



MONOGRAPHS ON THE  
PHYSICS AND CHEMISTRY  
OF MATERIALS

# Theory of Defects in Solids

Electronic Structure of  
Defects in Insulators and  
Semiconductors

A. M. Stoneham

# THEORY OF DEFECTS IN SOLIDS

ELECTRONIC STRUCTURE OF  
DEFECTS IN INSULATORS  
AND SEMICONDUCTORS

BY  
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## PREFACE

THE perfect crystal is one of the idealizations commonly found in theoretical physics and science fiction. Only after much experimental effort have the nature and properties of the commonest defects in real crystals been isolated. At the same time, the theory of defects has developed through a series of models, approximations, and assertions, and often the basis of these ideas has been forgotten in their evolution. In this book, I have tried to give a critical survey of defect theory, stressing assumptions made and attempting to assess their value. I hope that the book will be useful to the wide range of research workers and graduate students interested in solid state science, both to theorists who want to relate their own work to the many previous calculations, and to experimentalists who want to know what, if anything, they should believe of present theories.

The possible effects of defects on crystals are diverse, affecting the colours of gemstones and the strength of metals, so that a full discussion of all defect properties is beyond the scope of any one book. I have tried to compromise between breadth and depth of coverage by several broad restrictions. First, this book is primarily about defects. It does not try to be a textbook of general solid state physics, elementary quantum mechanics, or group theory. Thus the opening chapters on the perfect solid (Part I) merely define notation, state assumptions, and assert without proof results needed later. Secondly, I concentrate on the properties of point defects in insulators and semiconductors. Metals and heavily-doped semiconductors behave very differently because of the free carriers and, whilst most of the theory carries over to linear or planar defects, the experimental data in such cases are so much less satisfactory that detailed discussion is not yet worthwhile. Thirdly, it is the electronic properties of defects which are stressed. Optical and spin-resonance properties are discussed at length, the dynamics of lattices with defects in less detail, and defect production and mechanical properties largely ignored. Finally, this book is concerned with the *theory* of defects in solids. There are no vast tables of experimental results. The aim of the study of defects is surely to achieve a quantitative understanding of observed behaviour, and not the mere compilation of data. The discussion in Part IV attempts to see just how good our

present understanding is. To do this, a small number of classes of defect are considered in detail. The range is as wide as possible so, whilst I may have missed out the reader's favourite defect, I hope there will be some system discussed which is sufficiently similar to be helpful. I have felt under no obligation to discuss all defects seen or claimed, and I have intentionally spent less time on topics discussed in depth elsewhere, like the theory of transition-metal ions. Instead, I have tried to stress any important features treated sparsely in the literature, and to set out the arguments involved where controversy remains.

The bibliography should be reasonably complete up to late 1972, apart from inadvertent omissions. Later work has been included only when I have been able to see it before publication, or in rare cases of special importance. I have had to make arbitrary decisions in subjects at the borders of those I discuss and in topics treated in less detail, notably defect formation energies, dynamics of imperfect lattices, and transition-metal ions. And I have had no qualms about omitting work which I believe to be misleading, misguided, or simply wrong. It has been observed that there has rarely been a possible mistake which theorists have not made. Defect theory is no exception, and I should welcome corrections of errors or omissions.

*Dorchester-on-Thames,  
October, 1973*

A.M.S.

