

**EUROPEAN MINERALOGICAL UNION**



**EMU NOTES IN  
MINERALOGY**

**1**

**Modular Aspects  
of Minerals**

Edited by  
**STEFANO MERLINO**

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OF MINERALS**

UNIVERSITY TEXTBOOK

Edited by  
**Stefano Merlino**



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## Foreword

The European Mineralogical Union (EMU) was founded in 1989 to “further European cooperation in the Mineralogical Sciences” as stated in its constitution. Besides sponsoring European meetings (e.g. EMPG series) and organizing symposia (e.g., at the EUG conferences in Strasbourg), particular attention is paid to editorial initiatives as the foundation and the scientific management of the *European Journal of Mineralogy* (EJM). EMU officers began some years ago to discuss about the organization of Schools and annexed Notes. Now this Project is born and for sure the EMU Schools and the European Mineralogical Union Notes in Mineralogy, briefly *EMU Notes in Mineralogy*, shall contribute to realize the constitutional goal of EMU.

With the present book *Modular aspects of minerals*, edited by Stefano Merlino, appears the first volume of the EMU Notes in Mineralogy. The Notes are the edited version of the lectures presented at the first EMU School of Mineralogy in Budapest in December 1997. We experience herewith the start of a series of EMU Schools, which are planned to take place about once a year, and of EMU Notes in Mineralogy published in connection with and accompanying the Schools.

What do we intend by these EMU Notes? There are already excellent and successful series published by national mineralogical societies. Why an additional series? We think that there is still much need for high scientific quality and moderately priced books of this type on selected topics of the mineralogical sciences with contributions from experts in their field. The EMU Notes in Mineralogy shall serve as review volumes for university teachers preparing their lectures, and introduce students at different levels and advanced scientists into special fields of research. At the same time, the Notes will reflect the state of the art. Experience shows that – like in sport – there is no top science without a wide, deep and strong basement of well-trained students and scientists and vice versa. Therefore, it is quite natural that EMU, as umbrella organization of the mineralogical societies and groups in Europe, is engaged in ventures like Schools and Notes. We wish to communicate the achievements of our mineralogical sciences to as many mineralogists as possible and also to scientists of other fields, e.g. materials science.

We are very grateful to Stefano Merlino and the contributors of the lectures for starting the venture of EMU School and Notes in Mineralogy with the topic “Modular Aspects of Mineralogy”, and to Tamás G. Weiszburg, Secretary of EMU, for his untiring commitment in that matter, besides of many other things like locally organizing the School at Budapest. Particular thanks are due to the Editors and the Managing Committee of the *European Journal of Mineralogy* for advice and friendly support in the development of the project. Finally, we thank Gábor Papp for his patient and valuable work as technical editor and the Eötvös University Press at Budapest for its enterprise and cooperation in publishing the Notes.

*Giovanni Ferraris*  
Past-President of EMU

*Wolfgang Friedrich Müller*  
President of EMU

## **Conventions, recommendations and standards used in this volume**

**Mineral names:** Recommendations of the IMA CNMMN

**Crystallographic symbols:** As used in the *International Tables of Crystallography, Volume A, Space-Group Symmetry*; edited by Th. Hahn; fourth, revised edition; Dordrecht, Boston, London: Kluwer; 1995

**Transcription of Cyrillic characters:** British Standard 2979:1958

### **Notes on the usage of the References lists**

Multiple references to an author are listed in the following order: (1) publications of the author alone, in *chronological order*; (2) publications of the author with a single co-author, in *alphabetical order of the co-authors*; (3) publications of an author with more than one co-author in *chronological order*.

Journal names are abbreviated according to the ISDS standards (except for the usage of capital letters and the transcription of Cyrillic characters), wherever available.

# Contents

<b>Preface of the Editor</b> by <b>STEFANO MERLINO</b> .....	XIII
---	------

## **Chapter 1. OD theory: fundamentals and applications**

<b>Fundamentals of the OD theory</b> by <b>SLAVOMIL ĐUROVIČ</b> .....	3
Introduction – the notion of polytypism.....	3
Polytypes and OD structures.....	5
Case study 1: close packing of spheres.....	5
Polytype families and OD groupoid families.....	7
Standard polytypes and MDO polytypes.....	7
Case study 2: a hypothetical OD structure.....	9
Diffraction pattern – structure analysis.....	11
Superposition structures versus family structure.....	12
The vicinity condition.....	12
Categories of OD structures.....	13
OD structures of equivalent layers.....	13
Symbols for OD groupoid families.....	14
The <i>NFZ</i> relations.....	15
OD structures with more than one kind of layer.....	16
Symbols for OD groupoid families.....	17
The <i>NFZ</i> relations.....	19
OD packets.....	19
Derivation of MDO polytypes.....	19
Example 1: SiC.....	20
Example 2: hypothetical.....	21
Example 3: pyrophyllite.....	22
Desymmetrization of OD structures.....	24
Concluding remarks.....	24
Proposal for a definition of layer polytypism.....	25
A note for authors.....	26
References.....	26

