Materials Analysis by Ion Channeling

SUBMICRON CRYSTALLOGRAPHY

Leonard C. Feldman
James W. Mayer
S. Thomas Picraux

MATERIALS ANALYSIS BY ION CHANNELING

Submicron Crystallography

This page intentionally left blank

MATERIALS ANALYSIS BY ION CHANNELING

Submicron Crystallography

LEONARD C. FELDMAN
Bell Laboratories
Murray Hill, New Jersey

JAMES W. MAYER
Cornell University
Ithaca, New York

S. THOMAS PICRAUX
Sandia National Laboratories
Albuquerque, New Mexico

1982

ACADEMIC PRESS

A Subsidiary of Harcourt Brace Jovanovich, Publishers

New York London
Paris San Diego San Francisco São Paulo Sydney Tokyo Toronto

ACADEMIC PRESS, INC.
111 Fifth Avenue, New York, New York 10003

United Kingdom Edition published by
ACADEMIC PRESS, INC. (LONDON) LTD.
24/28 Oval Road, London NW1 7DX

Library of Congress Catloging in Publication Data

Feldman, Leonard C.
Materials analysis by ion channeling.

Bibliography: p.
Includes index.
1. Channeling (Physics) 2. Solids--Surfaces.
3. Crystals--Defects. 4. Ion beams.
5. Crystallography. I. Mayer, James W., Date. II. Picraux, S. T., Date.
III. Title.
QC176.8.C45F44 1982 620.1'1299 82-8723
ISBN 0-12-252680-5 AACR2

PRINTED IN THE UNITED STATES OF AMERICA

82 83 84 85 9 8 7 6 5 4 3 2 1

To Our Wives and Children

This page intentionally left blank

CONTENTS

Preface xi
Acknowledgments xv
Glossary of Symbols xvii

Introduction 1

General References 10

1. Interaction of Ion Beams with Surfaces

1.1 Introduction 12
1.2 Surface Interactions and the Formation of the Shadow Cone 13
1.3 Close-Encounter Probability 18
1.4 Computer Simulations of Surface Scattering 20
1.5 Surface Structure of a Crystal 26
1.6 Measurement of the Close-Encounter Probability 28
1.7 Adsorbate-Induced Reconstruction of the W(001) Surface 30
1.8 Perspectives 33
References 34

2. Channeling within the Crystal

2.1 Introduction 37
2.2 Energy Loss 37
2.3 Continuum Model 38
2.4 Transverse Energy 40
2.5 Critical Angle for Channeling 40
2.6 Minimum Yield 44
2.7 Blocking and Double Alignment 46
2.8 Angular Yield Curve: A Geometric Approach 49

2.9 Computer Simulations: Angular Width and Minimum Yield 52
2.10 Planar Channeling 54
2.11 Substitutional Impurity Location 55
2.12 Metastable Alloy Formation in Implanted Copper 56
2.13 Perspectives 59
References 60

3. Particle Distributions within the Channel

3.1 Introduction 61
3.2 Spatial Probability for a Channeled Particle 63
3.3 Spatial Flux Distribution—Parallel Incidence 66
3.4 Close-Encounter Probability—Parallel Incidence 72
3.5 Spatial Flux Distribution—Angular Dependence 73
3.6 Close-Encounter Probability—Angular Dependence 76
3.7 General Principles of Impurity Location 79
3.8 The Lattice Location of Hydrogen in Tungsten 81
3.9 Perspectives 85
References 86

4. Dechanneling by Defects

4.1 Introduction 88
4.2 Dechanneling in the Perfect Crystal 88
4.3 Dechanneling by Defects 90
4.4 Point Defects 91
4.5 Dislocation Lines 93
4.6 Dislocation Loops 101
4.7 Stacking Faults 103
4.8 Twins 105
4.9 Voids and Gas Bubbles 108
4.10 Precipitates 108
4.11 Amorphous Clusters 109
4.12 Amorphous and Polycrystalline Layers 110
4.13 Summary of Defect Dechanneling 114
References 115

5. Defect Depth Distributions

5.1 Introduction 117
5.2 Channeling Yield in Disordered Crystals 118
5.3 Random Fraction χ_R 119
5.4 Defect Scattering Factor f 121
5.5 Defects—Dechanneling Only 124
5.6 Defects—Dechanneling and Direct Scattering 125
5.7 Ion Implantation in Si 127
5.8 Ion Implantation in Al 131
5.9 Summary of Disorder Analysis 134
References 135

6. Surfaces

6.1 Introduction 136
6.2 Surface Reconstruction: Si(001) 137
6.3 Surface Relaxation: Si(111) 141
6.4 Substrate Shadowing: Epitaxial Au on Ag(111) 143
6.5 Adsorbate Location by the Blocking Technique: S on Ni(011) 145
6.6 Surface Reordering: H on W, Pt, and Si 147
6.7 Perspectives 149
References 150

