# MICAS: CRYSTAL CHEMISTRY and METAMORPHIC PETROLOGY

Editors: A Mottana, F P Sassi, J B Thompson, Jr & S Guggenheim

## Table of Contents

1. Mica Crystal Chemistry and the Influence of Pressure, Temperature, and Solid Solution on Atotlistic Models

   Maria Franca Brigatti, Stephen Guggenheim

**OVERVIEW**
- Treatment of the data and definition of the parameters used .......................... 1
- End-member crystal chemistry: New end members and new data since 1984 ........ 3
- Synthetic micas with unusual properties ....................................................... 11

**EFFECT OF COMPOSITION ON STRUCTURE**
- Tetrahedral sheet ............................................................................................... 11
- Tetrahedral rotation and interlayer region ....................................................... 19
- Tetrahedral cation ordering .............................................................................. 25
- Octahedral coordination and long-range octahedral ordering ......................... 27
- Crystal chemistry of micas in plutonic rocks ................................................ 37

**ATOMISTIC MODELS INVOLVING HIGH-TEMPERATURE STUDIES OF THE MICAS**
- Studies of samples having undergone heat treatment .................................... 39
- Dehydroxylation process for dioctahedral phyllosilicates ............................... 41
- Dehydroxylation models for *trans-vacant* 2:1 layers .................................... 43
- Dehydroxylation models for *cis-vacant* 2:1 layers ........................................ 44
- Compaison of Na-rich vs. K-rich dioctahedral forms ......................................... 49
- Heat-treated trioctahedral samples: The O,OH,F site and in situ high-temperature studies ......................................................... 50
- Heat-treated trioctahedral samples: Polytype comparisons ............................. 51

**ACKNOWLEDGMENTS** ..................................................................................... 51

**APPENDIX I: DERIVATIONS** ......................................................................... 52
- Derivation of "tetrahedral cation displacement", T₄sp ........................................ 52
- Derivation of f₁E₁, f₂E₂, f₃E₃ ............................................................................. 52
- Derivation of α .................................................................................................. 53
- Explanation of αₜₛ₀ .......................................................... ............................ 54
- Explanation of E₁ₜ₄₀ ....................................................................................... 54

**APPENDIX II: TABLES 1-4** ........................................................................... 55

<table>
<thead>
<tr>
<th>Table</th>
<th>Description</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>1a</td>
<td>Structural details of trioctahedral true micas-1M, space group C2/m</td>
<td>55</td>
</tr>
<tr>
<td>1b</td>
<td>Structural details of trioctahedral true micas-1M, space group C2</td>
<td>70</td>
</tr>
<tr>
<td>1c</td>
<td>Structural details of trioctahedral true micas-2M, space group C2/m</td>
<td>72</td>
</tr>
<tr>
<td>1d</td>
<td>Structural details of trioctahedral true micas-2M, space groups Cc, C1</td>
<td>74</td>
</tr>
<tr>
<td>1e</td>
<td>Structural details of trioctahedral true micas-2M, space group C2/m</td>
<td>74</td>
</tr>
<tr>
<td>1f</td>
<td>Structural details of trioctahedral true micas-3T, space group P3,12</td>
<td>74</td>
</tr>
<tr>
<td>2a</td>
<td>Structural details of trioctahedral true micas-1M, Mspace groups C2/m and C2</td>
<td>76</td>
</tr>
<tr>
<td>2b</td>
<td>Structural details of trioctahedral true micas-1M, space group C2</td>
<td>78</td>
</tr>
<tr>
<td>2c</td>
<td>Structural details of trioctahedral true micas-2M, space group C2/m</td>
<td>84</td>
</tr>
<tr>
<td>2d</td>
<td>Structural details of trioctahedral true micas-3T, space group P3,12</td>
<td>84</td>
</tr>
<tr>
<td>3a</td>
<td>Structural details of trioctahedral brittle micas</td>
<td>86</td>
</tr>
<tr>
<td>3b</td>
<td>Structural details of dioctahedral brittle micas</td>
<td>88</td>
</tr>
<tr>
<td>4</td>
<td>Structural details of boromuscovite-1M and -2M, calculated from the Rietveld structure refinement by Liang et al. (1995)</td>
<td>88</td>
</tr>
</tbody>
</table>

