



# X-Ray Metrology in Semiconductor Manufacturing

D. Keith Bowen  
Brian K. Tanner



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## *Preface*

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Semiconductor manufacturing technology in recent years has evolved to the point at which traditional metrologies, largely based upon optical techniques, are no longer adequate for process development or product monitoring. Thin films in current manufacturing processes may be less than 1 nm in thickness. Measuring these with a tool whose probing wavelength is several hundred nanometers is akin to measuring the thickness of a pencil line with a yardstick. X-rays, with their wavelengths around 0.1 nm, are clearly appropriate. Moreover, the constants that describe their interaction with materials are "Goldilocks" values, just right for the requirement. X-ray metrology (XRM) is now being rapidly adopted in manufacturing industry for semiconductor, magnetic, and other advanced thin-film materials.

This book is about wafer metrology for the semiconductor industry by x-ray methods. Its scope includes the highly accurate and traceable interferometric methods of diffraction and specular reflectivity, the methods of diffuse scatter that require detailed modeling but provide unique insights into film structure, and the simpler intensity methods, such as x-ray fluorescence, which require calibration but give valuable complementary information about material composition and mass density.

The metrologies that ensue are appropriate for measuring film thickness, composition, strain and its relaxation, crystallinity, mosaic spread, surface and interface roughness, and porosity and pore size. The techniques that have evolved include x-ray reflectivity (both specular and diffuse), high-resolution x-ray diffraction, diffraction imaging and interferometry, and fluorescence. The scope of this book is their application to measuring these parameters repeatably, accurately, and rapidly on development and production wafers.

Part 1 of the book, "The Applications," is intended to answer the following questions: Can I use x-rays to measure this parameter in my wafers? What are the limits of measurement? The key elements of the techniques are given by means of inset boxes in this part, which is organized by the parameters to be measured rather than by technique.

Part 2 of the book, "The Science," discusses the techniques and the basic theory underlying each. This is intended for the more specialized engineer or tool owner who wants to see whether a particular technique is well established in theory or is more speculative, or wants to discover whether it can be pushed to solve new materials problems. The theory is described and assessed, but detailed derivations are not given, since they are readily available in earlier publications.

Part 3 of the book, "The Technology," deals with the practical implementation of x-ray metrology. First, the technique of automated data analysis and modeling is covered, followed by the instrumentation fundamentals for the various techniques. Topics such as x-ray optics are discussed in terms of their contribution and potential to solve metrological problems, such as sufficient intensity in a small spot, rather than in academic detail. The concluding chapter covers the essential metrological questions of precision and repeatability, absolute accuracy, spot size, and throughput for each type of measurement.

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## *Acknowledgments*

It is a pleasure to acknowledge the assistance we have had from many colleagues in the preparation of this book.

We first thank those colleagues, and their publishers, who have given us permission to use their published figures and data. These are acknowledged individually in the figure captions.

This book contains a great number of previously unpublished figures from colleagues at Bede X-ray Metrology and we warmly thank those colleagues who have taken the data and prepared the figures and tables. We also owe them thanks for innumerable technical and scientific discussions over the years, which have greatly contributed to our own understanding of x-ray metrology. These are: Matthew Wormington, in particular, for figures and discussions on porosity, x-ray reflectivity and diffuse scatter, genetic algorithms, and data fitting; Paul Ryan, in particular, for figures, tables, and discussions on repeatability and reproducibility, SiGe diffraction, and x-ray fluorescence; Kevin Matney for many discussions and figures and, in particular, those on reciprocal space mapping and texture analysis; Tamzin Lafford for many discussions and figures on experimental measurements on x-ray diffraction and reflectivity throughout the book; Petra Feichtinger, for the discussions and all the experimental figures on x-ray diffraction imaging; David Joyce, for figures on x-ray reflectivity; Richard Bytheway for figures on x-ray fluorescence; and Ladislav Pina, Neil Loxley, and John Wall, for discussions and figures on x-ray sources and optics.

We likewise thank colleagues from the University of Durham for their similar cooperation, assistance, and discussions. They are: Dr. Tom Hase, who has been pivotal in the Durham high resolution scattering group for many years; Prof. Peter Hatton, whose individual approach to x-ray scattering is always stimulating; Drs. Ian Pape, Brian Fulthorpe, Andrea Li-Bassi, James Buchanan, Stuart Wilkins, Amir Rozatian, and Alex Pym and other research students who have borne the brunt of much experimental data collection.

We also thank Petra Feichtinger, David Joyce, Tamzin Lafford, Paul Ryan, and Matthew Wormington for reviewing the entire book and making critical comments on the manuscript. Their comments were invaluable. Needless to say, any errors are the responsibility of the authors.

Many customers of Bede X-ray Metrology allowed us to use data from their development samples. We may not name them individually but here we express our gratitude, since this enabled us to provide information on x-ray metrology in the most advanced materials.

We wish to thank the Directors of Bede plc for permission to publish this book and in particular Dr. Neil Loxley, CEO, for every encouragement and cooperation in its writing and preparation.

