

Serving the International Materials Research Community

A Publication of the Materials Research Society

February 1993, Volume XVIII, No. 2





https://doi.org/10.1557/S0883769400043530 Published online by Cambridge University Press

When High Voltage Engineering acquired General lonex a "cluster" in ion beam technology was born.

SUPERIOR F

OINT

D

Through integration and complementation of technologies an important step in the development of ion beam related equipment has been made.

> This joint technology has resulted in new generation Tandetrons™: reliable, compact and versatile tandem accelerator systems able to produce MeV ion beams of virtually all periodic-system elements for material modification and analysis in a research environment. <u>Circle no. 1</u> reader service card for new product literature.

DIVISIONS GENERAL IONEX DOWLISH DEVELOPMENTS More Energy for Research

HIGH VOLTAGE ENGINEERING EUROPA B.Y.

P.O. Box 99, 3800 AB Amersfoort, The Netherlands, Phone: (+31) 33 - 619741. Fax: (+31) 33 - 615291. Telex: 79100 HIVEC NL https://doi.org/for13apan: MARUBUN CORPURATION, 39 Ambinestin odentmacho, Chuo-ku, Tokyo, 103 Japan, Phone 03-3639-9861, Fax 03-3661-7473 For USA and Canada: HVEC, The Schrafft Center, Suite 602, 529 Main Street, Boston, MA 02129, Phone: (617) 241 5000, Fax: (617) 241 5005

HTT

February 1993

A Publication of the Materials Research Society Volume XVIII, Number 2 ISSN: 0883-7694 CODEN: MRSBEA

TRENDS IN **MATERIALS DATA:** REGULARITIES AND PREDICTIONS

27 Trends in Advanced Materials Data: Regularities and Predictions

> J.R. Rodgers and P. Villars, Guest Editors

- 31 Theory and Practice in the Prediction of New Materials K M Babe
- 38 Some Uses of **Crystallographic Databases** and Bibliographies J.C. Phillips and T. Siegrist

Prediction of Inorganic

40 **Compounds: Experiences** and Perspectives

N.N. Kiselvova

44 Data Compilation, Analysis, and Access: The Role of the Computer

J.H. Westbrook

RESEARCH REPORT

50 Portuguese-Spanish Collaboration on LiNbo₃ J.C. Soares and F. Agulló-López

INTERNATIONAL **UNION OF MATERIALS RESEARCH SOCIETIES**

- 52 **IUMRS-ICAM-93 Planned** for Tokyo—Abstracts Still **Being Accepted**
- 52 Yangtze Gorges Will Be Venue for IUMRS-ICA
- 53 **Electronic Materials Will Be Topic for Joint ICEM '94-ICA** Meeting in Taiwan
- 53 **IUMRS** Creates Lectureship

MRS NEWS

- 39 **New MRS Short Course** on Practical Electron Diffraction
- 54 **1992 MRS Fall Meeting** Extends Boundaries of Materials Science
- 67 Preview: 1993 Spring Meetina
- 75 Picraux, Bravman, Phillips, Hays Lead Slate of 1993 MRS Officials

MRS 20TH ANNIVERSARY

- 77 Foundations for the "Age of Materials"
- 77 **MRS Gains Effectiveness** and Flexibility through Empowerment

DEPARTMENTS

- 4 Material Matters
- 10 **Research/Researchers**
- 23 From Washington
- 25 **Editor's Choice**
- 25 Advertisers in This Issue
- 26 Resources
- 79 Upcoming Conferences
- 80 **Education Exchange**
- 82 **Historical Note**
- 85 **Book Reviews**
- 86 Classified



ON THE COVER: The cover shows the Quantum Structural Diagrams (QSD) for (clockwise, from top): high T, superconductors, stable quasicrystals and ferroelectric materials. The central diagram shows the distribution of the stable quasicrystals (Q), high T_c ferroelectrics (F), and high T_e superconductors (SA, SB, and SC) relative to each other and to the full database of known intermetallic compounds. For more on this topic, see "Theory and Practice in the Prediction of New Materials" by K.M. Rabe, starting on p. 31.

