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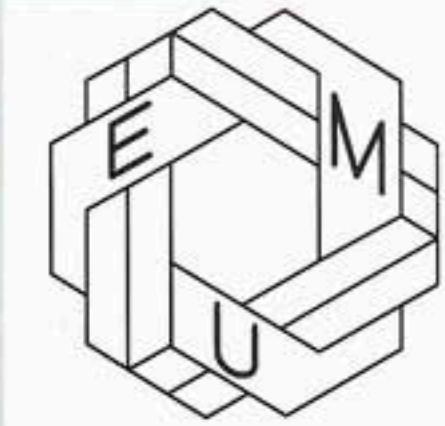
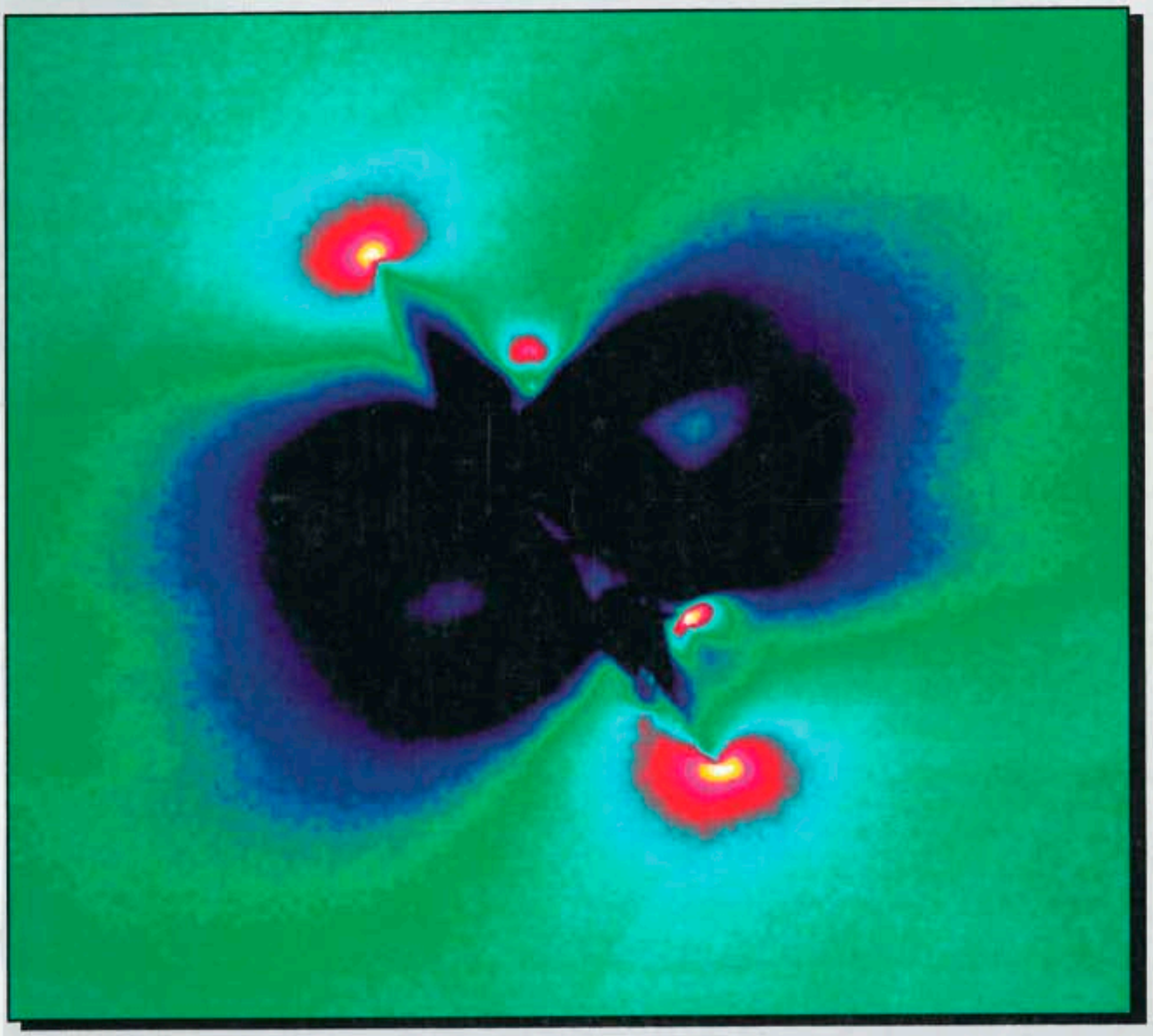


EMU NOTES IN MINERALOGY

6

Spectroscopic Methods in Mineralogy

Edited by
ANTON BERAN
and EUGEN LIBOWITZKY



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Volume 6

SPECTROSCOPIC METHODS IN MINERALOGY

UNIVERSITY TEXTBOOK

Edited by
Anton Beran
and
Eugen Libowitzky

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Initiator of the EMU Schools and the EMU Notes in Mineralogy
Giovanni Ferraris, Torino, President of the EMU 1992–1996

On the front cover: 2D-tomographic Raman map (size 779 × 700 μm) of a diamond crystal (Ekati diamond mine, Canada), revealing the diamond's internal pattern of pressure and strain around a graphite inclusion. The colour-coded plot shows the Raman shift of the diamond *LO=TO* mode (1332 cm^{-1} at ambient pressure; green). Increased Raman shifts (blue-black) indicate a halo of remnant enhanced pressure and compressive strain whereas decreased Raman shifts (red-yellow) indicate dilative strain near the ends of cracks (*cf.* Nasdala *et al.*, submitted). Sample courtesy by J.W. Harris and F. Glinnemann.

