Contents

1 Introduction
   1.1 General Aspects of Amorphous Semiconductors 1
   1.2 Chalcogenide Glasses 3
   1.3 Applications of Amorphous Semiconductors 3
   References 3

2 Preparation Techniques
   2.1 Growth of a-Si:H Films 5
      2.1.1 PECVD Technique 5
      2.1.2 HWCVD Technique 6
   2.2 Growth of Amorphous Chalcogenides 6
   References 8

3 Structural Properties of Amorphous Silicon and Amorphous Chalcogenides 11
   3.1 General Aspects 11
      3.1.1 Definitions of Crystalline and Noncrystalline 11
   3.2 Optical Spectroscopy 12
      3.2.1 Raman Scattering 12
      3.2.2 Infrared Absorption 13
   3.3 Neutron Diffraction 15
      3.3.1 Diffraction Measurements on Amorphous Silicon 17
      3.3.2 Diffraction Measurements on Hydrogenated Amorphous Silicon 18
      3.3.3 Diffraction Measurements on Amorphous Germanium 19
      3.3.4 Diffraction Measurements on Amorphous Selenium 19
### Contents

#### 3.4 Computer Simulations
- 3.4.1 Monte Carlo-Type Methods for Structure Derivation 20
- 3.4.2 Atomic Interactions 21
- 3.4.3 a-Si Models Constructed by Monte Carlo Simulation 25
- 3.4.4 Reverse Monte Carlo Methods 26
- 3.4.5 a-Si Model Constructed by RMC Simulation 28
- 3.4.6 a-Se Model Constructed by RMC Simulation 30
- 3.4.7 Molecular Dynamics Simulation 32
- 3.4.8 a-Si Model Construction by Molecular Dynamics Simulation 34
- 3.4.9 a-Si:H Model Construction by Molecular Dynamics Simulation 34
- 3.4.10 a-Se Model Construction by Molecular Dynamics Simulation 35
- 3.4.11 Car and Parrinello Method 38

References 38

#### 4 Electronic Structure of Amorphous Semiconductors 43
- 4.1 Bonding Structures 43
  - 4.1.1 Bonding Structures in Column IV Elements 44
  - 4.1.2 Bonding Structures in Column VI Elements 45
- 4.2 Electronic Structure of Amorphous Semiconductors 46
- 4.3 Fermi Energy of Amorphous Semiconductors 47
- 4.4 Differences between Amorphous and Crystalline Semiconductors 49
- 4.5 Charge Distribution in Pure Amorphous Semiconductors 49
- 4.6 Density of States in Pure Amorphous Semiconductors 52
- 4.7 Dangling Bonds 54
- 4.8 Doping 57

