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Materials Science of
Thermoelectric Materials:
Beyond Bismuth Telluride

FUNDAMENTAL MATERIALS RESEARCH

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*Michigan State University
East Lansing, Michigan*

Springer-Science+Business Media, LLC

New Thermoelectric Materials Workshop (2002: Traverse City, Mich.)

Chemistry, physics, and materials science of thermoelectric materials: beyond bismuth telluride/edited by Mercuri G. Kanatzidis, S.D. Mahanti, and Timothy P. Hogan.

p. cm. — (Fundamental materials research)

Lectures given at the New Thermoelectric (TE) Materials Workshop held in Traverse City, Michigan, from August 17–21, 2002.

Includes bibliographical references and index.

ISBN 978-1-4613-4872-6 ISBN 978-1-4419-9278-9 (eBook)

DOI 10.1007/978-1-4419-9278-9

I. Thermoelectric materials—Congresses. I. Kanatzidis, Mercuri G. II. Mahanti, S.D. III. Hogan, Timothy P. IV. Title. V. Series.

TK2950.N O 2003

620.1'1296—dc21

2003044720

Proceedings of the conference "Chemistry, Physics, and Materials Science of Thermoelectric Materials: Beyond Bismuth Telluride," held August 17–21, 2002, in Traverse City, Michigan

©2003 Springer Science+Business Media New York

Originally published by Kluwer / Plenum Publishers, New York in 2003

Softcover reprint of the hardcover 1st edition 2003

10 9 8 7 6 5 4 3 2 1

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SERIES PREFACE

This series of books, which is published at the rate of about one per year, addresses fundamental problems in materials science. The contents cover a broad range of topics from small clusters of atoms to engineering materials and involve *chemistry, physics, materials science, and engineering*, with length scales ranging from Ångstroms up to millimeters. The emphasis is on basic science rather than on applications. Each book focuses on a single area of current interest and brings together leading experts to give an up-to-date discussion of their work and the work of others. Each article contains enough references that the interested reader can access the relevant literature. Thanks are given to the Center for Fundamental Materials Research at Michigan State University for supporting this series.

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East Lansing, Michigan, November 2002

PREFACE

This volume records invited lectures given at the New Thermoelectric (TE) Materials Workshop held in Traverse City, Michigan from August 17-21, 2002. The theme of the workshop was *Chemistry, Physics and Materials Science of Thermoelectric Materials: Beyond Bismuth Telluride*. The objective of this symposium was threefold. First, to examine and assess the ability of solid state chemistry to produce new generation materials for TE applications. Second, to rationalize and predict the charge and heat transport properties of potential candidates and hypothetical systems through solid state theory and experiment. Third, to identify and prioritize research needed to reach various levels of requirements in terms of ZT and temperature. These objectives were addressed by a series of invited talks and discussions by leading experts from academia, government laboratories, and industry.

There were twenty-two invited and eight poster presentations in the workshop. Out of these, sixteen invited presentations are represented in this volume. They cover a wide range of subjects, starting from synthesis (based on different strategies) and characterization of novel materials to a careful study of their transport properties and electronic structure. Topics addressing the issue of making new materials are: synthetic search for new materials (di Salvo et al.) and synthetic strategies based on phase homologies (Kanatizidis). The different classes of materials covered are: bismuth nanowires (Dresselhaus et al.), unconventional high-temperature thermoelectrics, boron carbides (Aselage et al.), layered cobalt oxides (Fujii et al.), early transition metal antimonides (Kleinke et al.), skutterudites (Uher), and clathrate thermoelectrics (Nolas). Since an important part of thermoelectrics is a careful understanding of their thermal transport properties, several presentations (bismuth nano-wires by Heremans, superlattices by Chen, and skutterudites by Yang) have addressed this issue. The effect of pressure tuning on thermoelectric properties is discussed by Badding et al. Finally, the volume contains articles addressing several theoretical issues such as thermoelectrics with thermionic boundary conditions (Mahan), first-principles determination of transport coefficients (Sofa et al.), electronic structure of complex bismuth chalcogenide systems (Mahanti et al.), and calculation of thermoelectric figure of merit in a large class of materials using *ab initio* electronic structure results and transport models with and beyond relaxation time approximation (Metiu et al.).

Financial support for the Workshop was provided by Department of Physics and the Center for Fundamental Materials Research at Michigan State University, and Tellurex Corporation at Traverse City. We would like to thank the members of the advisory committee (M. Dresselhaus, F. DiSalvo, J-P. Fleurial, G. Mahan, G. Nolas, B. Sales, and

T. Tritt) for their thoughtful suggestions and encouragement. We are indebted to Ms. Lorie Newman for coordinating all the logistical aspects of the Workshop and to Ms. Janet King for editorial assistance and handling of the manuscripts for this publication.

Mercouri Kanatzidis
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Timothy P. Hogan
East Lansing, Michigan, November 2002

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