**REFERENCES** ................................................................................................ 90
Behavior of Micas at High Pressure and High Temperature
Pier Francesco Zanazzi, Alessandro Pavese

INTRODUCTION
Investigative techniques for the study of the thermoelastic behavior of micas
$p$- $V$ and $P$- $V$-$T$ equations of state
Dioctahedral micas
Trioctahedral micas
ACKNOWLEDGMENTS
REFERENCES

Structural Features of Micas
Giovanni Ferraris, Gabriella Ivaldi

INTRODUCTION
NOMENCLATURE AND NOTATION
MODULARITY OF MICA STRUCTURE
The mica module
CLOSEST-PACKING aspects
Closest-packing and polytypism
COMPOSITIONAL ASPECTS
SYMMETRY ASPECTS
Metric (lattice) symmetry
Structural symmetry
Symmetry and cation sites
Two kinds of mica layer: $M_1$ and $M_2$ layers
The interlayer configuration
Possible ordering schemes in the MDO polytypes
The phengite case
DISTORTIONS
The misfit
Geometric parameters describing distortions
Ditrigonal rotation
Other distortions
Effects of the distortions on the stacking mode
FURTHER STRUCTURAL MODIFICATION
Pressure, temperature and chemical influence
Thickness of the mica module
Ditrigonal rotation and interlayer coordination
Effective coordination number (ECoN)
CONCLUSIONS
APPENDIX I: MICA STRUCTURE AND POLYSOMATIC SERIES
Layer silicates as members of modular series?
Mica modules in polysomatic series
The heterophyllosicate polysomatic series
The palysepiole polysomatic series
Conclusions
APPENDIX II: OBLIQUE TEXTURE ELECTRON DIFFRACTION (OTED)
ACKNOWLEDGMENTS
REFERENCES
Crystallographic Basis of Polytypism and Twinning in Micas

Massimo Nespolo, Slavomír Durovic

INTRODUCTION 155
NOTATION AND DEFINITIONS 156
The mica layer and its constituents 157
Axial settings, indices and lattice parameters 158
Symbols 158
Symmetry and symmetry operations 159
THE UNIT LAYERS OF MICA 159
Alternative unit layers 160
MICA POLYPYTOPES AND THEIR CHARACTERIZATION 164
Micas as OD structures 164
SYMBOLIC DESCRIPTION OF MICA POLYPYTOPES 172
Orientational symbols 172
Rotational symbols 175
RETICULAR CLASSIFICATION OF POLYPYTOPES: SPACE ORIENTATION AND SYMBOL DEFINITION 178
LOCAL AND GLOBAL SYMMETRY OF MICA POLYPYTOPES FROM THEIR STACKING SYMBOLS 180
Derivation of MDO polytypes 180
The symmetry analysis from a polytype symbol 184
RELATIONS OF HOMOMORPHY AND CLASSIFICATION OF MDO POLYPYTOPES 189
BASIC STRUCTURES AND POLYPYTOPIDS. SIZE LIMIT FOR THE DEFINITION OF "POLYPYTYPE" 191
Abstract polytypes 192
Basic structures 193
HREM observations and some implications 193
IDEAL SPACE-GROUP TYPES OF MICA POLYPYTOPES AND DESYMME1RIZATION OF LAYERS IN POLYPYTOPES 193
CHOICE OF THE AXIAL SETTING 204
GEOME1RICAL CLASSIFICATION OF RECIPROCAL LATTICE ROWS 206
SUPERPOSITION S1RUCTURES, FAMILY S1RUCTURE AND FAMILY REFLECTIONS 209
Family structure and family reflections of mica polytypes 212
REFLECTION CONDITIONS 213
NON-FAMILY REFLECTIONS AND ORTHOGONAL PLANES 214
HIDDEN SYMMETRY OF THE MICAS: THE RHOMBOHEDRAL LATTICE 216
TWINNING OF MICAS: THEORY 217
Choice of the twin elements 219
Effect of twinning by selective merohedry on the diffraction pattern 220
Diffraction patterns from twins 223
Allotwinning 224
Tessellation of the hp lattice 224
Plesiotwinning 230
TWINNING OF MICAS. ANALYSIS OF THE GEOME1RY OF THE DIFFRACTION PATTERN 233
Symbolic description of orientation of twinned mica individuals. Limiting symmetry 235
Derivation of twin diffraction patterns 237
Derivation of allotwin diffraction patterns 243
IDENTIFICATION OF MDO POLYPYTOPES FROM THEIR DIFFRACTION PATTERNS 244
Theoretical background 244
Identification procedure 245
IDENTIFICATION OF NON-MOO POLYPYTOPES: THE PERIODIC INTENSITY DISTRIBUTION FUNCTION 247
PID in terms of TS unit layers 249
Derivation of PID from the diffraction pattern 251
5
Investigations of Micas
Using Advanced Transmission Electron Microscopy