References 58

#### 5 Electronic and Optical Properties of Amorphous Silicon 61
- 5.1 Introduction 61
- 5.2 Band Tails and Structural Defects 62
  - 5.2.1 Introduction 62
  - 5.2.2 Band Tails 62
  - 5.2.3 Structural Defects 66
- 5.3 Recombination Processes 68
  - 5.3.1 Introduction 68
  - 5.3.2 Radiative Recombination 68
<table>
<thead>
<tr>
<th>Section</th>
<th>Title</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>5.3.3</td>
<td>Nonradiative Recombination</td>
<td>70</td>
</tr>
<tr>
<td>5.3.4</td>
<td>Recombination Processes and Recombination Centers in a-Si:H</td>
<td>72</td>
</tr>
<tr>
<td>5.3.5</td>
<td>Spin-Dependent Recombination</td>
<td>73</td>
</tr>
<tr>
<td>5.4</td>
<td>Electrical Properties</td>
<td>74</td>
</tr>
<tr>
<td>5.4.1</td>
<td>DC Conduction</td>
<td>74</td>
</tr>
<tr>
<td>5.4.2</td>
<td>AC Conduction</td>
<td>80</td>
</tr>
<tr>
<td>5.4.3</td>
<td>Hall Effect</td>
<td>87</td>
</tr>
<tr>
<td>5.4.4</td>
<td>Thermoelectric Power</td>
<td>88</td>
</tr>
<tr>
<td>5.4.5</td>
<td>Doping Effect</td>
<td>89</td>
</tr>
<tr>
<td>5.5</td>
<td>Optical Properties</td>
<td>92</td>
</tr>
<tr>
<td>5.5.1</td>
<td>Fundamental Optical Absorption</td>
<td>92</td>
</tr>
<tr>
<td>5.5.2</td>
<td>Weak Absorption</td>
<td>94</td>
</tr>
<tr>
<td>5.5.3</td>
<td>Photoluminescence</td>
<td>96</td>
</tr>
<tr>
<td>5.5.4</td>
<td>Frequency-Resolved Spectroscopy (FRS)</td>
<td>96</td>
</tr>
<tr>
<td>5.5.5</td>
<td>Photoconductivity</td>
<td>101</td>
</tr>
<tr>
<td>5.5.6</td>
<td>Dispersive Photoconduction</td>
<td>109</td>
</tr>
<tr>
<td>5.6</td>
<td>Electron Magnetic Resonance and Spin-Dependent Properties</td>
<td>112</td>
</tr>
<tr>
<td>5.6.1</td>
<td>Introduction</td>
<td>112</td>
</tr>
<tr>
<td>5.6.2</td>
<td>Electron Magnetic Resonance</td>
<td>112</td>
</tr>
<tr>
<td>5.6.3</td>
<td>Spin-Dependent Properties</td>
<td>128</td>
</tr>
<tr>
<td>5.7</td>
<td>Light-Induced Phenomena and Light-Induced Defect Creation</td>
<td>131</td>
</tr>
<tr>
<td>5.7.1</td>
<td>Introduction</td>
<td>131</td>
</tr>
<tr>
<td>5.7.2</td>
<td>Light-Induced Phenomena</td>
<td>132</td>
</tr>
<tr>
<td>5.7.3</td>
<td>Light-Induced Defect Creation</td>
<td>134</td>
</tr>
<tr>
<td>6</td>
<td>Electronic and Optical Properties of Amorphous Chalcogenides</td>
<td>157</td>
</tr>
<tr>
<td>6.1</td>
<td>Historical Overview of Chalcogenide Glasses</td>
<td>157</td>
</tr>
<tr>
<td>6.1.1</td>
<td>Applications</td>
<td>157</td>
</tr>
<tr>
<td>6.1.2</td>
<td>Science</td>
<td>158</td>
</tr>
<tr>
<td>6.2</td>
<td>Basic Glass Science</td>
<td>159</td>
</tr>
<tr>
<td>6.2.1</td>
<td>Glass Formation</td>
<td>159</td>
</tr>
<tr>
<td>6.2.2</td>
<td>Glass Transition Temperature</td>
<td>160</td>
</tr>
<tr>
<td>6.2.3</td>
<td>Crystallization of Glasses</td>
<td>162</td>
</tr>
<tr>
<td>6.3</td>
<td>Electrical Properties</td>
<td>165</td>
</tr>
<tr>
<td>6.3.1</td>
<td>Electronic Transport</td>
<td>165</td>
</tr>
<tr>
<td>6.3.2</td>
<td>Ionic Transport</td>
<td>170</td>
</tr>
<tr>
<td>6.4</td>
<td>Optical Properties</td>
<td>175</td>
</tr>
<tr>
<td>6.4.1</td>
<td>Fundamental Optical Absorption</td>
<td>175</td>
</tr>
<tr>
<td>6.4.2</td>
<td>Urbach and Weak Absorption Tails</td>
<td>178</td>
</tr>
</tbody>
</table>
6.4.3 Photoluminescence
6.4.4 Photoconduction
6.5 The Nature of Defects, and Defect Spectroscopy
6.5.1 Electron Spin Resonance
6.5.2 Optical Absorption
6.5.3 Primary Photoconductivity
6.5.4 Secondary Photoconductivity
6.5.5 Electrophotography
6.5.6 Electronic Transport
6.6 Light-Induced Effects in Chalcogenides
6.6.1 Electron Spin Resonance
6.6.2 Optical Absorption
6.6.3 Photoluminescence
6.6.4 Photoconductivity
6.6.5 Electronic Transport
6.6.6 Defect Creation Kinetics
6.6.7 Structure-Related Properties
References

7 Other Amorphous Material Systems
7.1 Amorphous Carbon and Related Materials
7.1.1 Basic Structure of a-C (sp² Hybrids)
7.1.2 Preparation Techniques
7.1.3 Brief Review of Structural Studies on Amorphous Carbon
7.1.4 Applications
7.2 Amorphous Oxide Semiconductors
7.2.1 Preparation Techniques
7.2.2 Optical Properties
7.2.3 Electronic Properties
7.2.4 Applications
7.3 Metal-Containing Amorphous Chalcogenides
7.3.1 Preparation Techniques
7.3.2 Structure of Ag-Chs and Related Physical Properties
7.3.3 Photodoping
7.3.4 Applications
References

8 Applications
8.1 Devices Using a-Si:H
8.1.1 Photovoltaics
8.1.2 Thin-Film Transistors
8.2 Devices Using a-Chs
   8.2.1 Phase-Change Materials 249
   8.2.2 Direct X-ray Image Sensors for Medical Use 257
   8.2.3 High-Gain Avalanche Rushing Amorphous Semiconductor Vidicon 258
   8.2.4 Optical Fibers and Waveguides 260
References 261

Index 265