## **OD approach in minerals: examples and applications**

by <b>STEFANO MERLINO</b> .....	29
Introduction.....	29
OD structures consisting of equivalent layers.....	30
OD character of wollastonite.....	31
Structures with maximum degree of order (MDO structures) in wollastonite family.....	33
Derivation of the OD groupoid family of wollastonite from the diffractive features.....	35
Polytypism in brochantite, revealed through an OD approach.....	36
OD character of CSH compounds.....	39

## VI

Clinotobermorite: discussion of its OD character and derivation of the MDO polytypes.....	39
Symmetry of the two MDO polytypes in clinotobermorite.....	41
OD character of the structural family of hillebrandite .....	42
Family of hillebrandite OD structures built up by $Pmn2_1$ layers .....	44
OD families of shattuckite and planchéite.....	46
Shattuckite OD family .....	46
Planchéite OD family.....	49
Conclusion .....	50
Acknowledgements.....	50
Appendix.....	50
A1. Diffraction effects in clinotobermorite.....	50
A2. Application of the OD procedure to the family (A) in hillebrandite .....	52
References.....	53

## Chapter 2. Modular aspects of layer silicates

### Theoretical derivation and identification of possible two-layer lizardite polytypes

by ISTVÁN DÓDONY.....	57
Introduction.....	57
The one- and two-layer lizardite polytypes .....	59
Calculated X-ray diffraction patterns .....	60
SAED pattern simulations.....	60
Identification of lizardite polytypes by X-ray powder diffraction.....	65
Identification of lizardite polytypes by SAED and TEM .....	66
Conclusions.....	69
Acknowledgements .....	69
References.....	69
Appendix.....	69

### Crystallography of mica polytypes

by MASSIMO NESPOLO, HIROSHI TAKEDA and GIOVANNI FERRARIS.....	81
Introduction.....	81
Mica unit layer .....	82
General classification of mica polytypes .....	85
Twin laws for mica polytypes .....	86
Alternative description of $\sigma$ twin laws .....	89
Diffraction patterns from twins .....	91
Reticular classification of mica polytypes.....	92
Axial settings for mica polytypes .....	93
Class <i>a</i> .....	93
Class <i>b</i> .....	94
Fixed-angle setting for Class <i>a</i> .....	95
Fixed-angle setting for Class <i>b</i> .....	97
Axial settings for 3 <i>K</i> -layer polytypes.....	98
Axial transformations.....	99
Inconsistent choice of the axial setting.....	101
Geometrical features of $2M_1$ lattice.....	104
Geometrical features of $2M_2$ lattice.....	107
Ambiguity of the axial choice for $2M_1$ and $2M_2$ polytypes .....	110

Geometrical features of 3T lattice .....	111
Indexing of 4M <sub>1</sub> polytype .....	112
Discussion .....	113
Appendix .....	115
Symbols .....	115
Matrix formalism .....	115
Acknowledgements .....	116
References .....	116
<b>Equilibrium and kinetic processes for polytype and polysome generation</b> by ALAIN BARONNET .....	119
Introduction .....	119
What are polytypes? .....	119
What are polysomes? .....	122
Topologic features relevant to polytypism and polysomatism .....	123
Linear defects .....	123
Planar defects .....	124
Physical faults .....	125
<i>Intrinsic faults</i> 125 • <i>Extrinsic faults</i> 125 • <i>Growth faults</i> 125	
<i>Deformation faults</i> 125 • <i>Layer displacement faults</i> 126	
Chemical faults .....	126
Recognizing stacking order-disorder .....	127
Ordered or regular sequences .....	128
Basic structures and long-period polytypes .....	130
Regular and long-period polysomes .....	131
Disordered polytypes and polysomes, and faulted sequences .....	132
The special case of cylindrical lattices .....	134
<i>Radial polytypism in chrysotile</i> 135 • <i>A rosette of polytypes</i>	
<i>in polygonal serpentine</i> 136 • <i>Layer rotations in conical serpentine</i> 137	
Polytypes and polysomes: equilibrium or disequilibrium structures? .....	138
Some arguments for a thermodynamic influence .....	138
Some models based on thermodynamic control .....	138
The Jagodzinski's disorder theory .....	138
The ANNNI model .....	139
Selje's model based on phase transition theory .....	140
Arguments for disequilibrium .....	140
Models on growth around screw dislocations .....	140
The perfect-matrix model of spiral growth (PMM) .....	141
The faulted-matrix model of spiral growth (FMM) .....	142
PMM and FMM models facing real growth patterns .....	142
Extension of the concept of growth spiral .....	144
Extensions to polysomes? .....	145
Limitations of spiral growth models .....	145
Model on transformation around screw dislocations .....	146
Detailed stacking sequences as chaotic arrangements .....	147
Models for polytypes .....	147
Possible model for polysomes .....	148
Summary and conclusion .....	148
References .....	149