Finally, we thank Nora Konopka and the editing and publication team at Taylor & Francis for their encouragement, cooperation, and skill in the production of this book.



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## *About the Authors*

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**Professor Keith Bowen, F.R.Eng., F.R.S.,** obtained his M.A. and D.Phil. in metallurgy at Oxford University, working on mechanical properties of metals. He then held academic positions at Warwick University from 1968 onward, culminating in his appointment as professor of engineering and director of the Center for Nanotechnology and Microengineering, which he held until 1997. He has held visiting professorships at Massachusetts Institute of Technology, University of Paris, and University of Denver. He is currently emeritus professor of engineering at Warwick University and visiting professor in physics at Durham University. He has authored over 130 publications on the theory and application of x-ray characterization techniques, theory of dislocations, x-ray interferometry, and ultraprecision engineering, including the book *High-Resolution X-Ray Diffraction and Topography* with Professor Brian Tanner. He joined Bede Scientific part-time in 1983, was engineering director from 1984 to 2000, was president of Bede Scientific, Inc. from 1995 to 2002, and was group director of technology from the flotation of Bede plc in 2000 until he retired in 2005. During this period he was responsible for the strategic development of science and technology in the Bede plc group of companies, for the development of the industry's first fully automated x-ray metrology tools, and for numerous inventions in x-ray technology, including the BedeScan™ method of digital x-ray diffraction imaging. Professor Bowen is a fellow of the Royal Society, fellow of the Royal Academy of Engineering, fellow of the Institute of Physics, and fellow of the Institute of Materials, Minerals and Mining.

**Professor Brian Tanner** moved to Durham in 1973 as a university lecturer, after holding a junior research fellowship at Linacre College, Oxford. Promoted to senior lecturer in 1983, reader in 1986, and professor in 1990, he served as head of the Physics Department from 1996 to 1999. From 1999 to 2000 he held a Sir James Knott Foundation Fellowship, and from 2000 to 2001 he was a Leverhulme research fellow. Since 2000, part of his time has been spent as director of the North East Centre for Scientific Enterprise. He has served on numerous research council committees and panels, and from 1998 to 2000 was chairman of a scientific review committee at the European Synchrotron Radiation Facility in Grenoble. In 1978 he co-founded a spin-off company, Bede Scientific Instruments Ltd., that floated on the London Stock Exchange in November 2000 as Bede plc. It is the largest spin-off company from the University of Durham, now employing about 150 people in the U.K., U.S., China, and Czech Republic. Professor Tanner is a non-executive director of Bede plc. He has published over 300 papers in refereed



international scientific journals, written two books, co-authored a third, and edited three more. His research interests lie in understanding the relationship between magnetic, optical, and structural properties of advanced materials, making particular use of high-resolution x-ray scattering. He is a fellow of the Institute of Physics and a fellow of the Royal Society of Arts.

Professors Bowen and Tanner have between them over 80 years experience in x-ray analysis of materials, and have collaborated for over 25 years. Both are enthusiastic amateur musicians and claim that their long collaboration in science and industry began by playing a clarinet and piano duet at the NATO ASI conference on Characterization of Crystal Growth Defects by X-Ray Methods, which they jointly organized in Durham in 1979.

In 2005, their distinction and collaboration were recognized when they jointly received the biennial C.S. Barrett Award at the Denver X-Ray Conference for "seminal contributions to the theory, instrumentation and computerized analysis of x-ray scattering and x-ray reflectivity and for unceasing efforts in teaching and popularizing these topics" from the International Committee for Diffraction Data.



Brian Tanner, pianist. Keith Bowen, clarinetist. (Photograph courtesy of Ruth Tanner.)

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## **Part 1**

# **The Applications**





# 1

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## Introduction

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### 1.1 Scope of X-ray Metrology (XRM)

This book is about wafer metrology for the semiconductor industry using x-ray methods. Its scope includes the highly accurate and traceable interferometric methods of diffraction and specular reflectivity, the methods of diffuse scatter that require detailed modeling but provide unique insights into film structure, and the simpler intensity methods, such as x-ray fluorescence, which require calibration but give valuable complementary information about material composition and mass density.

Interferometric methods work by splitting the x-ray wavefront at some discontinuity in the material and detecting the recombined component waves, normally by the intensity of scattering as a function of angle. They are analogous to optical interference, but no external optical element is required to split the wavefront; a natural feature such as an interface or a crystal plane is used. Such methods include specular x-ray reflectivity, diffuse scatter, high-resolution diffraction, x-ray topography, and x-ray interferometry. The interference of x-rays allows us to make three fundamental measurements, from which several others derive. These are *thickness*, from the interference fringes generated by rays reflected from pairs of interfaces, *strain*, and *tilt*, from the positions (and displacements) of Bragg diffraction peaks. The parameters that we can measure or infer include:

- Thickness
- Strain
- Composition
- Mosaic spread
- Lateral nanostructure dimensions, including critical dimension (CD) measurements
- Porosity