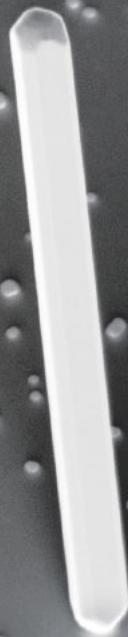




Diffusion in Materials DIMAT-2017

10th International Conference
on Diffusion in Materials



Edited by
Eugen Rabkin, Amy Novick-Cohen,
Leonid Klinger and Nachum Frage

Diffusion in Materials

DIMAT-2017

10th International Conference on
Diffusion in Materials

Edited by
Eugen Rabkin
Amy Novick-Cohen
Leonid Klinger
Nachum Frage

Diffusion in Materials DIMAT-2017

10th International Conference on
Diffusion in Materials

Selected, peer reviewed papers from the
10th International Conference on
Diffusion in Materials (DIMAT-2017),
Haifa, Israel, May 7-12, 2017.

Edited by

**Eugen Rabkin, Amy Novick-Cohen, Leonid Klinger
and Nachum Frage**

■
■ *Scientific.Net*
■

Copyright © 2018 Trans Tech Publications Ltd, Switzerland

All rights reserved. No part of the contents of this publication may be reproduced or transmitted in any form or by any means without the written permission of the publisher.

Trans Tech Publications Ltd
Reinhardstrasse 18
8008 Zurich
Switzerland
<http://www.scientific.net>

Volumes 383 of
Defect and Diffusion Forum
ISSN print 1012-0386
ISSN cd 1662-9515
ISSN web 1662-9507
(Pt. A of Diffusion and Defect Data – Solid State Data ISSN 0377-6883)

Full text available online at <http://www.scientific.net>

Distributed worldwide by

Trans Tech Publications Ltd
Reinhardstrasse 18
8008 Zurich
Switzerland
Phone: +41 (44) 922 10 22
Fax: +41 (44) 922 10 33
e-mail: sales@scientific.net

Preface

These proceedings contain a selection of papers presented at the 10th International Conference on Diffusion in Materials (DIMAT-2017) held at the Dan Panorama Hotel in Haifa, Israel between May 7th and 12th, 2017. The conference was attended by 117 participants from 20 different countries. The largest group was from the host country, Israel (31), followed by the Russian Federation (21) and Germany (18).

DIMAT is an internationally recognized conference series for diffusion and mass transfer in solids. The first two conferences (Diffusion in Metals and Alloys, DIMETA) were held in Hungary in 1982 and 1988, and since then the conferences were held on a regular basis every three to four years in: Kyoto, Japan (1992), Münster, Germany (1996), Paris, France (2000), Cracow, Poland (2004), Lanzarote, Spain (2008), Dijon, France (2011), and Münster, Germany (2014). The aim of DIMAT is to bring together researchers working in diverse areas of Materials Science and Solid State Physics, in which the kinetics of atom movements within materials plays a major role. One of the aims of DIMAT 2017 was to reach out to the less-traditional field of science and technology where the atomic random walks are important, such as mineralogy, energy storage and conversion, polymers and hybrid organic-inorganic materials, and more. We were particularly happy that several organizers of previous DIMAT conferences attended DIMAT-2017: Prof. D. Beke (DIMETA 1982 and 1988), Prof. H. Mehrer (DIMAT-1996), Prof. N.A. Stolwijk (DIMAT-1996 and 2014), and Prof. S.V. Divinski (DIMAT-2014).

The proceedings contain contributions presented at DIMAT-2017 in the following fields:

- Bulk diffusion and reactions;
- Computer simulations of diffusion and diffusion-controlled processes;
- Diffusion and surface diffusion in thin films, nanoparticles, and grain boundaries;
- Diffusion in solid-gas systems;
- Diffusion in materials processing.

The contributions published in these proceedings reflect only a partial picture of the talks presented at the DIMAT-2017 meeting. In the past, it was customary to publish a short conference paper, to be followed by the extended, more in depth publication in a “regular” journal. In the age before searchable, on-line publication databases became widely available, this publication strategy made perfect sense: while the conference paper set the authors’ priority and targeted the limited, but highly relevant audience of the conference attendees, it was hardly available beyond this group. The extended follow-up publication in “regular” journal was then aimed at disseminating the results to a wider readership. During the recent decade, the rapid development of searchable publication databases has led to all published material becoming instantaneously available. This resulted in stricter enforcement of copyright laws, and to the general understanding that copy-pasting of the relevant parts of the authors’ own work (self-plagiarism) is unacceptable. Naturally, this drastically reduced the motivation of researchers to publish their work in conference proceedings. In this respect, we would like to extend our sincere thanks to those DIMAT attendees who did decide to publish their work in the DIMAT-2017 proceedings, and who invested their time and efforts in preparation of high-quality manuscripts. All of the manuscripts in this volume have undergone a strict peer-review process comparable to that of “regular” journals.