7. Surface Layers and Interfaces

7.1 Introduction 151
7.2 Detection of Thin Surface Layers 153
7.3 Reaction of Metal with Semiconductor: Ni on Si 155
7.4 Oxide–Semiconductor Interface: SiO_2 on Si 157
7.5 Channeling in Thin Crystals: SiO_2 on Si 160
7.6 Composition of Semiconductor Oxides: GaP 166
7.7 Perspectives 167
References 169

8. Epitaxial Layers

8.1 Introduction 171
8.2 Epitaxial Silicides 173
8.3 Thermal Anneal of Implanted Si 178
8.4 Molecular Beam Deposition of Silicon Layers 181
8.5 Laser Annealing of Silicon 185
8.6 Silicon on Sapphire 187
8.7 Superlattices and Heteroepitaxial Structures 188
8.8 Perspectives 191
References 191

9. Impurity–Defect Interactions

9.1 Introduction 193
9.2 Metal–Solute Interactions with Interstitials and Vacancies 194
9.3 Hydrogen Trapping at Point Defects in Metals 200
9.4 Analysis Beam-Induced Damage 205
9.5 Perspectives 209
References 211

Appendix A. Atomic Scattering Concepts

A.1 Introduction 213
A.2 Impact Parameter, Scattering Angle, and Cross Section 213

A.3 Energy Loss of Charged Particles 215
A.4 Random Spectrum in Backscattering Analysis 217
References 220

Appendix B. Lecture Notes on Channeling and the Continuum Potential

B.1 Introduction 221
B.2 Surface Interaction via a Two-Atom Model 223
B.3 Channeling in the Bulk: The Continuum Potential 226
B.4 Channeling in the Bulk: Transverse Energy and the Critical Angle 228
B.5 Channeling in the Bulk: Fraction Channeled 229
B.6 Channeling Flux Distribution 231

Bibliography 235

Index 297

PREFACE

Nuclear physicists have developed the art of producing energetic ion beams; solid state physicists have developed the art of producing single-crystal solids. These two disciplines come together in the "world" of channeling. Channeling is defined as the influence of a crystal lattice on the trajectories of energetic particles. The major applications of channeling concern the crystallographic structure of the near surface region (submicron depths) of solids.

The historical evolution of channeling and its application to materials studies is typical in science. The idea that a crystal lattice could influence an energetic ion trajectory was suggested as early as 1912 by Stark and then essentially forgotten. The actual "discovery" of the channeling effect occurred in the period 1960–1965. At least two stories suggest that it may have been an accidental discovery. In one instance it was found that computer simulations of ion ranges in solids took an extraordinarily long time when the incident ion was directed along a major crystallographic direction of the crystal model (within the computer). This was eventually explained as an enhanced penetration along these channeling directions. In another case, scientists developing thin, single-crystal particle detectors for nuclear physics applications observed a relatively small, anomalous behavior in the energy lost by the ion in traversing the crystal. The "anomaly" was found to be strongly dependent on the orientation of the crystal. The pursuit of this small effect resulted in one of the early demonstrations of the channeling behavior of mega-electron-volt ions.

Once established, the channeling phenomenon was studied in detail through experiments primarily aimed at testing the evolving channeling theory. Suggestions for application of the channeling effect to problems in

nuclear physics, atomic physics, and materials science quickly followed.

The applications to materials have been the most extensive. This is probably the result of the coming together of a number of interests. The advent of ion implantation as a technological process required a probe of cystal structure sensitive in the first 0.1 micron of the solid. Furthermore, in the backscattering mode, channeling is a mass-dispersive structure probe so that the crystallographic site of the implanted impurity as well as the host crystal could be explored. In recent years, the ability to detect the lattice position of impurities has been extended to many other problems of interest in materials science. Ion implantation is no longer the sole driving force for channeling studies; the realm has extended to the general problem of the lattice position of impurities in crystalline solids.

The characterization and use of thin films is another area of materials science that has grown increasingly important in the past fifteen years. Such films, either crystalline or amorphous, are ideal structures for study by channeling techniques. Crystalline films can be grown by a variety of deposition techniques; the unique aspect of the channeling/backscattering methods is the ability to analyze these films in depth without layer removal. Using these techniques one can characterize interfacial solid–solid reactions, determine crystal structure at buried interfaces, and analyze for extended defects that may arise in growth procedures. This book focuses on the methods involved in these structural analyses.