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# CONTENTS

## I. THE PERFECT SOLID

1. CRYSTALS AND LATTICE GEOMETRY	3
1.1. Introduction: types of crystal	3
1.2. Structure of simple lattices	4
1.2.1. NaCl structure	4
1.2.2. CsCl structure	5
1.2.3. $\text{CaF}_2$ structure	6
1.2.4. Diamond and zincblende structures	8
1.2.5. Wurtzite structure	9
1.3. Geometric properties: lattice potentials	11
2. ELECTRONIC STRUCTURE OF THE PERFECT LATTICE	14
2.1. Basic equations and approximations	14
2.1.1. Static lattice approximation	14
2.1.2. The one-electron approximation	15
2.1.3. Koopmans' approximation	16
2.1.4. Approximations for exchange	17
2.1.5. Coulomb correlation	18
2.2. Band theory	22
2.2.1. Basic assumptions	22
2.2.2. Band structures: general features	22
2.2.3. Band structures: wavefunctions	26
2.2.4. Band structure: examples	29
2.2.5. Correspondence between electrons and holes	33
3. LATTICE DYNAMICS	36
3.1. Adiabatic approximations	36
3.1.1. The Born-Oppenheimer approximation	36
3.1.2. Adiabatic approximations for degenerate systems	37
3.1.3. Accuracy of adiabatic approximations	38
3.2. The harmonic approximation	40
3.2.1. Normal modes	41
3.2.2. General results in the harmonic approximation	42
3.2.3. Limits of the harmonic approximation	44
3.3. The dipole approximation	45
3.3.1. Introduction	45
3.3.2. Lattice dynamics	46

3.4. Models for interatomic forces	48
3.4.1. Introduction	48
3.4.2. Ionic crystals	48
3.4.3. Valence crystals	50
3.4.4. Partly-ionic crystals	51
3.4.5. Rare-gas crystals	52
3.5. Lattice dynamics	52
3.5.1. Dispersion curves	52
3.5.2. Density of states	53
3.6. The electron-phonon interaction	54
3.6.1. The Hellman-Feynman theorem	54
3.6.2. Electron-phonon interaction: delocalized case	55
3.6.3. Local models for electron-lattice coupling	59
<b>II. ELECTRONIC STRUCTURE OF ISOLATED DEFECTS</b>	
4. EFFECTIVE-MASS THEORY	65
4.1. Introduction	65
4.2. Simple effective-mass theory	65
4.2.1. Fundamental equations for the defect lattice	65
4.2.2. Approximations of effective-mass theory	67
4.2.3. The function $\Delta(\mathbf{r})$	68
4.2.4. The effective-mass equation	69
4.2.5. The wavefunction	70
4.2.6. More complicated band structures	71
4.2.7. Matrix elements in effective-mass theory	75
4.3. The quantum-defect method	76
4.4. Effective-mass theory for a many-body system	77
4.4.1. Many-body eigenfunctions for the perfect lattice	78
4.4.2. Fundamental equations for the defect lattice	79
4.4.3. Approach using exact many-body states as a basis	80
4.4.4. Approach using Hartree-Fock states as a basis	83
4.5. The accuracy of the effective-mass approximation	84
5. GREEN'S FUNCTION METHODS	87
5.1. Introduction	87
5.1.1. Choice of basis	87
5.1.2. The Green's function	87
5.1.3. Matrix elements of the Green's function	87
5.2. Bound states: the Koster-Slater model	90
5.2.1. The one-band, one-site model	90
5.2.2. The eigenvalue equation	91
5.3. Resonant states	95
5.3.1. The Green's function	97
5.3.2. The scattering problem	98

5.4. Band structures with subsidiary minima	103
5.4.1. General theory: minima at different points of the zone	104
5.4.2. Resonant states	105
5.4.3. Expressions for $\Delta E_n$	107
5.5. Other approaches using Green's function methods	108
5.5.1. The Bassani, Iadonisi, and Preziosi method	108
5.5.2. KKR and <i>T</i> -matrix methods	109
5.6. Choice of potential: validity of Green's function methods	112
6. VARIATIONAL METHODS	115
6.1. Introduction	115
6.1.1. Basic theorems	115
6.1.2. The few-electron approximation	116
6.2. The orthogonality constraint	117
6.2.1. Modulated band functions	117
6.2.2. Atomic orbital methods	118
6.2.3. Explicit orthogonalization	119
6.2.4. The pseudopotential method	121
6.2.5. Defects with several electrons	126
6.3. The accuracy of a variational calculation	126
6.4. Choice of a variational wavefunction	130
7. MOLECULAR METHODS AND MODEL CALCULATIONS	133
7.1. Introduction	133
7.2. General methods	133
7.2.1. Molecular-orbital and valence-bond methods	133
7.2.2. Separation of singlet and triplet states	135
7.2.3. Localized bonds and hybridization	136
7.3. Approximate methods	138
7.3.1. Approximations for matrix elements	138
7.3.2. Semi-empirical approaches	141
7.3.3. Model calculations	144
7.4. Weak covalency	146
7.5. Method of localized orbitals	149
7.5.1. The density operator	150
7.5.2. Self-consistent solutions	152
7.5.3. Conditions on the orbitals	153
7.5.4. Application of localized orbitals methods	155
7.5.5. Approximate methods and local orbitals	157
8. LATTICE DISTORTION FOR DEFECT SYSTEMS	159
8.1. Introduction	159
8.2. Linear coupling	161



