



UNIVERSITÉ
DE GENÈVE

Archive ouverte UNIGE

<https://archive-ouverte.unige.ch>

Livre

2007

Extract

Open Access

This file is a(n) Extract of:

Physics of ferroelectrics : a modern perspective

Rabe, Karin M.; Ahn, Charles; Triscone, Jean-Marc

This publication URL:

<https://archive-ouverte.unige.ch/unige:12885>

© This document is protected by copyright. Please refer to copyright holders for terms of use.

Contents

Modern Physics of Ferroelectrics:

Essential Background

Karin M. Rabe, Matthew Dawber, Céline Lichtensteiger, Charles H.

Ahn, and Jean-Marc Triscone	1
1 Introduction	1
2 Switching and Hysteresis Loops	2
3 Crystallographic Signature of Ferroelectricity	6
4 Materials	8
4.1 Perovskite Oxides	8
4.2 LiNbO_3	14
4.3 Layered Oxide Ferroelectrics	15
4.4 Other Ferroelectric Oxide Families	17
4.5 Magnetic Ferroelectric Oxides	18
4.6 Electronic Ferroelectrics	19
4.7 Nonbulk Ferroelectrics	19
5 Applications of Ferroelectric Materials	20
5.1 Pyroelectric and Piezoelectric Devices	20
5.2 Ferroelectric Memory Technology	21
5.3 Potential Future Applications	21
5.3.1 Ferroelectric Nanostructures	21
5.3.2 Field-Effect Devices	22
5.3.3 Ferroelectric Device Fabrication Using Atomic Force Microscopy	22
5.3.4 Ferroelectric Cooling Devices	23
6 Note from the Editors	23
References	23
Index	29

Theory of Polarization: A Modern Approach

Raffaele Resta and David Vanderbilt	31
1 Why is a Modern Approach Needed?	31
1.1 Fallacy of the Clausius–Mossotti Picture	32
1.2 Fallacy of Defining Polarization via the Charge Distribution	34
2 Polarization as an Adiabatic Flow of Current	36
2.1 How is Induced Polarization Measured?	36

2.2	How is Ferroelectric Polarization Measured?	38
2.3	Basic Prescriptions for a Theory of Polarization	40
3	Formal Description of the Berry-Phase Theory	41
3.1	Formulation in Continuous $\mathbf{k}$ -Space	42
3.2	Formulation in Discrete $\mathbf{k}$ -Space	44
3.3	The Quantum of Polarization	46
3.4	Formal Polarization as a Multivalued Vector Quantity	48
3.5	Mapping onto Wannier Centers	50
4	Implications for Ferroelectrics	52
4.1	Spontaneous Polarization	53
4.2	Anomalous Dynamical Charges	54
4.3	Piezoelectric Properties	55
5	Further Theoretical Developments	57
5.1	Polarization in an Applied Electric Field	57
5.2	Interface Theorem and the Definition of Bound Charge	58
5.3	Many-Body and Noncrystalline Generalizations	61
5.4	Polarization in Kohn–Sham Density-Functional Theory	62
5.5	Localization, Polarization, and Fluctuations	63
6	Summary	64
	References	65
	Index	67

A Landau Primer for Ferroelectrics

	Premi Chandra, Peter B. Littlewood	69
1	Introduction	69
2	Landau–Devonshire Theory	74
2.1	General Phenomenology	74
2.2	Second-Order (Continuous) Transition	75
2.3	First-Order (Discontinuous) Transition	76
2.4	Coupling to Strain	79
2.5	Domains	81
3	Landau–Ginzburg Theory	84
3.1	General Considerations	84
3.2	The Polarization Correlation Function	85
3.3	The Levanyuk–Ginzburg criterion	86
3.4	Displacive and Order–Disorder Transitions	88
3.5	Recent Developments in Bulk Ferroelectricity	91
4	Reduced Size and Other Boundary Effects	92
4.1	General Discussion	92
4.2	The Polarization at the Boundary	93
4.3	Depolarization Effects	96
4.4	Misfit Epitaxial Strain	100
4.5	Inhomogeneous Effects	102
5	Summary and (Some) Open Questions	104
	References	106

Index	115
-------------	-----

First-Principles Studies of Ferroelectric Oxides

Karin M. Rabe and Philippe Ghosez	117
1 Introduction	117
2 First-Principles Methods	118
3 Results for Perovskite Oxide Compounds	123
3.1 Ground-State Structure	124
3.2 Phonons, Lattice Instabilities and Polarization	127
3.3 Polarization–Strain Coupling	136
3.4 Dielectric and Piezoelectric Responses	137
3.5 Results at Nonzero Temperature	140
4 Results for Other Ferroelectric Oxide Compounds	143
5 Results for Solid Solutions	146
6 Results for Defects	150
7 Results for Surfaces, Thin Films, Superlattices, Nanowires and Nanoparticles	152
8 Challenges and Prospects	154
References	156
Index	172

