

Contents

Introduction	1
Outline of this Work	2
1 Some Facts about Silicon Carbide	3
1.1 Historical Facts and Applications	3
1.2 Doping of SiC	6
1.3 Crystal Structure: the Polytypes of SiC	8
2 Theoretical Description of Defect Dynamics	13
2.1 Some General Aspects of Point Defects	13
2.1.1 Point defects at thermodynamic equilibrium	13
2.1.2 The situation after an implantation process	14
2.1.3 Migration of defects	15
2.1.4 Jump probabilities	16
2.1.5 Charge state effects on the migration of defects	16
2.2 Density Functional Theory	17
2.3 SCC-DFTB	20
2.4 Modeling of Defects	22
2.5 The Diffusion Algorithm	24
2.5.1 The constrained relaxation technique	25
2.5.2 The activation relaxation technique (ART)	26
2.6 Lattice Vibrations and Free Energies	26
2.7 Applications and Test Calculations	28
2.7.1 The vibrational spectrum of 3C-SiC bulk	28
2.7.2 Heat capacity of diamond, silicon, and SiC	30
2.7.3 Absolute entropy in different methods	31
2.7.4 Formation entropy	32
2.7.5 The vacancy in diamond and silicon	37

3	Vacancies and Interstitials	41
3.1	Vacancies	41
3.1.1	Formation energies	41
3.1.2	Migration of vacancies	45
3.1.3	Vacancy – antisite pair formation	48
3.2	Interstitials	50
3.3	Interstitial Recombination with Vacancies	52
4	Aggregation of Antisites	55
4.1	The Antisite Pair $C_{Si} Si_C$	55
4.1.1	Formation Energy of $C_{Si} Si_C$	55
4.1.2	Properties of the Antisite Pair	57
4.1.3	Creation of the $C_{Si} Si_C$ Pair in the perfect Si_C -lattice	59
4.1.4	Migration of Antisites in the ideal lattice	60
4.1.5	Pair creation by vacancy migration	60
4.2	Larger Aggregates of Antisites	62
4.2.1	Stability of various arrangements	62
4.2.2	A Vacancy's Spiral Walk	65
4.3	Contributions of the Vibrational Entropy	69
4.4	Mobility of Isolated Antisites	72
4.4.1	The vacancy assisted mechanism	73
4.4.2	The $Si_C (C_{Si})_2$ complex	75
4.5	Influence of other Defects on Migration Processes	77
4.6	Conclusions for the Formation of Antisite Aggregates	79
5	Nitrogen-related Defects	83
5.1	Nitrogen-related Pair Defects	84
5.1.1	Pair formation by aggregation of V_{Si} and N_C	85
5.1.2	Mobilizing N_C — Creation of N-interstitials	86
5.1.3	Recombination of $(NC)_C$ with divacancies $V_C V_{Si}$	87
5.1.4	$(NC)_C$ meeting isolated vacancies	89
5.1.5	The $C_{Si} N_C$ pair as an alternative	90
5.2	Dissociation or Aggregation	91
5.2.1	Dissociation of $N_C V_{Si}$ pairs	91
5.2.2	$V_{Si} (N_C)_n$ -complexes	92
5.2.3	Formation of $C_{Si} (N_C)_n$ complexes	94
5.3	Correlation of Activation Energies and Temperatures	95
5.3.1	Definition of an assignment	96
5.3.2	Correlation of the calculated values with experimental findings	97

5.3.3 Entropy effects on nitrogen migration	98
5.4 Implantation with Phosphorus	99
6 Summary and Outlook	103
A Formation Energies	105
B Calculation of the Gibbs Free Enthalpy	107
C Basic Properties of Strain Fields	109
D Summary: Activation Energies	111
Acknowledgment	119