8.3. Static distortion near defects	164
8.3.1. Linear response formalism	164
8.3.2. Methods for calculating static distortion	166
8.3.3. Long-range distortion from point defects	181
8.4. The Jahn-Teller instability	186
8.4.1. Introduction: the quasi-molecular hypothesis	186
8.4.2. Potential energy surfaces	187
8.4.3. Static and dynamic Jahn-Teller effects	197
8.4.4. Matrix elements of electronic operators: the Ham effect	218
8.5. Other asymmetric systems	223
8.5.1. Introduction	223
8.5.2. Fast- and slow-rotation limits	224
8.5.3. Other energy levels for rotating systems	229
8.5.4. Choice of potential for rotating systems	230
8.6. The bound polaron	231
8.6.1. Introduction	231
8.6.2. Weak electron-lattice coupling	233
8.6.3. Intermediate coupling: more advanced models	237
8.6.4. Strong coupling	248
8.6.5. The Toyozawa-Haken-Schottky model	250
8.6.6. Local phonon modes associated with bound polarons	252
8.6.7. The bound polaron: final comments	253
9. GENERAL RESULTS	256
9.1. Introduction	256
9.2. Number of bound states	256
9.3. Nature of the ground state	259
9.4. Order of energy levels	262
9.5. Scaling relations and the virial theorem	264
9.6. Symmetry	266

### III. CALCULATION OF OBSERVABLE PROPERTIES OF DEFECTS

10. OPTICAL PROPERTIES	271
10.1. Optical absorption by atoms	271
10.2. Optical properties of centres in a solid	276
10.3. The Condon approximation	277
10.4. The line-shape function	280
10.5. Smakula's formula and the effective-field correction	282
10.6. Einstein coefficients and the principle of detailed balance	289
10.7. The line-shape function with electron-lattice interaction	291
10.7.1. Introduction	291
10.7.2. Linear electron-lattice coupling	294
10.7.3. Beyond linear coupling	309

10.8.	Method of moments	310
10.8.1.	Introduction	310
10.8.2.	Non-degenerate states: linear and quadratic coupling	312
10.8.3.	The configuration-coordinate diagram	315
10.9.	Forbidden transitions: non-degenerate states	317
10.10.	Electronic degeneracy	320
10.10.1.	Introduction	320
10.10.2.	Splitting of optical bands due to degeneracy	323
10.10.3.	The Huang-Rhys factor with orbital degeneracy	328
10.10.4.	Antiresonances	328
10.11.	Photoionization of defects	331
10.11.1.	Introduction	331
10.11.2.	Dependence on the conduction band	333
10.11.3.	Dependence on the defect wavefunction	334
10.11.4.	Photoionization with phonon assistance	340
11.	DYNAMICS OF IMPERFECT LATTICES	342
11.1.	Introduction	342
11.2.	Comparison with electronic defect systems	345
11.3.	Defects in a linear chain	345
11.4.	The method of classical Green's functions	348
11.5.	The method of thermodynamic Green's functions	350
11.5.1.	Introduction	350
11.5.2.	Equations of motion	351
11.5.3.	Correlation functions	353
11.6.	Response functions	354
11.6.1.	Introduction	354
11.6.2.	Relation to classical Green's functions	355
11.6.3.	Absorption of energy from external forces	356
11.7.	The isotopic impurity	359
11.8.	Asymptotic expansions	361
11.8.1.	Local modes	363
11.8.2.	The existence of local modes	365
11.8.3.	Bounds on local modes	365
11.8.4.	Low-frequency resonance modes	368
11.8.5.	Anharmonicity of local modes and resonances	370
11.9.	Infrared absorption	375
11.9.1.	The dipole moment	375
11.9.2.	Charged defect in a homopolar lattice	376
11.9.3.	Charged defect in a polar lattice	377
11.10.	The $T$ -matrix	382

