# International Conference on the Structure and Properties of Internal Interfaces

1985

JOURNAL DE PHYSIQUE

Tome 46 Colloque C4, supplément au n° 4 Avril 1985

# International Conference on the Structure and Properties of Internal Interfaces

August 19-23, 1984
Schwäbisches Bildungszentrum
Irsee, W. Germany

les éditions de physique

Avenue du Hoggar,
Zone Industrielle de Courtabœuf,
B.P. 112,
91944 Les Ulis Cedex, France

## FOREWORD

This Proceedings is a collection of papers presented at an "International Conference on the Structure and Properties of Internal Interfaces", which was held August 20-23, 1984 in Irsee, West-Germany. The purpose of the conference was to critically examine the current knowledge in the field of internal interfaces, with particular emphasis on grain boundaries. The conference was timely since several powerful experimental tools, including high resolution electron microscopy and X-ray diffraction, have provided new information on the atomic structure of interfaces. Innovative computer modeling approaches have also been developed to calculate the atomic structure. The conference offered an opportunity for the comparison of computer modeling predictions with experimental observations. Discrepancies between theory and experiment appeared, and these were often the starting point of intensive discussions. Solid State theoretists also participated in the conference giving ideas for future directions for fundamental theoretical studies of internal interfaces. The results of those studies may contribute to a better understanding of the structure of internal interfaces. The final portion of the conference was dedicated to a detailed examination of the relationship between interface structure and properties.

It is hoped that this Proceedings will provide a comprehensive view of current interface science both for the expert and any persons contemplating entering the field. We hope that the stimulating atmosphere during the conference at the former monastery in Irsee may also stimulate the reader of this Proceedings.

All invited and contributed papers published in the Proceedings have been reviewed by at least one referee. We would like to thank all authors and colleagues who quickly reviewed the papers so that the Proceedings could be published within a reasonable time after the conference.

The conference was organized by the Max-Planck-Institut für Metallforschung, Institut für Werkstoffwissenschaften, Stuttgart and it was sponsored by the Deutsche Forschungsgemeinschaft (DFG), FRG ; National Science Foundation (NSF), USA ; Centre National de Recherches Scientifiques (CNRS), France ; and the Max-Planck-Society, FRG.

Finally, it is a pleasure to thank Mrs. Susanne Schneeweiss and Mrs. Christa Schreiner from the Max-Planck-Institut für Metallforschung for sustantial assistance before, during and after the conference. The help of Mrs. Schneeweiss during the preparation of this Proceedings is gratefully acknowledged.

M. Rühle
R.W. Balluffi
H. Fischmeister
S.L. Sass

## ODE TO AN INTERFACE

Oh metal metal when entwined
To volume change though be inclined
The wolf, beheld he this aloft
And gave a sigh so soft
Oh soothe he did exclaim
From pair potentials I now refrain

Oh ceramic ceramic when ye doth stick
Nasty muck doth hither come, so thick
Our ruhler, thence he came and he did yell
Ye dislocation, I cannot tell.
A foreign clark he did then appear
And saith, the glass be very thin, O dear

Oh metal, ceramic when thou do join
Be it coincidence thy do seek
Oh no did they exclaim, to win
Close pack thy showed and then lock in

A.G. EVANS

Conference Banquet
Irsee Conference
August 23, 1984

## LIST OF PARTICIPANTS

ANDERSEN, O.K.- MPI für Festkörperforschung, Heisenbergstrasse 1, D-7000 Stuttgart 80, F.R.G.

ARZT, E.- MPI für Metallforschung, Inst. für Werkstoffwissenschaften, Seestrasse 92, D-7000 Stuttgart 1, F.R.G.

AST, D.- Cornell University, Bard Hall, Ithaca, NY 14853, U.S.A.

ATKINSON, A.- MDD, Bldg. 552, AERE Harwell, Didcot, Oxon OX11 ORA, U.K.

