

*Advanced Computing  
in Electron Microscopy*

# *Advanced Computing in Electron Microscopy*

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The files are organized into the following directories: [1] win32exe; [2] macPPC; [3] mfiles; [4] csource. For details on using the CD-ROM, please refer to Chapter 8.

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# Preface

Image simulation has become a common tool in HREM (High Resolution Electron Microscopy) in recent years. However, the literature on the subject is scattered among many different journals and conference proceedings that have occurred in the last two or three decades. It is difficult for beginners to get started in this field. The principle method of image simulation has come to be known as simply *the multislice method*. This book attempts to bring the diverse information on image simulation together into one place and to provide a background on how to use the multislice method to simulate high resolution images in both conventional and scanning transmission electron microscopy. The main goals of image simulation include understanding the microscope and interpreting high resolution information in the recorded micrographs. This book contains sections on the theory of image formation and simulation as well as a more practical introduction on how to use the multislice method on real specimens. Also included with this book is a CD-ROM with working programs to perform image simulation. The source code as well as the executable code for IBM-PC and Apple Macintosh computers is included. Although the programs may not have a very elegant user interface by today's standards (simple command line dialog), the source code should be very portable to a variety of different computers. It has been compiled and run on Mac's, PC's and several different types of UNIX computers.

This book is intended to be at the level of first year graduate students or advanced undergraduates in physics or engineering with an interest in electron microscopy. It assumes a familiarity with quantum mechanics, Fourier transforms and diffraction, some simple optics and basic computer skills (although not necessarily programming skills) at the advanced undergraduate level. Prior experience with electron microscopy is also helpful. The material covered should be useful to students learning the material for the first time as well as to experienced researchers in the field. The programs provided on the CD can be used as a black-box without understanding the underlying programs (with a primary goal of understanding the transmission electron microscope image) or the source code can be used to understand how to write your own version of the simulation programs.

Although an effort was made to include references to most of the appropriate publications on this subject, there are undoubtedly some that were omitted. I apologize in advance for leaving out some undoubtedly outstanding references. I also apologize for the as yet undiscovered errors that remain in the text.

I wish to acknowledge the support of various funding agencies (principally DOE, NSF and NIH) that have supported my research efforts over the past several decades. My

research experience has substantially contributed to my understanding of the material covered in this book.

I also wish to thank Dr. David A. Muller and Dr. Richard R. Vanfleet for providing many helpful suggestions and help in proof reading the manuscript and to thank Dr. M. A. O'Keefe for providing helpful comments on electron microscopy and image simulation.

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