1
Introduction

1.1
Style

The style of the first edition of this book, which carries the same title as this second edition, consisted of a mixture of TEX-like equations and equations generated by *Mathematica* computational output, interwoven between each other. There were two reasons for this choice of style. The first reason is that at the time when the first edition was written, the newest version of *Mathematica* was version 2.2, which was limited in its ability to produce as an output the traditional form of equations. It was found necessary, therefore, to print most of the equations using TEX. This new edition of the book is using *Mathematica* version 5.2, whose text form is close enough to TEX to make the equations appear similar to the traditional form. The second, and more important reason for having equations printed in a combination of TEX and *Mathematica* computational output was the belief that the reader will benefit from having the code running the simulations in each chapter transparent to him. Consequently, the text was interwoven with the segments of the chapter's code, making it easy to modify each segment "on the run."

After 6 years of using this book as both a research and a teaching resource, it became apparent that the code and the text should be completely separated. There were two reasons for the need of this separation. The first reason stems from the fact that expertise in both *Mathematica* and scanning probe microcopy (SPM) is not as prevalent among the SPM community as originally thought. The second and more important reason for the need of this separation is based on the fact that the styles required for coding and composing text are very different. It is much easier to compose the code that runs a chapter without having to pay attention to the demands required by composing a text. In contrast, it is much easier to compose the text without having to be limited by the shortcomings of the style of the *Mathematica* computational output.

This second edition of the book has 20 chapters, each of which consists of three components. The first component, titled *Mathematica* Preparation, is a code that is common to all the chapters in this book. This code, as will be described in detail, is a collection of bits of information needed by the specific code belonging to all the chapters. This code is attached to the code associated with each of the chapters. The second component is the code that is specific to each chapter. This code generates the tables and figures appearing in the chapters using typical parameters. These parameters can be changed within a reasonable range, generating new tables and figures. Although there is no text embedded in the code, it is clear what is the function of each *Mathematica* instruction it contained when read together with its associated text. The third component consists of the printed text of the chapters of the book that contains no code at all. The equations appearing in this component are renditions of the *Mathematica* code that were rearranged to appear close to the TEX form.

By dividing each chapter into these three components, one gains several advantages that were proven time and again to be extremely useful in both research and teaching. Having the first component shared by all the chapters insures a common style to the parameters, tables, and figures. Having the code of each chapter separated from its text makes it easier to develop research ideas and test them based only on the merit of the results presented by table and figures. Following this method requires no attention to a clear presentation of computational results. After the code is developed, one can compose a code-free text with traditionally recognized equations, making the presentation of scientific arguments clear and simple.

1.2 *Mathematica* Preparation

1.2.1 General

The first step in running the code belonging to each chapter consists of **Clearing** previous computational results and turning off comments addressing usage of similar names for different routines. The code belonging to each chapter may require the use of several **Packages,** all of which will therefore be loaded. The code uses a standard notation of **Units** for numerical calculations. To facilitate algebraic solutions, we use a numerical subroutine, **NSub**, as a replacement rule for all the **Physical constants** used in the chapters. Thus, one can develop a model of a physical problem and obtain algebraic results. By using the replacement rule, the results are rendered numerically. A collection of material constants used or can be used in the code includes **Young's modulus**, E, **Poisson's ratio**, ν, **Mass density**, ρ, **Electric conductivity and resistivity**, σ_e and ρ_e, respectively, **Thermal conductivity**, κ, and **Thermal expansion**, α. To each of these the designated material name is appended. To shorten the code of the figures in the book, we use a **Plotting Style** and options that contain the most common plotting commands. These options include **General option, Option for solid lines, Option for dashed lines**, and **Simple option**. The *Mathematica* **Preparation** code is included in the code of each chapter.

1.2.2 Example

Figure 1.1 is an example of plots of three functions, $\sin x$, $\sin 2x$ and $\sin 3x$, using the option **opt1**. The code sets the minimum and maximum values of the horizontal and vertical axes, has a frame label that reads a given parameter, $a = 2.345\,6$, for example, and uses **Epilog** to have text embedded in the figure that reads a given parameter. The presented values of the parameters can also be controlled by **IntegerPart** .

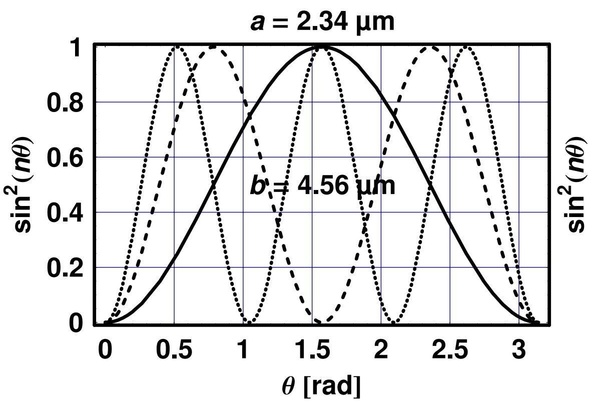

Fig. 1.1 An example of a figure using the option **opt1**.