The book is organized into two parts: Chapters 1–5 emphasize the fundamental channeling principles necessary for materials analysis. Chapters 6–9 give a broader view of materials science applications of the channeling technique. In the first part Chapter 1 includes descriptions of the interaction of an ion beam at the surface of a solid and the use of these interactions in investigations of the structure of surfaces. Channeling within the bulk of the solid is described qualitatively in Chapter 2 and quantitatively in Chapter 3. The influence of defects and crystal imperfections on the channeling process is discussed in Chapter 4, while in Chapter 5 use is made of the results to show how channeling can yield the depth profile of defects. Each of these first chapters contains a materials application to illustrate the concepts discussed within the chapter.

The second part of the book contains examples of the channeling technique as a materials science tool. Chapter 6 is concerned with clean surface applications and the question of the atom positions in the first monolayer of a solid. Chapter 7 has a description of the use of channeling in thin film and interface analysis with examples from metal silicide formation and Si/SiO_2 stoichiometry and structure determinations. Epitaxial thin film structures are discussed in Chapter 8. These examples come from molecular beam epitaxy, from a heteroepitaxial system, Si on sap-

phire, and from solid phase epitaxial growth of silicon and silicides. The chapter includes examples of the study of regrowth of damaged layers by laser or furnace annealing. Chapter 9 describes the use of channeling determinations of the lattice location of impurities in a metallic solid in studies of impurity interactions with crystal defects. Such defects can be created by the ion beam itself, and a discussion of beam-induced defect production is also given in this chapter of the book.

Appendix A is a brief review of the fundamentals that govern ion scattering in solids. It provides background information for understanding ion scattering in crystals. The essentials of channeling as they were presented in a graduate course on modern materials analysis are given as course notes in Appendix B. The Bibliography includes conference proceedings reviews, books, and papers that are primarily concerned with applications of channeling to solid state science.

Our intention has been to write a book that would be useful to people with a variety of levels of interest in this subject. Clearly it should be useful to both graduate students and workers in the field. We have attempted to bring together many of the concepts used in channeling beam analysis with an indication of the origin of the ideas within fundamental channeling theory. The level of the book is appropriate to senior undergraduates and graduate students who have had a modern physics course and some solid state physics. A second audience is those scientists who work in related areas of materials science and wish to learn more about the "channeling" probe, its strengths, weaknesses, and areas of further potential application. To them we hope we have explained this apparent paradox of using mega-electron-volt ions to probe solid state phenomena that have characteristic energies of electron volts.

This page intentionally left blank

ACKNOWLEDGMENTS

The three authors were drawn together by our common interest in applications of channeling. We owe a special debt of gratitude to those who provided initial insights into channeling: W. M. Gibson (L. C. F.) and J. A. Davies (S. T. P. and J. W. M.). The three of us gained from our association with the free spirit and insights of Jens Ulrik Andersen.

One of the joys of being in this area of science is the opportunity to collaborate with many different scientists. These include not only colleagues based in our home laboratories but the frequent international visitors to our institutions and collaborations resulting from our visits to other laboratories. We want to acknowledge the exciting times we have enjoyed during these periods and want to thank our good friends. Some of the major institutes and people involved in our collaborations in channeling investigations of solids include, at Aarhus University: J. U. Andersen, H. H. Andersen, B. Bøgh, Jens Lindhard, E. Uggerhøj, I. Stensgaard, P. Sigmund, and J. Bøttinger; at Chalk River Nuclear Labs: J. Davies, T. Jackman, I. Mitchell, M. Swanson, and J. Whitton; at Bell Labs: W. L. Brown, T. Buck, W. M. Gibson, J. Poate, J. MacDonald, N. Tolk, R. Haight, R. Culbertson, J. Williams, J. Hirvonen, and E. Kaufmann; at Cal Tech: Marc Nicolet, S. S. Lau, W. K. Chu, L. Csepregi, J. Gyulai, O. Meyer, E. Kennedy, T. Sigmon, E. Lugujjo, N. Cheung, B. Scherzer, G. Ottaviani, C. Canali, and W. Van de Weg; at Oak Ridge: B. R. Appleton, C. W. White, S. Datz, and J. Barrett; at F.O.M.: F. Saris; at Catania: E. Rimini, G. Foti, and S. Campisano; at Sandia Labs: F. Vook, J. Ellison, D. Brice, J. Borders, D. Follstaedt, J. A. Knapp, and S. Myers; at Rockwell Science Center: F. Eisen; at Research Institute for Physics: B. Domeij, L. Eriksson, D. Sigurd, and N. G. E. Johansson.

We have enjoyed the interactions and the long hours around the accelerator. These collaborators helped in the development of the subject of this book. We thank all of them!

This book rests on the support of our laboratories, Bell Labs and Sandia National Labs; the encouragement of our management; the patience and expertise of the typists; and the excellence and skill of the technical illustrators.