Analogies and Differences between Ferroelectrics and Ferromagnets

Nicola A. Spaldin	175
1 Fundamentals	177
1.1 Understanding the Origin of Spontaneous Polarization	177
1.1.1 What Causes Ferroelectricity?	177
1.1.2 What Causes Ferromagnetism?	184
1.2 Domains	188
2 Applications	194
2.1 Ferroelectric Random Access Memories	196
2.2 Magnetoresistive Random Access Memories	196
3 Multiferroics	198
3.1 The Scarcity of Ferromagnetic Ferroelectrics	199
3.2 Magnetoelectric Coupling	200
3.3 Some Materials Examples	201
3.3.1 BiFeO ₃	201
3.3.2 BiMnO ₃	204
3.3.3 YMnO ₃	206
3.3.4 TbMnO ₃	209
3.4 Composites	209
4 Outlook	210
References	211
Index	216

Growth and Novel Applications of Epitaxial Oxide Thin Films

Agham-Bayan Posadas, Mikk Lippmaa, Fred J. Walker, Matthew

Dawber, Charles H. Ahn, and Jean-Marc Triscone	219
1 Introduction	219
2 Thin-Film Growth of Complex Oxides	221
2.1 Vacuum Chamber	221
2.2 Temperature Control and Monitoring	222
2.3 Pulsed Laser Deposition	227
2.3.1 Laser	228
2.3.2 Targets	230
2.3.3 Ablation Process	232
2.3.4 Film Growth Using PLD	235
2.4 Sputter Deposition	238
2.4.1 Sputtering Process	238
2.4.2 The Sputtering of Insulators	239
2.4.3 Process Gas	240
2.4.4 Preferential Sputtering	242
2.4.5 Technical Considerations in Sputter Deposition	242
2.4.6 Reactive Sputtering	244
2.5 Oxide Molecular Beam Epitaxy	244
2.5.1 Hardware	246
2.5.2 RHEED	247
2.5.3 Fundamentals of Growth	249
2.5.4 Alkaline-Earth Oxide Growth	253
2.5.5 Perovskite Growth	254
3 Substrates	257
4 Applications of Epitaxial Oxide Thin Films	269
4.1 Strain Engineering and Superlattices	270
4.1.1 Strain Engineering in Epitaxial Thin Films	270
4.1.2 Strain in Superlattices	271
4.1.3 Electrostatic Coupling Between Layers	274
4.1.4 Selected Examples of Material Combinations	274
4.1.5 X-Ray Characterization of Superlattices	277
4.2 Crystalline Oxides on Semiconductors (COS)	279
4.2.1 Layer-Sequenced COS Growth	281
4.2.2 How the Silicide Facilitates Epitaxy	285
4.3 Conclusions	289
References	290
Index	304

Ferroelectric Size Effects

Céline Lichtensteiger, Matthew Dawber, and Jean-Marc Triscone	305
1 Size Effects in Ferroelectrics	305
2 Size Effects in the Ginzburg–Landau–Devonshire Theory	306
3 Extrinsic Size Effects	307
4 Effect of Screening	308
4.1 Recent Experimental Work: Ultrathin Films on Metallic Electrodes	310
4.1.1 Results of Combined Experimental and Theoretical Investigations	316
4.1.2 Other Similar Studies	320
4.2 Scaling of the Coercive Field	321
4.3 Thin Films on Insulating Substrates	322
5 Superlattices	324
6 Other Geometries	326
6.1 Nanoparticles	327
6.2 Areal Size Effects	328
6.3 Self-Patterning	328
6.4 Novel Ferroelectric Geometries	329
6.4.1 Nanotubes	329
6.4.2 Nanowires – Nanorods	329
References	330
Index	336

Nanoscale Studies of Domain Walls in Epitaxial Ferroelectric Thin Films

Patrycja Paruch, Thierry Giamarchi, and Jean-Marc Triscone	339
1 Introduction	339
2 Ferroelectric Domain Walls as Elastic Disordered Systems	340
3 Static and Dynamic Behavior of Elastic Disordered Systems	341
4 Experimental Observation of Domain-Wall Creep	344
5 Domain-Wall Creep in a Commensurate Potential	347
6 Domain-Wall Creep in a Random Potential	351
7 Experimental Observation of Domain-Wall Roughness	354
8 Domain Walls in the Presence of Random-Bond Disorder and Dipolar Interactions	357
9 Recent Studies of Ferroelectric Domain-Wall Dynamics	358
10 Conclusions	359
References	360
Index	362

APPENDIX A –

Landau Free-Energy Coefficients

Long-Qing Chen 363

1 BaTiO₃ 364

2 SrTiO₃ 365

3 PbZr_{1-x}Ti_xO₃ (PZT) 366

4 PbTiO₃ 368

5 LiTaO₃ and LiNbO₃ 368

6 Sr_{0.8}Bi_{2.2}Ta₂O₉ 369

7 SrBi₂Nb₂O₉ 369

References 370

Index 371

Appendix B – Material–Substrate Combinations Tables

Céline Lichtensteiger and Matthew Dawber 373

Index 385

Physics of Ferroelectrics

A Modern Perspective

(Eds.) K. M. Rabe; C. H. Ahn; J.-M. Triscone

2007, XII, 390 p. 123 illus., 36 in color., Hardcover

ISBN: 978-3-540-34590-9