1.3 Recommended Books

1.3.1 Mathematica Programming Language

The following is a selected list of books on the *Mathematica* programming language that can be used both as a teaching and a refresher tool.

1 Stephen Wolfram, *Mathematica, A System for Doing Mathematics by Computer*, 2nd Edition, Addison-Wesley, Reading, MA, 1991.

2 R. E. Crandall, *Mathematica for the Sciences*, Addison-Wesley, Reading, MA, 1991.

3 N. Blachman, *Mathematica: A Practical Approach*, Prentice Hall Series in Innovative Technology, Prentice Hall, Englewood Cliffs, NJ, 1992.

4 W. T. Shaw and J. Tigg, *Applied Mathematica: Getting Started, Getting It Done*, Addison-Wesley, Reading, MA, 1994.

5 S. Kaufmann, *Mathematica as a Tool: An Introduction with Practical Examples*, Birkhauser, Basel, 1994.

6 T. B. Bahder, *Mathematica for Scientists and Engineers*, Addison-Wesley, Reading, MA, 1995.

7 P. P. Tam, *A Physicist's Guide to Mathematica*, Academic Press, New York, 1997.

8 B. F. Torrence and E. A. Torrence, *The Student's Introduction to Mathematica: A Handbook for Precalculus, Calculus, and Linear Algebra,* Cambridge University Press, Cambridge, 1999.

9 S. Wagon, *Mathematica in Action*, Springer, Telos, 2000.

10 M. H. Hoft and H. F. W. Hoft, *Computing with Mathematica*, Academic Press, New York, 2002.

11 S. Wolfram, *Mathematica Book*, 5th Edition, Cambridge University Press, Cambridge, 2003.

12 C. -K. Cheung, et al., *Getting Started with Mathematica*, 2nd Edition, Wiley, New York, 2003.

13 G. Baumann, *Mathematica for Theoretical Physics: Classical Mechanics and Nonlinear Dynamics*, Springer, New York, 2005.

14 M. Trott, *The Mathematica Guidebook for Programming*, Springer, Berlin, 2004.

1.3.2 Scanning Probe Microscopies

The literature on scanning probe microscopies, which grew almost exponentially in the past decade, includes papers, review articles, and books. Of these we selected a list of those books that cover the topics dealt with in this book.

1 R. J. Behm, N. Garcia, and H. Rohrer, eds., *Scanning Tunneling Microscopy and Related Methods*, NATO ASI Series E 184, Kluwer, Dordrecht, 1990.

2 D. Sarid, *Scanning Force Microscopy with Applications to Electric, Magnetic, and Atomic Forces*, Oxford University Press, New York, 1991.

3 H.-J. Guntherodt and R. Wiesendanger, eds., *Scanning Tunneling Microscopy I*, Springer Series in Surface Sciences 20, Springer, New York, 1992.

4 R. Wiesendanger and H. J. Guntherodt, eds., *Scanning Tunneling Microscopy II*, Springer Series in Surface Sciences 28, Springer, New York, 1992.

5 R. Wiesendanger and H. J. Guntherodt, eds., *Scanning Tunneling Microscopy III*, Springer Series in Surface Sciences 29, Springer, New York, 1993.

6 Ph. Avouris, ed., *Atomic and Nanometer-Scale Modification of Materials: Fundamentals and Applications*, NATO ASI Series E 239, Kluwer, Dordrecht, 1993.

7 C. Julian Chen, *Introduction to Scanning Tunneling Microscopy*, Oxford University Press, New York, 1993.

8 D. W. Pohl and D. Courjon, eds., *Near Field Optics*, NATO ASI Series E 242, Kluwer, Dordrecht, 1993.

9 D. Sarid, *Scanning Force Microscopy with Applications to Electric, Magnetic, and Atomic Forces*, Revised Edition, Oxford University Press, New York, 1994.

10 R. Wiesendanger, *Scanning Probe Microscopy and Spectroscopy, Methods and Application*, Cambridge University Press, Cambridge, 1994.

11 Y. Martin, ed., *Scanning Probe Microscopes, Design and Applications*, SPIE Milestone Series, Volume MS 107, 1995.

12 M. A. Paesler and P. J. Moyer, *Near-Field Optics*, Wiley, New York, 1996.

13 S. N. Magonov and M.H. Whangbo, *Surface Analysis with STM and AFM, Experimental and Theoretical Aspects of Image Analysis*, VCH, New York, 1996.

14 D. Sarid, *Exploring Scanning Probe Microscopy with Mathematica*, Wiley, NY, 1997.

15 C. Bai, *Scanning Tunneling Microscopy and Its Applications*, New York, Springer, 2000.

16 S. Morita, R. Wiesendanger, and E. Meyer, *Noncontact Atomic Force Microscopy*, Springer, New York, 2002.

17 Ernst Meyer, Hans J. Hug, and Roland Bennewitz, *Scanning Probe Microscopy: The Lab on a Tip*, Springer, New York, 2004.