Toshihiro Kogure

INTRODUCTION

TEMs AND RELATED TECHNIQUES FOR THE INVESTIGATION OF MICA
Transmission electron microscopy
New recording media for beam-sensitive specimens
Sample preparation techniques
Image processing and simulation

ANALYSES OF POLYTOPES

DEFECT STRUCTURES

CONCLUSION

ACKNOWLEDGMENTS

REFERENCES

6
Optical and Mossbauer Spectroscopy of Iron in Micas

M. Darby Dyar

INTRODUCTION

OPTICAL SPECTROSCOPY
Current instrumentation
Review of existing work
Summary

MOSSBAUER SPECTROSCOPY (MS)
Current instrumentation
Recoil-free fraction effects
Thickness effects
Texture effects and other sources of error
Techniques for fitting Mossbauer spectra
Review of existing Mossbauer data
Summary

COMPARISON OF TECHNIQUES

CONCLUSIONS

ACKNOWLEDGMENTS

APPENDIX: Other techniques for measurement of Fe³⁺/Fe in Micas
X-ray photoelectron spectroscopy (XPS)
Electron energy-loss spectroscopy (EELS)
X-Ray absorption spectroscopy (XAS

REFERENCES
INTRODUCTION

LATTICE VIBRATIONS
  Far-IR region
  Mid-IR region

OH STRETCHING VIBRATIONS
  Polarized measurements
  Quantitative water determination
  Hydrogen bonding
  Cation ordering
  OH-F replacement
  Dehydroxylation mechanisms
  Excess hydroxyl
  NH\textsubscript{3} groups

ACKNOWLEDGMENTS

REFERENCES

8 X-Ray Absorption Spectroscopy of the Micas
Annibale Mottana, Augusto Marcelli, Giannantonio Cibin, and M. Darby Dyar

INTRODUCTION

OVERVIEW OF THE XAS METHOD
  EXAFS
  XANES
  Experimental spectra recording
  Optimization of spectra
  Systematics

ACKNOWLEDGMENTS

REFERENCES

9 Constraints on Studies of Metamorphic K-Na White Micas
Charles V. Guidotti, Francesco P. Sassi

INTRODUCTION

EFFECTS OF PETROLOGIC FACTORS ON WHITE MICA CHEMISTRY
  Important compositional variations
  Controls of mica composition by petrologic factors

MAXIMIZING INFORMATION FROM MICA STUDIES:
  SAMPLE SELECTION CONSTRAINTS
    Petrologic studies
    Mineralogic studies

DISCUSSION
  Common failings in petrology studies
  Common failings in mineralogy studies
  "Standard starting points" for the compositional variations of
    rock-forming dioctahedral and trioctahedral micas

ACKNOWLEDGMENTS

REFERENCES