

Contents

Preface 7

Introduction 11

Chapter 1 Principles of the one-electron theory

Part 1

Theoretical principles of the pseudopotential method

Chapter 2. Scattering theory for “solid-state people”

2.1. Mathematical formalism 23

2.2. Scattering on an isolated potential 31

2.3. Pseudism and scattering 46

2.4. Bound states, pseudopotentials and the convergence of series 54

2.5. Scattering theory and potential formfactors 61

Chapter 3. Theory of potential

3.1. Potential seen by an atomic electron 69

3.2. Dielectric screening 83

3.3. The self-consistency of pseudopotential and additive screening 99

3.4. Muffin-tin potential 107

3.5. Average value of the screened potential 124

Chapter 4. Theory of pseudopotential formfactors

4.1. Nonlocality, the energy dependence of formfactors and perturbation theory 132

4.2. The OPW formfactor 144

4.3. Phase-shift formfactors 157

4.4. Effective medium and pseudopotential formfactors 173

Chapter 5. Pseudism and the secular equations of band theory

5.1. The Green’s function (or KKR) method 181

5.2. Pseudopotential secular equations 196

Part 2

The use of pseudopotential theory for crystal-structure calculations

Chapter 6. Formalism of crystal-structure energy calculations

6.1. Basic assumptions 205

6.2. Band structure energy of pure metals and binary alloys 205

6.3. Electrostatic energy 223

Contents

- 6.4. The total internal energy of an alloy: second-order perturbation theory and the locality approximation 227
 - 6.5. Higher-order perturbation analysis 232
 - 6.6. OPW nonlocal alloy theory 236
- Chapter 7. Pseudopotential theory of alloys. Structure stability application
- 7.1. Phase boundaries in terms of pseudopotential theory 241
 - 7.2. Ordered phases, their structures, and existence conditions 245
 - 7.3. Short-range order problems 256
 - 7.4. Crystal structure stability in the OPW approach 261
- Chapter 8. Pseudopotential theory and imperfections in crystals
- 8.1. Introductory remarks 267
 - 8.2. Crystal lattice vibrations 267
 - 8.3. Static imperfections 279
- Chapter 9. Principles of pseudopotential calculations of the properties of metals
- 9.1. General 287
 - 9.2. Calculation of the atomic properties of crystalline metals and alloys 287
 - 9.3. Transport properties of noncrystalline metals and alloys 297
- References 317
- Index 331