

Table of Contents

Symbols and Abbreviations.....	xii
Introduction.....	1
Chapter I. The classical grain boundary diffusion models.....	5
Introduction.....	5
1.1 Grain boundary model. Guggenheim or Fisher?.....	6
1.1.1 Isolated grain boundary model.....	7
1.1.2 Mathematical description of grain boundary diffusion in the isolated grain boundary model.....	8
1.1.3 Transformations made to obtain Fisher's system.....	9
1.1.4 An alternative derivation of Fisher's system.....	12
1.1.5 Whipple's solution.....	13
1.2 Diffusion kinetic regimes.....	14
1.3 Deducing the grain boundary diffusivity from the diffusion profile.....	21
Chapter II. Finite Element Model.....	27
Introduction.....	27
2.1 General aspects with respect to continuum problems.....	28
2.2 Fisher's system expressed in the form suitable for finite element calculation.....	28
2.2.1 Finite element method formulation of space charge layer problem.....	30
2.3 Finite element calculation by using FLUX-EXPERT.....	32
Chapter III. Nonlinearity effect.....	35
Introduction.....	35
3.1 Important definitions.....	35
3.1.1 The C- or B-regime?.....	36
3.2 Integrating Whipple's solution.....	36
3.3 Errors in determining the grain boundary diffusivity.....	43
3.3.1 Nonlinearity and small values of dimensionless parameter w.....	50
3.3.2 Analyzing the errors of using Le Claire's constant.....	54

3.4 Discussing new procedures for finding the grain boundary diffusivity.....	59
3.4.1 An analytical expression for $\partial \ln C_{av} / \partial W^{6/5}$ at the maximum.....	59
3.4.2 The reason of observing a constant value for $\partial \ln C_{av} / \partial W^{6/5}$. Discussing procedures used in the literature.....	62
3.4.3 On important dependences for finding the grain boundary diffusivity.....	67
Summary.....	73
 Chapter IV. Realistic microstructures.....	75
Introduction.....	75
4.1 Finite Element Calculation. To get started.....	76
4.1.1 Main characteristics of the geometrical model of isolated boundary used in the finite element program.....	77
4.1.2 A comparison of Whipple's solution and FLUX-EXPERT's simulation results.....	78
4.1.3 The accuracy of results obtained in FLUX-EXPERT.....	79
4.1.3.1 The averaging of concentration C_g	79
4.1.3.2 The effect of the finite element mesh.....	81
4.1.3.3 The effect of the time interval.....	82
4.2 Realistic polycrystalline microstructures.....	84
4.2.1 A comparison of the model of parallel boundaries with the model of square grains under conditions of type-B kinetics.....	86
4.2.1.1 The model of parallel boundaries at short diffusion times.....	86
4.2.1.2 The model of square grains at short diffusion times.....	89
4.2.2 General geometrical models.....	94
4.2.2.1 Main characteristics of general geometrical models.....	94
4.2.2.2 Simulation results obtained in the general geometrical models.....	97
4.2.3 A comparison of the model of parallel boundaries with the model of square grains under conditions of type-A kinetics.....	101
4.2.3.1 Analyzing the boundary condition at the bottom.....	102
4.2.3.2 Analyzing Hart's equation and Maxwell-Garnett's equation.....	105
4.2.3.3 Segregation effects under conditions of type-A kinetics.....	110
Summary.....	116

Chapter V. Space charge layer problems in grain boundary diffusion studies.....	117
Introduction.....	117
5.1 Mathematical model to describe diffusion in a polycrystal including space charge layers.....	119
5.2 Accuracy of the simulated diffusion profiles and effect of coordinate-dependent space charge layer diffusivity.....	121
5.2.1 The finite element mesh and diffusion barrier at the bottom of the geometrical model.....	121
5.2.2 The reason of using constant space charge layer diffusivity.....	126
5.3 How diffusion proceeds in the models of parallel boundaries and square grains.....	128
5.3.1 The model of parallel boundaries under conditions of type-B kinetics.....	130
5.3.2 The model of square grains under conditions of type-B kinetics.....	138
5.3.3 The model of parallel boundaries and the model square grains under conditions of type-A kinetics.....	139
Summary.....	147
Conclusions.....	149
Kurzfassung der Dissertation in deutscher Sprache.....	155
1. Einführung.....	155
2. Physikalische und geometrische Modelle, die in der numerischen Untersuchung benutzt wurden.....	158
3. Ergebnisse und Diskussion.....	164
3.1 Nichtlinearitätseffekt.....	164
3.2 Realistische Mikrostrukturen.....	168
3.3 Probleme durch Raumladungszonen.....	170
4. Zusammenfassung.....	173
References.....	177
Curriculum Vitae.....	185