MRS BULLETIN

Materials Research Society • 9800 McKnight Road • Pittsburgh, PA 15237

MRS BULLETIN

Editorial Assistants E.M. Benec, M. M. Costello, J. Dininny

Advertising and Circulation M. E. Kaufold

Associate Editor—Europe I. W. Boyd University College London Dept. of Electronic and Electrical Engineering Torrington Place London WCI E7 JE United Kingdom 71-387-7050 ext. 3956 or 7304

L. C. lanniello

Editorial and Advertising Offices 9800 McKnight Road Pittsburgh, PA 15237 Telephone (412)-367-3036 Fax (412) 367-4373

MRS Office of Public Affairs 1025 Thomas Jefferson St. NW Washington, DC 20007 Telephone (202) 337-0910

Guest Editors J. R. Rodgers and P. Villars Special Contributors

Pennsylvania State University

University Park, Pennsylvania, USA

R. Roy

T. Sugano

Toyo University

University of Dublin

Tokyo, Japan

D. L. Weaire

S. Namba

J. Soares

Dublin, Ireland

Osaka University

A. D. Romig Jr. Sandia National Laboratories

Universidade de Lisboa

Lisboa, Portugal

W. H. Sutton

C. W. White

United Technologies

Research Center

Oak Ridge, Tennessee

East Hartford, Connecticut

Oak Ridge National Laboratory

Albuquerque, New Mexico, USA

K. C. Taylor General Motors Research Laboratories Warren, Michigan, USA

Osaka, Japan

H. Alten, K.J. Anderson, F.S. Myers

Research Society The Materials Research Society (MRS), a nonprofit scientific association founded in 1973, promotes interdisciplinary goal-oriented basic research on materials of techno-

About

the Materials

ented basic research on materials of technological importance. Membership in the Society includes nearly 11,000 scientists, engineers, and research managers from industrial, government, and university research laboratories in the United States and nearly 50 countries.

The Society's interdisciplinary approach differs from that of single-discipline professional societies because it promotes information exchange across the many technical fields touching materials development. MRS sponsors two major international annual meetings encompassing approximately 50 topical symposia, and also sponsors numerous single-topic scientific meetings. The Society recognizes professional and technical excellence, conducts short courses, and fosters technical interaction in local geographic regions through Sections and University Chapters.

MRS participates in the international arena of materials research through the International Union of Materials Research Societies (IUMRS). MRS is an affiliate of the American Institute of Physics.

MRS publishes symposium proceedings, MRS Bulletin, Journal of Materials Research, and other publications related to current research activities.

MRS Bulletin (ISSN: 0883-7694) is published 12 times a year by the Materials Research Society, 9800 McKnight Road, Pittsburgh, PA 15237. Application to mail at Pittsburgh, PA and at additional mailing offices. POSTMASTER: Send address changes to MRS Bulletin in care of the Materials Research Society, at the address listed; phone (412) 367-3003; Fax (412) 367-4373

Membership in MRS is \$70 annually for regular members, \$25 for students and retired members. Dues include an allocation of \$25 (\$15 for students and retirees) to a subscription to *MRS Bulletin*. Individual member subscriptions are for personal use only. Non-member subscription rates are \$106 for one calendar year (12 issues) within the U.S.A. and \$156 elsewhere. Single copies may be purchased for \$16 each. Send subscription orders to Subscription Department, Materials Research Society, 9800 McKnight Road, Pittsburgh, PA 15237.

MRS Bulletin is included in Current Contents/Physical, Chemical & Earth Sciences™, Research Alert, and the Materials Science Citation Index™. Back volumes of MRS Bulletin are available in 16mm microfilm, 35mm microfilm, or 105mm microfiche through University Microfilms Inc., 300 North Zeeb Road, Ann Arbor, Michigan 48106.

Publisher Ed G. A. Oare E.I. Technical Editor J. E. L. Fleischer Ad Assistant Editor M. J. M. Guenther As Copy Editors I. N. L. A. Krysinski, D. M. Varner Ur Art Director De C. Love To Design/Production Lo S. B. Franklin, S. O. Franklin, Ur H.J. Miller H.J. Miller T1

E. N. Kaufmann • Argonne National Laboratory • Argonne, Illinois, USA

INTERNATIONAL ADVISORY BOARD

M. Balkanski University of Pierre and Marie Curie Paris, France R. G. Elliman Australian National University Canberra, Australia S. Hsu Chung Shan Institute of Science and Technology Taiwan, China