The success of the conference is determined first and foremost by participants themselves – by the quality of their presentations and by their willingness to interact and to contribute to the discussions. We would like to express our gratitude to all of the DIMAT attendees for their valuable contributions to the conference success. For the foreign DIMAT participants, attendance involved an overseas trip, with all the associated hassles of trip planning and financial expenses. We highly

appreciate the efforts of our foreign guests who made the effort to come to DIMAT. We would like to thank the members of the International Advisory Board for their help, and especially for their valuable suggestions of the names of invited speakers. Organizing an international conference entails dealing with a number of large and small problems and unexpected situations. It would have been impossible to handle all of this by ourselves, and we would express our gratitude to the team of the event organizer, Diesenhaus Ltd., and especially to Ms. T. Laxer, Ms. A. Reshef, and Ms. M. Mizrahi for their highly professional help. The team of the Dan Panorama Hotel headed by Ms. D. Steinmetz was accommodating to all of our requests. Finally, the wonderful team of students and post-docs of the Solid State Thermodynamics Laboratory at the Technion was always there to help with critical issues such as web and graphical design, logistics, technical support with audio-visual equipment, photography, and much more: Dr. A. Kosinova, Dr. A. Sharma, Ms. H. Barda, Mr. O. Kovalenko, Mr. N. Gazit, and Mr. E. Almog.

We learned with a great sadness that on May 22nd 2017, shortly after the DIMAT meeting, our colleague and friend Prof. Dr. Nicolaas A. Stolwijk from the Institute of Materials Physics, University of Münster, unexpectedly passed away. It was very difficult to fathom this news since during the DIMAT meeting, Nico was in a good mood, appeared to be in excellent physical shape, and presented excellent talks, as usual in his unforgettable, inspiring manner. Prof. Stolwijk is renowned in the diffusion community for his groundbreaking results on diffusion in ordered intermetallics, semiconductors, polymers and thin films. In parallel to his highly accurate experimental work, Prof. Stolwijk contributed to fundamental understanding of the correlation effects in diffusion by numerical simulations. He co-organized two DIMAT meetings, and during the last several years he worked intensively on diffusion in solid electrolytes and minerals, and on computer simulations of diffusion in ionic materials. He will be sorely missed in our community.

Organizing the conference always requires financial resources. We were happy to receive generous support from several organizations. This allowed us to keep the registration fee at a reasonable level, to provide free accommodation and registration for nine early career researchers, and to waive the registration fee for retired participants. The financial support of following bodies is heartily acknowledged:

- Ministry of Science, Technology and Space, State of Israel;
- Office of Naval Research Global (USA);
- Technion – Israel Institute of Technology;
- Department of Materials Science and Engineering, Technion;
- Department of Materials Engineering, Ben-Gurion University of the Negev.

During the meeting of the International Advisory Board it was decided that the upcoming 11th DIMAT conference will be organized in the year 2020 by the team of Prof. Zoltán Erdélyi from the University of Debrecen, Hungary. Thus, after 38 years the DIMAT will return to the place where everything began! The fact that the DIMAT conference series has survived for so long, and has traveled across so many different cities and countries, is a clear sign of the vitality of our community.

E. Rabkin, DIMAT-2017 Chairman;

Local Organizing Committee:

N. Frage, Ben Gurion University of the Negev;

L. Klinger, Technion;

A. Novick-Cohen, Technion.

Committees

DIMAT International Advisory Board

D. Beke (Hungary)

B. Bokstein (Russia)

M. Danielewski (Poland)

S. Divinski (Germany)

C. Girardeau (France)

S. Greenbaum (USA)

A. Gusak (Ukraine)

P. Heitjans (Germany)

G. Impellizzeri (Italy)

J. Kärger (Germany)

R. Kozubski (Poland)

D. Mangelinck (France)

H. Mehrer (Germany)

Y. Mishin (USA)

G. Murch (Australia)

R. Nakamura (Japan)

A. Paul (India)

O. Politano (France)

V. Popov (Russia)

G. Roma (France)

H. Schmidt (Germany)

W. Sprengel (Austria)

N. Stolwijk (Germany)

B. Straumal (Russia)

Z. Wang (China)

Conference Sponsors

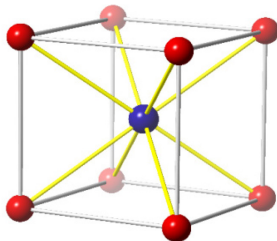
Ministry of Science, Technology and Space, State of Israel	
Office of Naval Research Global (USA)	
Technion – Israel Institute of Technology	
Department of Materials Engineering, Ben Gurion University of the Negev	
Department of Materials Science and Engineering, Technion – Israel Institute of Technology	