## VIII

### Mixed-layer minerals

by VICTOR A. DRITS .....	153
Introduction.....	153
Types of mixed-layer structures .....	154
Irregular mixed-layer structures .....	157
Statistical models .....	157
Degree of homogeneity-heterogeneity for a powder of thin interstratified crystals .....	159
Methods for the structural and crystallochemical study of mixed-layer minerals .....	160
Diffraction effects and Mering's principles .....	162
The Q rule, a reflection broadening description.....	164
Simulation of XRD patterns; advantages and limitations .....	165
Structural study of mixed-layer minerals; basal reflection analysis .....	170
A peak migration technique.....	171
Qualitative comparison of calculated and experimental XRD patterns .....	171
Quantitative comparison of calculated and experimental XRD patterns .....	173
Structural study of mixed-layer minerals by SAED and EDA .....	174
Structural study of irregular mixed-layer minerals by HRTEM .....	178
Geological occurrence of mixed-layer minerals .....	179
Expandable mixed-layer mica minerals .....	180
Illite/smectite .....	180
Leucophyllite/smectite.....	182
Fe <sup>3+</sup> -rich dioctahedral mica/smectites (celadonite/nontronites, glauconite/nontronites).....	182
Mixed-layer kaolinite/montmorillonite and kaolinite/montmorillonite/illite .....	183
Trioctahedral mica/vermiculites and mica/smectites .....	183
Expandable mixed-layer chlorite minerals.....	184
Trioctahedral chlorite/smectite .....	184
Dioctahedral chlorite/smectite (tosudite).....	184
Non-expandable mixed-layer chlorite minerals .....	184
Serpentine/chlorites .....	184
Biotite/chlorites .....	185
Conclusions.....	185
Acknowledgements .....	186
References .....	186

## Chapter 3. Modular aspects of sulphides and sulphosalts

### Modular structures in sulphides: sphalerite/wurtzite-, pyrite/marcasite- and pyrrhotite-type minerals

by MIHÁLY PÓSFÁI and PETER R. BUSECK .....	193
Introduction.....	193
Sphalerite/wurtzite group .....	194
Basic structures .....	194
Models of planar defects .....	195
Observed stacking defects.....	199
Ordering in sphalerite- and wurtzite-type structures .....	205
Ordering of Sb and Cu at stacking faults in luzonite and in ordered 24R enargite .....	207
Sb-content and the structure of enargite/luzonite.....	209

Pyrite/marcasite group .....	211
The structures of pyrite and marcasite .....	211
Mixed pyrite/marcasite structures with disordered and ordered stackings.....	213
Ordered substitutions in the S positions .....	214
Non-cubic symmetry and As in pyrite .....	217
Effects of marcasite lamellae on the symmetry and composition of pyrite.....	218
Forbidden reflections and domain structure .....	220
Pyrrhotite .....	220
The structures of ordered pyrrhotite types .....	221
Intergrowths of nC pyrrhotite types.....	223
Disordered vacancy distribution in nA pyrrhotite.....	225
Structure and magnetic properties .....	227
Structural relationship between pyrrhotite and marcasite.....	228
Conclusions .....	230
Acknowledgements.....	230
References.....	230

