manufacturing processes.
I. Levi, A. F. J. (Anthony Frederic John), 1959– II. Haas, Stephan.
TS171.O78 2010
658.5´752 – dc22 2009036991

ISBN 978-0-521-11660-2 Hardback

Contents

Preface

Dramatic advances in the control of physical systems at the atomic scale have provided many new ways to manufacture devices. An important question is how best to design these ultra-small complex systems. Access to vast amounts of inexpensive computing power makes it possible to accurately simulate their physical properties. Furthermore, high-performance computers allow us to explore the large number of degrees of freedom with which to construct new device configurations. This book aims to lay the groundwork for a methodology to exploit these emerging capabilities using optimal device design. By combining applied mathematics, smart computation, physical modeling, and twenty-first-century engineering and fabrication tools it is possible to find atomic and nanoscale configurations that result in components with performance characteristics that have not been achieved using other methods.

Imagine you want to design and build a novel nanoscale device. How would you go about it? A conventional starting point is to look at a macroscopic component with similar functionality, and consider ways to make it smaller. This approach has several potential pitfalls. For one, with continued reduction in size, device behavior will become quantum in character where classical concepts and models cease to be applicable. Moreover, it is limited by ad hoc designs, typically rooted in our unwillingness to consider aperiodic configurations, unless absolutely mandated by physical constraints. Most importantly this conventional approach misses the enormous opportunity of exploring the full landscape of possible system responses, offered by breaking all conceivable symmetries.

Computational resources, realistic physical models, and advanced optimization algorithms now make it possible to efficiently explore the properties of many more configurations than could be tested in a typical laboratory. This is the new paradigm: explore the most improbable, most nonintuitive, system configurations and you will likely be rewarded not only with unprecedented optimized device performance but also with new physical insights into how these small complex systems work.

Preface

This book is for those not satisfied with incremental scientific progress but instead willing to explore a vibrant and exciting new direction that acknowledges the richness inherent to small complex systems. We are particularly eager to reach and inspire an emerging generation of computer-savvy individuals who recognize the shortcomings of conventional disciplinary thinking and ad hoc engineering. As incomplete as this book may be in many respects, we wish to show a possible direction out of the science-as-usual mentality. The approach leverages computational resources and advances in controlling and manipulating nanoscale objects. It develops an analysis non-convex via optimization that we believe changes the way one thinks about physical problems.

Chapter 1 offers a statement of the set of problems considered, surveys the mathematical and computational approaches used, and discusses specific applications and designs. The following chapters explore these issues one by one in greater depth, touching on topics at the forefront of our current understanding of nanoscale devices. Of course, as we sincerely hope that this will inspire your scientific thinking and approach towards research, the final word, dear reader, is for you to write.

California S. H. and A. F. J. L.

Acknowledgements

Stephan Haas and Tony Levi are particularly grateful to Dennis Healy for unflinching encouragement and inspiration in many aspects of the research endeavor that made this book possible. They would also like to thank Alexander Balatsky for his insights into how correlated many-body systems work, Ilya Grigorenko for providing powerful computational implementation of adaptive design concepts, and Peter Littlewood for enlightening discussions of complex phenomena.

Dimitris Bertsimas and Omid Nohadani would like to thank J. Birge, F. Kärtner, and K.M. Teo for fruitful discussions and collaboration on some of the projects that are discussed in Chapter 6.