

Contents

1 Crystallographic Aspects of Interfaces in Ferroelectrics and Related Materials	1
1.1 Domain Structures and Interfaces	2
Between Polydomain Regions	2
1.1.1 Formation of Domain Structures in Ferroelectric Single Crystals	2
1.1.2 Elastic-Matching Concept and Its Application to Domain Boundaries	4
1.1.3 Classification of Domain Boundaries in Ferroelectric Single Crystals.....	8
1.1.4 Crystallographic Interpretation of Interfaces in the Case of Complicated Domain Structures.....	8
1.2 Phase Coexistence at First-Order Phase Transitions	12
1.2.1 Elastic Matching of Phases and Zero-Net-Strain Planes	12
1.2.2 Stress Relief and Conical Interphase Boundaries.....	16
1.3 Polydomain/Heterophase Ferroelectrics.....	18
References	19
2 Two-Phase States.....	23
2.1 Elastic Matching of Morphotropic Phases in $\text{Pb}(\text{Zr}_{1-x}\text{Ti}_x)\text{O}_3$	25
2.1.1 Tetragonal–rhombohedral Phase Coexistence and Crystallographic Interpretation	25
2.1.2 Elastic Matching and Stress Relief in the Presence of the Intermediate Monoclinic Phase.....	28
2.2 Phase Coexistence in $(1 - x)\text{Pb}(\text{Mg}_{1/3}\text{Nb}_{2/3})\text{O}_3 - x\text{PbTiO}_3$ Near the Morphotropic Phase Boundary	32
2.2.1 Phase Coexistence Without the Monoclinic Phase	32
2.2.2 Phase Coexistence in the Presence of the Monoclinic Phases	36
2.2.3 Effect of Non-180° Domains on Phase Coexistence	39
2.2.4 Different Scenarios of Stress Relief	44

2.3	Model of Interpenetrating Phases: Application to $(1 - x)\text{Pb}(\text{Mg}_{1/3}\text{Nb}_{2/3})\text{O}_3 - x\text{PbTiO}_3$ Near the Morphotropic Phase Boundary	49
2.4	Domain and Heterophase States in $(1 - x)\text{Pb}(\text{Zn}_{1/3}\text{Nb}_{2/3})\text{O}_3 - x\text{PbTiO}_3$ Near the Morphotropic Phase Boundary	53
2.4.1	Phase Transitions and Intermediate Phases	53
2.4.2	Crystallographic Study of Elastic Matching of Morphotropic Phases.....	55
2.4.3	Interpenetrating Phases in $0.90\text{Pb}(\text{Zn}_{1/3}\text{Nb}_{2/3})\text{O}_3 - 0.10\text{PbTiO}_3$ Single Crystals	57
	References	60
3	Phase Coexistence Under Electric Field	65
3.1	Heterophase $\text{Pb}(\text{Mg}_{1/3}\text{Nb}_{2/3})\text{O}_3$ at the Induced Phase Transition ...	65
3.2	Domain State: Interface Relationships at Electric Field $E \parallel [001]$	68
3.2.1	Heterophase $(1 - x)\text{Pb}(\text{Mg}_{1/3}\text{Nb}_{2/3})\text{O}_3 - x\text{PbTiO}_3$	68
3.2.2	Heterophase $(1 - x)\text{Pb}(\text{Zn}_{1/3}\text{Nb}_{2/3})\text{O}_3 - x\text{PbTiO}_3$	79
3.3	Domain State: Interface Relationships at Electric Field $E \parallel [110]$	83
3.4	Domain State: Interface Relationships at Electric Field $E \parallel [111]$	87
3.5	Role of Intermediate Phases in Heterophase States.....	92
	References	93
4	Three-Phase States.....	97
4.1	Model of Three-Phase Single Crystal	97
4.2	Application of Model Concepts to PbZrO_3 and $\text{Pb}(\text{Zr}_{1-x}\text{Ti}_x)\text{O}_3$ ($x \approx 0.22$)	100
4.2.1	Phase Coexistence in PbZrO_3 Single Crystals	100
4.2.2	Phase Coexistence in $\text{Pb}(\text{Zr}_{1-x}\text{Ti}_x)\text{O}_3$ Single Crystals ($x \approx 0.22$)	101
4.3	Application of Model Concepts to $(1 - x)\text{Pb}(\text{Mg}_{1/3}\text{Nb}_{2/3})\text{O}_3 - x\text{PbTiO}_3$	102
4.4	Three-Phase Coexistence and Complete Stress Relief in $(1 - x)\text{Pb}(\text{Zn}_{1/3}\text{Nb}_{2/3})\text{O}_3 - x\text{PbTiO}_3$	103
4.5	Thermodynamic Description of Three-Phase States in Ferroelectric Solid Solutions	108
4.6	Crystallographic and Thermodynamic Studies of Three-Phase States	114
	References	115

5	Overlapping Structures and Transition Regions	119
5.1	Overlapping Structures in $\text{Pb}(\text{Zn}_{1/3}\text{Nb}_{2/3})\text{O}_3$	119
5.2	S_j : Interface Relationships in $\text{Pb}(\text{Zn}_{1/3}\text{Nb}_{2/3})\text{O}_3$	121
5.3	Transition Regions in $(1 - x)\text{Pb}(\text{Zn}_{1/3}\text{Nb}_{2/3})\text{O}_3 - x\text{PbTiO}_3$	124
5.4	Stress Relief at Variable Unit-Cell Parameters	128
	References	129
6	Conclusions	131
6.1	A Way from a Unit Cell to Morphotropic Polydomain/Heterophase Structures	131
	References	133
A	Methods for Description of Heterophase and Polydomain Single Crystals	135
A.1	Concepts on the Zero-Net-Strain Plane	135
A.2	Comparison of Data	141
	References	147
B	Optimal Volume Fractions in Terms of Angles Between Spontaneous Polarization	149
B.1	Optimal Volume Fractions and Polarization Rotations	149
	References	152
	Index	153
	About the Author	155