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Foreword

The present volume of the EMU Notes in Mineralogy is dedicated to different spectroscopic methods frequently applied in mineralogy. It is the first volume of this series dealing especially with the basics of spectroscopic techniques and applications. This book follows five volumes devoted to different aspects of mineralogy. Volume 1, edited by S. Merlino, was dedicated to *Modular Aspects of Minerals*, Volume 2, edited by D.J. Vaughan and R.A. Wogelius, to *Environmental Mineralogy*, Volume 3, edited by C.A. Geiger, to *Solid Solutions in Silicate and Oxide Systems*, Volume 4, edited by C.M. Gramaccioli, to *Energy Modelling in Minerals* and Volume 5, edited by D.A. Carswell and R. Compagnoni, to *Ultrahigh Pressure Metamorphism*. The present volume contains the contributions of the lectures given at the 6th School of the European Mineralogical Union (6th EMU School) on *Spectroscopic Methods in Mineralogy*, held at the University of Vienna from August 30 to September 8, 2004. The School includes the 5th European Conference on Mineralogy and Spectroscopy (ECMS 2004), held from September 4 to 8, 2004, where students will be provided with additional examples of state-of-the-art applications of spectroscopic methods.

Spectroscopic methods provide information about the local structure of minerals. The methods do not depend on long-range periodicity or crystallinity. The geometric arrangement of atoms in a mineral phase is only one aspect of its constitution. Its vibrational characteristic, electronic structure and magnetic properties are of greatest importance when we consider the behaviour of minerals in dynamic processes. The characterisation of the structural and physico-chemical properties of a mineral requires the application of several complementary spectroscopic techniques. However, it is one of the main aims of this School to demonstrate that different spectroscopic methods work on the same basic principles. Spectroscopic techniques represent an extremely rapidly evolving area of mineralogy and many recent research efforts are similar to those in materials science, solid state physics and chemistry. Applications to different materials of geoscientific relevance have expanded by the development of microspectroscopic techniques and by *in situ* measurements at low- to high-temperature and high-pressure conditions.

We feel bound to thank David J. Vaughan, Past President of the EMU and the Executive Committee of the EMU for their support and encouragement. For her tireless commitment we are indebted to Herta S. Effenberger, Secretary of the EMU. Giovanni Ferraris strongly supported this venture. We would like to thank the European Commission through the EU Socrates/Erasmus Intensive Programme (IP) managed by the project coordinator Tamás G. Weiszburg, for providing scholarships to students and support funds for the teachers. Financial support from the Österreichische Mineralogische Gesellschaft (ÖMG), the Deutsche Gesellschaft für Kristallographie (DGK) and Universität Wien is also gratefully acknowledged. In addition, the European Mineralogical Union provided financial aid.

Particular thanks are due to the series editors of the EMU Notes in Mineralogy, Tamás G. Weiszburg and Gábor Papp, for their efforts in the production of this volume published by the Eötvös University Press and to Tamás Váczi for his patient and competent work as technical editor. It should be noted that the authors and editors are responsible for any errors remaining in this volume. The chapters underwent peer review

by the authors of the book and by the "external" referees H. Annersten, G. Di Lonardo, U. Hålenius, C.M.B. Henderson, U. Kolitsch, D.J. Newman, G.R. Rossman, M. Schmücker, H. Skogby, M.E. Smith, J.F. Stebbins, G.A. Waychunas and A. Woodland. Our sincere thanks are due to the reviewers and last but not least to all colleagues who agreed to take part in the EMU School, thereby contributing to its success.

It is our hope that the present volume will contribute to the specific development of spectroscopic methods in geosciences and that it will stimulate numerous scientists who are concerned with detailed structural investigations of solid state materials with respect to their physical and chemical properties.

Anton Beran and *Eugen Libowitzky*
Vienna, July 2004

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Conventions, recommendations and standards used in this volume

Spelling: British English
Mineral names: Recommendations of the IMA CNMMN
Symbols (abbreviations) for rock-forming minerals: In accordance with the Appendix of *The nomenclature of minerals: A compilation of IMA reports*; edited by R.F. Martin; Ottawa: Mineral. Assoc. Can., 1998.
Crystallographic symbols: In accordance with the *International tables of crystallography, Volume A, Space-group symmetry*; edited by Th. Hahn; fourth, revised edition; Dordrecht: 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*. Different authors with the same surname are not considered separately.
Journal names are abbreviated according to the ISDS standards (with a few exceptions in the usage of capitals and in the transcription of Cyrillic characters).