Table of Contents

Preface

Chapter 1: Bulk Diffusion and Reactions

Constructing an Introductory Course on Diffusion R. Ghez	3
Interdiffusion, Reactions, and Phase Transformations Observed during Fabrication of Low Enriched Uranium Monolithic Fuel System for Research and Test Reactors R. Newell, A. Mehta, Y.J. Park, D.D. Keiser Jr. and Y.H. Sohn	10
Redistribution of Metallic Impurities in Si during Annealing and Oxidation: W and Fe A. Portavoce, A. de Luca, N. Burle and M. Texier	17
On the Analysis of Composition Profiles in Binary Single-Phase Diffusion Couples: Systems with a Strong Compositional Dependence of the Interdiffusion Coefficient B. Tas Kavakbasi, I.S. Golovin, A. Paul and S.V. Divinski	23
Formation of Intermediate Phases and Supersaturated Solid Solution in Al-Cu System during Diffusion A. Rodin and N. Goreslavets	31
High-Throughput Determination of Interdiffusivities for Ni-Al-Cr Alloys at 1173 K through a Combination of Diffusion Multiple and Numerical Inverse Method W.M. Chen and L.J. Zhang	36
Moisture Sorption and Desorption in Epoxy Composites Reinforced with Triangular and V-Shaped Bars: Determination of Diffusion Coefficient and Effect of Varied Factors B.B. Pajarito, M.T. de Leon and E.R.A. Pacumio	43

Chapter 2: Computer Simulations of Diffusion and Diffusion-Controlled Processes

Numerical Analysis of Diffusion-Controlled Internal Corrosion by the Cellular Automata Approach U. Krupp, K. Jahns, K. Balinski and J. Wübbelmann	51
Tracer Diffusion and Ordering in FCC Structures - Stochastic Kinetic Mean-Field Method vs. Kinetic Monte Carlo V. Bezpalchuk, R. Abdank-Kozubski, M. Pasichnyy and A. Gusak	59
A Coupling Interface between Phase-Field Model with Finite Interface Dissipation and CALPHAD Thermodynamic and Atomic Mobility Databases J. Zhong, K. Wang and L.J. Zhang	66
Diffusion Equations for Early Stages of Solid Solutions Decay Based on the Markovian Theory of Random Walk D.M. Levin and Y.N. Kolmakov	74

Chapter 3: Diffusion and Surface Diffusion in Thin Films, Nanoparticles, and Grain Boundaries

Study of the Very First Stages of Mg Growth onto Si(100) C. Girardeaux, B. Sarpi and S. Vizzini	83
Spinodal Decomposition in Nanoparticles - Experiments and Simulation B.D. Gajdics, J.J. Tomán, F. Misják, G. Radnóczy and Z. Erdélyi	89
Effect of Equal Channel and Dynamic Channel Angular Pressing of Ni and Further Heat Treatment on its Structure and Grain Boundary Diffusion V.V. Popov, G. Reglitz, E.V. Shorohov, E.N. Popova, A.V. Stolbovsky, S.V. Divinski and G. Wilde	96
Effect of Atomic Complexes Formation in Grain Boundaries on Grain Boundary Diffusion A. Itckovich, M. Mendelev, A. Rodin and B. Bokstein	103

Mullins' Self-Similar Grooving Solution Revisited V. Derkach and A. Novick-Cohen	112
The Role of Interfaces in Evolution of Structure and Thermal Stability of Cu-Nb Composite Processed by High-Pressure Torsion E.N. Popova, I.L. Deryagina, E.G. Valova-Zaharevskaya and A.V. Stolbovsky	118

Chapter 4: Diffusion in Solid-Gas Systems

Hydrogen Sorption Kinetics in MgH₂ and TiH₂ Thin Films E. Hadjixenophontos, L. Michalek, A. Weigel and G. Schmitz	127
On the Mechanism of Oxidation Resistance of W-Cr-Pd Alloys A. Kafri, A. Makonovitsky and R.Z. Shneck	133
<i>In Situ</i> XRD Experiments on the Growth of Expanded Austenite Using Different Process Gases Z. Balogh-Michels, A. Faelt, S. Kleiner, P. Margraf, A. Dommann and A. Neels	142
Oxidation Kinetics of Nitrogen Doped TiO_{2-δ} Thin Films: Analysis on the Basis of Oxygen Activity Dependence of the Chemical Diffusion Coefficient M. Sinder, J.M. Shi and K.D. Becker	147
Properties of Species Profiles during Oxygen Chemical Diffusion in Oxides M. Sinder	153

Chapter 5: Diffusion in Materials Processing

Influence of Ion Nitriding Regimes on Diffusion Processes in Titanium Alloy Ti-6Al-4V R.D. Agzamov, A.F. Tagirov and K.N. Ramazanov	161
Influence of Ultrafine-Grained Structure of Martensitic and Austenitic Steels on Diffusion Processes at Low-Temperature Ion Nitriding U.G. Khusainov, K.N. Ramazanov and R.S. Esipov	167
Impact of a Constant Magnetic Field on Decomposition of Cu-Be-Ni-Based Solid Solution R. Post, J.V. Osinskaya, S.V. Divinski, A.V. Pokoev and G. Wilde	173
Manifestation of Magnetoplastic Effect in Some Metallic Alloys A.V. Pokoev and J.V. Osinskaya	180
Resonant Behavior of Sn Diffusion Coefficient in α-Fe in Pulsed Magnetic Field at 730-750 °C A.A. Fedotov, A.V. Pokoev and S.V. Divinski	185
Heat Transfer and Phase Formation through EBM 3D-Printing of Ti-6Al-4V Cylindrical Parts V. Popov, A. Katz-Demyanetz and M. Bamberger	190

CHAPTER 1:

Bulk Diffusion and Reactions