TECHNICAL EDITORIAL BOARD

J. C. Bravman Stanford University Stanford, California, USA C. W. Draper AT&T Engineering Research Center Princeton, New Jersey, USA E. Fogarassy Centre de Recherches Nucléaires Strasbourg, France

MRS BULLETIN PUBLICATIONS SUBCOMMITTEE

A. Barkatt Catholic University of America Washington, DC A. J. Hurd Sandia National Laboratories Albuquerque, New Mexico

M. R. Libera Stevens Institute of Technology Hoboken, New Jersey

President S. T. Picraux Sandia National Laboratories First Vice President and President-Elect J. C. Bravman Stanford University Second Vice President J. M. Phillips AT&T Bell Laboratories U. S. Department of Energy Washington, DC, USA H-D. Li National Science Foundation—China Beijing, China P. Rama Rao Ministry of Science and Technology New Delhi, India

F. Y. Fradin Argonne National Laboratory Argonne, Illinois, USA B. M. Léon Universidade de Vigo Vigo, Spain G. L. Liedl Purdue University West Lafayette, Indiana, USA

G. J. McCarthy North Dakota State University Fargo, North Dakota J. M. Phillips AT&T Bell Laboratories Murray Hill, New Jersey S. M. Prokes Naval Research Laboratory Washington, DC

1993 MRS EXECUTIVE COMMITTEE

Secretary L. A. Boatner Oak Ridge National Laboratory Treasurer A. K. Hays Sandia National Laboratories Immediate Past President G. S. Cargill III IBM T. J. Watson Research Center Executive Director Materials Research Society John B. Ballance

INTERNATIONAL UNION OF MATERIALS RESEARCH SOCIETIES

Secretary Rodney C. Ewing University of New Mexico, USA Tel. (505) 277-4163; **Vice President Immediate Past President** President Treasurer Shigeyuki Somiya The Nishi-Tokyo University, Japan Tel. (81) 3 417 2866; R. P. H. Chang Masao Doyama The Nishi-Tokyo University, Japan Paul Siffert Centre de Recherches Nucléaires, Northwestern University, USA Tel. (708) 491-3598; Fax (708) 491-4181 Tel. (81) 3 3339 0519; France Fax (81) 3 3310 0931 Fax (505) 277-0090 Fax (81) 3 415 6619 Tel. (88) 28 65 43; Fax (88) 28 09 90 **IUMRS ADHERING BODIES** Materials Research Society of Korea (MRS-Korea) Australian Materials Research Society (A-MRS) Materials Research Society (MRS) J. S. Williams S. T. Picraux Min Che Chon Materials Research Society of Taiwan (MRS-T) Chinese Materials Research Society (C-MRS) Materials Research Society of India (MRS-I) Hengde Li P. Rama Rao Li-chung Lee Mexican Materials Research Society (Mexican-MRS) European Materials Research Society (E-MRS) Materials Research Society of Japan (MRS-J) M. J. Yacaman P. A. Glasow M. Doyama

https://doi.org/10.1557/S0883769400043530 Published online by Cambridge University Press

We Go To Extremes In Isostatic Pressing MARIA

UNIFORM RAPID COOL

VESSEL FATIGUE = (C (2-m)(Tr) 7/2 S LIFE = 300,000 cycles Only ABB Autoclave offers you a line

COMPUTER CONTROLS

of isostatic pressing equipment with the widest range of size, temperature and pressure needed to meet your processing requirements, from aluminum to zirconia. We lead the industry with advances such as workzone dilatometers, uniform rapid cooling capability, reliable high temperature measurement systems, high temperature furnaces, reactive gas HIPping

SYSTEM STA

and computer-based control systems.

135,000

Our extremes extend beyond process flexibility. Our products are as dependable as they are innovative. No one goes to the extremes of service, safety and support like the professionals from ABB Autoclave.

MORK ZUNE

14.7 PSI

PRECISION NET SHAPES

Contact ABB for your hot and cold isostatic pressing needs. Let us go to extremes for you.



Research





Advanced Materials



Bus. (614) 891-2732 • Telex. 241341 • Fax. (614) 891-4568

https://doi.org/10.1557/S0883769400043530 Published online by Cambridge University Press Circle No. A on Reader Service Card.