

Contents

1 Relation of $A^{II}B_2^{III}X_4^{VI}$ Compounds to Other Materials, Their Properties and Applications (Instead of Introduction)	1
V. V. Ursaki and I. M. Tiginyanu	
1.1 $A^{II}B_2^{III}X_4^{VI}$ Compounds Among Other Ternary and Multinary Compounds	2
1.2 Crystal Growth	13
1.3 Crystal Structure	19
1.4 Energy Band Structure	23
1.5 Optical and Radiative Properties	31
1.6 Vibrational Properties	39
1.7 Applications	41
1.8 Trends in Temperature- and Pressure-Induced Phase Transitions	44
1.9 Conclusions	45
References	47
Part I Spinel-Structured AB_2X_4 Chalcogenide Compounds	
2 AB_2O_4 Compounds at High Pressures	53
Daniel Errandonea	
2.1 Introduction	53
2.2 Isothermal Compression of the Spinel Phase: X-ray Diffraction Studies	55
2.3 High Pressure Phases of Oxospinels	59
2.4 Lattice Vibrations in Spinels	62
2.5 High-Pressure Raman Scattering Studies	65
2.6 Raman of Post-Spinel Phases	66
2.7 Elastic Constants	67
2.8 Miscellaneous	69
2.9 Summary	69
References	70

3 AB₂S₄ and AB₂Se₄ Compounds at High Pressures	75
David Santamaría-Pérez and Javier Ruiz-Fuertes	
3.1 Introduction	75
3.2 High-Pressure Studies in Sulfide and Selenide Spinels	78
3.2.1 High-Pressure Studies on Thiospinels	78
3.2.2 High-Pressure Studies on Selenospinels	79
3.3 High-Pressure Structural Study of Indium Thiospinels	81
3.3.1 Low-Pressure Spinel Phase.	81
3.3.2 Phase Transition and the High-Pressure Post-Spinel Phase.	85
3.4 High-Pressure Vibrational Study of Indium Thiospinels	86
3.4.1 Low-Pressure Spinel Phase.	87
3.4.2 High-Pressure Phase	91
3.5 Experimental High-Pressure Optical Absorption Study of Indium Thiospinels	93
3.5.1 Low-Pressure Spinel Phase.	93
3.5.2 High-Pressure Phase	98
3.6 Conclusions	98
References	99
4 Theoretical Ab Initio Calculations in Spinels at High Pressures	103
P. Rodríguez-Hernández and A. Muñoz	
4.1 Introduction	103
4.2 Crystal Structure. Calculations of the Spinel Phase	104
4.3 Elastic Properties.	109
4.4 Electronic Structure	112
4.5 Vibrational Analysis	116
4.6 Pressure-Induced Phase Transitions in Spinels.	120
4.7 Conclusions	125
References	125

Part II Ordered-Vacancy AB₂X₄ Chalcogenide Compounds

5 AB₂S₄ Ordered-Vacancy Compounds at High Pressures	133
Francisco Javier Manjón and Rosario Isabel Vilaplana	
5.1 Introduction	133
5.2 Isothermal Compression of AB ₂ S ₄ OVCs: X-ray Diffraction Studies	138
5.3 Pressure-Induced Phase Transitions in Adamantine OVCs	141
5.4 High-Pressure Raman Studies of AB ₂ S ₄ OVCs	150
5.5 Conclusions	157
References	158

6 AB₂Se₄ Ordered-Vacancy Compounds at High Pressures	163
Óscar Gomis and Francisco Javier Manjón	
6.1 Introduction	163
6.2 Isothermal Compression of AB ₂ Se ₄ OVCs: X-ray Diffraction Studies	166
6.3 Pressure-Induced Phase Transitions in Adamantine OVCs	171
6.4 High-Pressure Raman Studies of AB ₂ Se ₄ OVCs	173
6.5 High-Pressure Optical Absorption Studies of AB ₂ Se ₄ OVCs	178
6.6 Conclusions	180
References	181
7 Theoretical Ab Initio Calculations in Ordered-Vacancy Compounds at High Pressures	185
A. Muñoz and M. Fuentes-Cabrera	
7.1 Introduction	185
7.2 Theoretical Background	186
7.3 Structural Considerations	188
7.4 Electronic Band Structure and Optical Properties	189
7.5 Vibrational Properties Under Hydrostatic Pressure	191
7.6 Elastic Properties Under Pressure	194
7.7 Theoretical Study of CdIn ₂ Se ₄ in the Pseudo-Cubic Phase	200
7.8 Conclusions	207
References	207
Part III AB₂X₄ Chalcogenide Compounds with Other Types of Structures	
8 AB₂X₄ Compounds with Other Types of Structures at High Pressures	213
V. V. Ursaki and I. M. Tigranyan	
8.1 A Comparison of Pressure Induced Phase Transitions in Wutrzite and Spinel Phases of the ZnAl ₂ S ₄ Compound	213
8.2 Raman Scattering Study of Pressure Induced Phase Transitions in ZnAl _{2(1-x)} Ga _{2x} S ₄ Solid Solutions	222
8.3 Raman Scattering Study of Layered AlInGaS ₄ (A = Zn, Cd, Mg) Compounds Under Hydrostatic Pressure	228
8.4 Conclusions	233
References	234
9 Epilogue	237
Francisco Javier Manjón, Ion Tigranyan and Veaceslav Ursaki	
Index	239