### **Modular crystal chemistry of sulphosalts and other complex sulphides**

by EMIL MAKOVICKY .....	237
Crystal structures of sulphosalts and other complex sulphides .....	237
Sulphide families with recombination structures.....	237
Typical coordination polyhedra.....	238
Large-scale crystal chemistry: archetypes and structure building principles .....	240
The homologous series and higher categories.....	242
The accretional series .....	242
The variable-fit series .....	243
The plesiotype and merotype families .....	243
Case studies .....	244
The lillianite accretional series .....	244
The pavonite accretional series.....	247
The sartorite combinatorial series.....	248
The meneghinite accretional series.....	252
Rod-based sulphosalts: a plesiotype family.....	254
The hutchinsonite family of merotypes .....	257
Plesiotypes derived from cannizzarite by crystallographic shear and out-of-phase boundaries.....	259
Solutions to the problems on meneghinite homologues .....	265
Solutions to the problems on derivatives of cannizzarite .....	266
Weibullite plesiotypes.....	266
Weibullite 266 • $Pb_4In_3Bi_7S_{18}$ 266 • $PbBi_2S_4$ (galenobismutite) 266	
Junoite plesiotypes .....	266
Junoite 266	
Rod-based plesiotype family.....	266
Cosalite $\sim Pb_2Bi_2S_5$ 266	
Epilogue and acknowledgements.....	267
References.....	267

## Chapter 4. Polysomatic approach in minerals: examples and applications

<b>Polysomatism as a tool for correlating properties and structure</b> by GIOVANNI FERRARIS .....	275
Introduction.....	275
Carlosturanite.....	276
Structural model.....	276
The inophite polysomatic series.....	278
Solid state reactions.....	278
Revisiting the structural model? .....	279
Nafertisite and related titanosilicates.....	279
Nafertisite .....	279
The heterophyllosilicate polysomatic series.....	280
Further modular interpretations .....	282
Seidozerite derivatives.....	282
Solid state reactions and oriented growths.....	284
Kalifersite.....	285
Structural model.....	286
Polysomatic interpretations.....	288
Minerals related to palysepioles.....	288
Tungusite.....	290
Reyerite derivatives .....	290
Conclusions.....	291
Acknowledgements .....	292
References.....	292
 <b>Polysomatic approach in the crystal chemical study of minerals</b> by STEFANO MERLINO and MARCO PASERO .....	 297
Introduction.....	297
Pyroxene–spinel family (two-module polysomes).....	297
The sapphirine–aenigmatite group.....	298
Structure of sapphirine–aenigmatite ( <i>PS</i> ) .....	299
Polytypic features of sapphirine–aenigmatite .....	300
Surinamite ( <i>PPS</i> ) .....	301
CaFe <sub>3</sub> AlO <sub>7</sub> ( <i>SSP</i> ) .....	302
Phase A and Phase B .....	302
A unifying way to describe polysomatism and polytypism in the pyroxene–spinel family ...	303
Lintisite family (three-module polysomes).....	303
Lintisite.....	303
Vinogradovite.....	304
Lorenzenite.....	305
Silinaite.....	305
Polysomatic relationships .....	305
A note on kukisvumite.....	306
Shattuckite and planchéite.....	307
Acknowledgements .....	310
Appendix.....	310
References.....	310

## Chapter 5. Different approaches to modularity

### Modularity – different types and approaches

by <b>EMIL MAKOVICKY</b> .....	315
Introduction .....	315
Hierarchical description. Configuration levels.....	316
Modular description. Types of homologous/polysomatic series .....	319
Accretional series .....	319
Polysomatism .....	323
Variable-fit homologous series and series with a combined character .....	325
Polytypy.....	327
Merotype and plesiotype series .....	332
Examples and applications .....	333
Conclusions .....	337
Acknowledgements.....	339
References.....	339

### Modular analysis of crystal structures

by <b>BORIS B. ZVYAGIN</b> .....	345
Introduction .....	345
The notion of modular structures.....	347
Alternation and stacking of building modules (Spatial arrangement of modules) .....	348
Some considerations on the terminology in the modular structure (MS) diversity in relation to its nature.....	349
The nature of the modular structure diversity and principles of the modular analysis of crystal structures (MACSs) .....	350
Symmetry relationships and symbols as analytical means for operating with modular structures.....	353
Lattice characteristics of modular structures.....	353
Instructive examples .....	357
Derivation of modular structures .....	364
Diffractional features of modular structures .....	366
Acknowledgements.....	370
References.....	371

### Structural aspects of oxide and oxysalt minerals

by <b>FRANK C. HAWTHORNE</b> .....	373
Introduction .....	373
Crystal structures as graphs.....	373
Topological aspects of molecular-orbital theory.....	375
Molecules .....	375
Molecular building blocks.....	377
Crystals.....	377
The method of moments .....	378
Topological aspects of crystal chemistry .....	380
Pauling's rules .....	381
Ionicity and covalency.....	382
Bond-valence theory.....	382