11.11. Thermal conductivity	383
11.11.1. Introduction: the relaxation time	383
11.11.2. The long-wavelength limit: Rayleigh scattering	385
11.11.3. The peak theorem	386
11.11.4. Summary and comparison with infrared absorption	389
<b>12. EXTERNAL FIELDS AND THEIR EFFECTS</b>	<b>390</b>
12.1. Introduction	390
12.2. Electric and optic fields: the Stark effect	390
12.2.1. Introduction: linear and quadratic Stark effects	390
12.2.2. Linear Stark effect	392
12.2.3. Effects of electric fields on wavefunctions	395
12.2.4. Reorientation of defect under electric fields	397
12.2.5. External optical fields	397
12.2.6. Secondary radiation: the Raman effect and hot luminescence	400
12.3. Magnetic fields: the Zeeman effect	402
12.3.1. Introduction	402
12.3.2. Zeeman effect in atoms and effective-mass systems	403
12.3.3. Linear Zeeman effect: general defects	413
12.3.4. Faraday rotation and related phenomena	416
12.4. Stress fields	422
12.4.1. Effects of stress on energy levels	423
12.4.2. Effects of stress on wavefunctions	426
12.5. Strong electron-lattice coupling: moment methods	428
12.5.1. Introduction	428
12.5.2. Zero-phonon lines	428
12.5.3. Broad-band transitions	429
12.5.4. Raman effect	434
12.5.5. The rigid-shift hypothesis	437
<b>13. ELECTRON-SPIN RESONANCE</b>	<b>438</b>
13.1. Introduction	438
13.2. The spin Hamiltonian	439
13.3. The Zeeman effect	442
13.3.1. Orbital angular momentum	444
13.3.2. Examples of g-factors	447
13.4. The zero-field splitting	450
13.5. Electron-nucleus interaction: hyperfine structure	455
13.5.1. Isotropic hyperfine interaction	457
13.5.2. Anisotropic hyperfine interaction	462
13.5.3. Coupling of nuclear moment to the electronic orbital moment	465

13.6. Quadrupole interaction	466
13.6.1. The electric field gradient	467
13.7. Measurement of lattice distortion by spin resonance	473
<b>14. NON-RADIATIVE PROCESSES AND INTERACTION OF FREE CARRIERS WITH DEFECTS</b>	477
14.1. Introduction	477
14.2. Non-radiative transitions	477
14.2.1. General theory	477
14.2.2. Paramagnetic relaxation	490
14.2.3. Resonant and non-resonant absorption	501
14.2.4. Temperature dependence of the zero-phonon line	505
14.3. Scatter of conduction electrons	512
14.3.1. Introduction	512
14.3.2. Limiting cases	514
14.3.3. Scatter by neutral impurities	515
14.3.4. Scatter by ionized impurities	517
14.3.5. Other approaches	519
14.4. Capture of electrons in solids	520
14.4.1. Introduction	520
14.4.2. Capture by phonon emission	522
14.4.3. The Auger effect and related phenomena	539
14.5. Kinetics	547
<b>IV. COMPARISON OF THEORY AND EXPERIMENT</b>	
<b>15. THE F-CENTRE AND RELATED ONE-CARRIER SYSTEMS</b>	555
15.1. Introduction	555
15.1.1. The hydrogen atom model of the F-centre	555
15.1.2. Empirical rules for optical absorption	556
15.1.3. Optical emission and the relaxed excited state	558
15.1.4. Empirical rules for optical emission	561
15.1.5. Other one-carrier centres	561
15.2. The ground-state configuration of the F-centre	562
15.2.1. Introduction	562
15.2.2. Optical absorption	562
15.2.3. Electron spin resonance	571
15.2.4. Spin-orbit coupling	574
15.2.5. Response to stress	577
15.2.6. Response to electric fields	581
15.2.7. Optical absorption line-shapes	583

15.3. Excited-state configuration of the F-centre	595
15.3.1. Introduction	595
15.3.2. Calculations of the relaxed excited state	596
15.3.3. Model calculations of the F-centre excited states	602
15.4. Perturbed F-centres	608
15.4.1. Introduction	608
15.4.2. The $F_A$ -centre	608
15.4.3. Photochromic centres in $\text{CaF}_2$	613
15.4.4. The $M^+$ -centre	613
15.4.5. The $Z_1$ -centre	614
15.5. Antimorphs of the F-centre: trapped-hole centres	615
15.5.1. Trapped-hole centres in oxides	615
15.5.2. The zinc vacancy in ZnSe	618
16. CENTRES WITH TWO CARRIERS	620
16.1. Introduction	620
16.2. The $F'$ -centre	620
16.2.1. Bound states in the alkali halides	620
16.2.2. Bound states in the alkaline earth oxides	623
16.3. Two electrons at close anion vacancies	625
16.3.1. The M-centre	625
16.3.2. The $F_1$ -centre in alkaline earth oxides	627
16.4. Two-hole centres in the alkaline earth oxides	629
17. THE R-CENTRE	631
17.1. Introduction	631
17.2. Electronic structure of the R-centre	632
17.2.1. The Kern-Bartram model	632
17.3. The R-centre and the Jahn-Teller effect	638
17.3.1. Introduction	638
17.3.2. Wavefunctions	638
17.3.3. Optical matrix elements and transition probabilities	640
17.3.4. Response to external fields	640
17.3.5. Comparison of LHOPS theory with the R-centre: summary	651
18. THE $V_k$ -CENTRE AND THE RELAXED EXCITON	653
18.1. Introduction	653
18.2. Atomic configuration of the $V_k$ -centre	655
18.3. Optical transitions	658
18.4. Spin resonance	661
18.5. The $V_k$ -centre as a molecule in a crystal	663
18.6. Motion of the $V_k$ -centre	664
18.7. The relaxed exciton in ionic crystals: $[V_k e]$	667

19. THE H-CENTRE AND OTHER INTRINSIC INTERSTITIALS	670
19.1. Introduction	670
19.2. Anion interstitials in ionic crystals	670
19.2.1. Defect structures	670
19.2.2. Theory of the H-centre lattice configuration	672
19.2.3. Interactions with other defects	674
19.2.4. Electronic structure of the H-centre	675
19.3. Interstitials in valence crystals	677
19.3.1. Experiment and the interstitial	677
19.3.2. Theories of interstitial migration	678
19.3.3. Theories of interstitial electronic structure	680
20. HYDROGEN IN IONIC CRYSTALS: $U^-$ , $U_1^-$ , AND $U_2$ -CENTRES	681
20.1. Introduction	681
20.2. The interstitial atom $H_1^0$ ( $U_2$ -centre)	682
20.2.1. Nature of the ground state: spin resonance	682
20.2.2. Optical properties of $H_1^0$	687
20.3. The substitutional hydrogen ion $H_s^-$ ( $U$ -centre)	688
20.3.1. Optical properties	688
20.3.2. Infrared absorption: the local mode	692
21. THE REORIENTATION OF DEFECTS IN SOLIDS	699
21.1. Introduction	699
21.2. Electric dipole centres	699
21.2.1. $CN^-$ and $OH^-$ in alkali halides	699
21.2.2. Hydrogen halides in rare-gas hosts	703
21.3. Elastic dipole centres: the $O_2^-$ molecular ion	704
21.4. Off-centre ions	710
21.4.1. The KCl: Li system	710
21.4.2. Occurrence of off-centre ions	712
21.4.3. Oxygen interstitial in silicon	714
22. TRANSITION-METAL IONS	717
22.1. Introduction	717
22.2. Classes of theory and coupling schemes	718
22.3. The iron-group in cubic symmetry	720
22.3.1. The cubic field splitting	720
22.3.2. Theories of the cubic field splitting	721
22.3.3. Distribution of electrons over orbitals	725
22.3.4. Optical properties	727
22.3.5. Spin resonance parameters	733