## XII

Bond-valence relationships .....	383
Bond-valence theory as a molecular-orbital model .....	384
Network solids.....	384
Characteristic bond-valences.....	385
Lewis acid and base strengths.....	385
The valence-matching principle.....	387
Simple applications of the valence-matching principle .....	387
A hierarchical approach to structure .....	388
A general hypothesis .....	388
Dimensional polymerization.....	388
Unconnected-polyhedra structures .....	390
Finite-cluster structures .....	390
Infinite-chain structures.....	392
Infinite-sheet structures .....	395
Framework structures .....	396
(OH) and (H <sub>2</sub> O) in oxysalt structures.....	398
(OH) and (H <sub>2</sub> O) as components of the structural unit .....	398
(H <sub>2</sub> O) groups bonded to interstitial cations .....	401
Hydrogen-bonded interstitial (H <sub>2</sub> O) groups .....	402
Occluded (H <sub>2</sub> O) groups .....	404
Structural and chemical predictions.....	404
Binary structural representation.....	404
(H <sub>2</sub> O) as a bond-valence transformer .....	406
Interstitial (H <sub>2</sub> O).....	406
Bond-valence controls on interstitial cations.....	407
Summary.....	409
Acknowledgements.....	410
References.....	410
Appendix .....	418
<b>Name index.....</b>	<b>431</b>
<b>Subject and mineral index.....</b>	<b>437</b>
<b>Corrigenda &amp; addenda .....</b>	<b>449</b>

## Preface of the Editor

Since the first beginning of the crystal chemical study of the inorganic compounds, a simple modular approach was developed, by looking at the crystal structures as built up through the assembling of polyhedral units. This approach was not only useful for a vivid and insightful description of the complex atomic arrangements of natural and synthetic compounds, but, through the use of simple and powerful rules for assembling the polyhedral units, it displayed an extraordinary heuristic power, suggesting reliable models for many complex structural assemblages.

The polyhedral approach also laid the basis for meaningful classifications which were applied to all the classes of inorganic compounds.

More complex modular systems were developed by applying the same theoretical scheme, namely combining polyhedral units in stable complex modules and determining the ways to firmly connect those modules. Once again useful applications were found in the three directions previously indicated:

- insightful description of complicated crystal structures;
- careful prevision of possible new assemblages;
- meaningful classifications.

For example, in looking at the large variety of zeolite structures realized in nature or in the laboratory, it clearly appears that nature and man play with a limited number of modules (rings, cages, chains) built up by the connection of the primary units (namely  $\text{SiO}_4$ ,  $\text{AlO}_4$ , or, more rarely,  $\text{BO}_4$ ,  $\text{PO}_4$ ,  $\text{BeO}_4$ ,... tetrahedra). Once the kind of these modules is clarified, the description of the various structures is reduced to the 'modular play' of enumerating the various ways through which they interconnect, leading to rational classification, simple description and careful prediction.

An additional vigorous stimulus to pay due attention to the modular aspects has been given by the wide access of crystal chemists to the new techniques of structural investigation offered by the electron diffraction and even more by the high resolution electron microscopy, which allow the investigation of inhomogeneities, stacking faults, microtwining, intergrowths, domain structures, namely all those microstructural aspects which are so frequent in inorganic compounds and especially in minerals: new possible structural arrangements, as suggested by a modular approach, may in fact be present as small domains or may be realized at fault or twin boundaries.

Under the action of these various spurs the 'modular play' slowly developed into a definite research theme in crystal chemistry and the original ingenious looseness in assembling the building modules was progressively substituted by a more systematic approach with rigorous rules to select the modules and to combine them.

The most common and, therefore, the most important and investigated modular systems are those which present infinite two dimensional layers as building blocks and include OD structures, polytypes, polysomatic families, homologues series,....

The systematic approach previously mentioned is, in all these cases, particularly evident, especially in OD structures, where rigid constraints in the choice of the modules and in their assembling are imposed by strict requirements of symmetry.

## XIV

These rational, systematic approaches now provide us with reliable procedures to effectively deal with modular problems and therefore it seems necessary that these procedures be part of the cultural equipment of every crystal chemist, no matter whether active on natural or synthetic products.

The lectures held at the School on Modular Aspects of Minerals, collected in the five chapters of this volume, have just the aim to show the wide range of modular problems in mineralogy and to indicate the procedures to deal with them.

*Stefano Merlino*

Chapter 1

**OD theory: fundamentals  
and applications**