22.4. Rare-earth ions	742
22.4.1. Free rare-earth ions	742
22.4.2. Crystal fields for rare-earth ions	745
23. SHALLOW DONORS AND ACCEPTORS IN SEMICONDUCTORS	751
23.1. Introduction	751
23.2. The application of effective-mass theory : non-degenerate bands	751
23.2.1. Energy levels	752
23.2.2. Wavefunctions	755
23.2.3. Response to perturbations	757
23.3. Applications of effective-mass theory : degenerate bands	758
23.3.1. Energy levels and wavefunctions	758
23.4. Corrections to effective-mass theory	762
23.4.1. Terms which depend only on the host	764
23.4.2. Corrections which depend in detail on the electronic structure of the defect	766
23.4.3. Lattice deformation	775
24. ISOELECTRONIC IMPURITIES	781
24.1. Introduction	781
24.2. Binding mechanisms	782
24.2.1. Mechanisms independent of lattice distortion	782
24.2.2. Mechanisms which involve lattice distortion	787
24.3. The one-band, one-site model	790
24.3.1. Band structure	790
24.3.2. Energy levels : bound states and resonances	792
24.3.3. Optical line-shapes	794
24.4. Beyond the one-band, one-site model	800
24.4.1. The single impurity bound state	800
24.4.2. The nitrogen pair bound state	801
24.4.3. Phenomenology : use of an effective range and depth potential	802
24.5. Phonon structure in optical spectra	803
25. DIPOLAR SYSTEMS AND DONOR-ACCEPTOR PAIRS	806
25.1. Introduction	806
25.1.1. Lattice geometry	807
25.2. Transition energies	808
25.2.1. One carrier bound to a finite dipole	808
25.2.2. Pair recombination spectra	813
25.3. Transition probabilities	822
25.3.1. Basic theory	822

# CONTENTS

xix

25.3.2. Time dependence of recombination	826
25.3.3. Other transitions	827
26. BOUND EXCITONS	829
26.1. Introduction	829
26.2. Quantum chemistry of the bound exciton	829
26.2.1. Introduction	829
26.2.2. Basic transition energies	830
26.2.3. Electron bound to a neutral donor, and its antimorph	831
26.2.4. Exciton bound to ionized donor, and its antimorph	832
26.2.5. Exciton bound to neutral donor, and its antimorph	838
26.2.6. Other systems	842
26.3. Other properties of bound-exciton systems	843
26.3.1. The Jahn-Teller effect	843
26.3.2. Optical line-shapes	844
26.3.3. Undulation spectra	846
26.4. Response to external fields	848
26.4.1. Zeeman effect	848
26.4.2. Response to stress	850
27. VACANCIES IN VALENCE CRYSTALS	851
27.1. Introduction	851
27.2. Vacancy centres in silicon	852
27.3. Other observations of vacancy centres	857
27.4. Electronic structure in the undistorted lattice	860
27.4.1. Defect-molecule models	860
27.4.2. Cluster models	865
27.4.3. Other methods	869
27.4.4. The one-electron approximation	871
27.4.5. Summary	872
27.5. Electronic structure with lattice distortion	873
27.5.1. Basic assumptions	873
27.5.2. Forces causing distortion	874
27.5.3. Effective frequencies: the lattice response	875
27.5.4. Consequences of lattice relaxation	878
27.6. Summary of problems	882
APPENDIX I	
Sum rules	884
APPENDIX II	
The factorization of secular equations	887
REFERENCES	889
AUTHOR INDEX	925
SUBJECT INDEX	945



I  
THE PERFECT SOLID