ATKINSON, H.V.- MDD, Bldg. 552, AERE Harwell, Didcot, Oxon OX11 ORA, U.K.

BALLUFFI, R.W.- Department of Materials Science, Massachusetts, Institute of Technology, Room 13-5078, Cambridge, MA 02139, U.S.A.

BEAUNIER, L.-GR4 - CNRS, Université de Paris VI, 4, placeJussieu, 75230 Paris Cedex 05, France.

BERNARDINI, J.- Laboratoire de Métallurgie, ERA 552, Faculté des Sciences et Techniques, Rue Henri Poincaré, 13397 Marseille Cedex 13, France.

BIRRINGER, R.- Universität des Saarlandes, Werkstoffphysik, FB 12.1, Bau 2, D-6600 Saarbrücken, F.R.G.

BISCONDI, M.- Ecole Nationale Supérieure des Mines, 158 Cours Fauriel, 42023 St Etienne, France.

BÖGEL, A.- MPI für Metallforschung, Inst. für Werkstoffwissenschaften, Seestrasse 92, D-7000 Stuttgart 1, F.R.G.

BOLLMANN, W.- 22, Chemin Vert, CH-1234 Pinchat, GENF, Switzerland.

BONNET, R.- Institut National Polytechnique, LTPCM, Domaine Universitaire, B.P. 75, 38402 Saint-Martin-d'Hères, France.

BOUCHET, D.- Laboratoire de Métallurgie, 3 Rue Yvart, 75015 Paris, France.

BOURRET, A.- CEN-Grenoble, DRF, Physique du Solide, 85 X, 38041 Grenoble, France.

BRISTOWE, P.D.- Massachusetts Institute of Technology, Department of Materials Science and Engineering, Room 13-5157, Cambridge, MA 02139, U.S.A.

BROKMAN, A.- Hebrew University, Graduate School of Applied Science, Giv. Ram, 91904 Jerusalem, Israel.

CABANE, F.- Laboratoire de Métallurgie, ERA 552, Faculté des Sciences et Techniques, Rue Henri Poincaré, 13397 Marseille Cedex 13, France.

CAERS, J.F.J.M.- Center for Manufacturing Technology, SAQ p421, Philips Bedrijven B.V., 5600 MD Eindhoven, The Netherlands.

CHUANG, T.-H.- MPI für Metallforschung, Inst. für Werkstoffwissenschaften, Seestrasse 92, D-7000 Stuttgart 1, F.R.G.

CLARKE, D.R.- IBM T.J. Watson Research Center, 21-239, Yorktown Heights, NY 10598, U.S.A.

COBLE, R.L.- Department of Materials Science and Engineering, Massachusetts Institute of Technology, Cambridge, MA 02139, U.S.A.

DEYMIER, P.A.- Department of Materials Science and Engineering, Massachusetts Institute of Technology, Cambridge, MA 02139, U.S.A.

DIVINCENZO, D.P.- Department of Physics, Cornell University, Bard Hall, Ithaca, NY 14853, U.S.A.

DOLLAR, M.- Universität des Saarlandes, Werkstoffphysik, FB 12.1, Bau 2, D-6600 Saarbrücken, F.R.G.

DUPEUX, M.- L.T.P.C.M. - E.N.S.E.E.G., B.P. 75, 38402 Grenoble, France.

ELSSNER, G.- MPI für Metallforschung, Inst. für Werkstoffwissenschaften, Seestrasse 92, D-7000 Stuttgart 1, F.R.G.

ERBUDAK, M.- ETH, Festkörperphysik, CH-8093 Zürich, Switzerland.

EVANS, A.G.- Department of Materials Science and Mineral Eng., University of California, Hearst Mining Building, Berkeley, CA 94720, U.S.A.

EXNER, H.E.- MPI für Metallforschung, Inst. für Werkstoffwissenschaften, Seestrasse 92, D-7000 Stuttgart 1, F.R.G.

FECHT, H.-J.- Universität des Saarlandes, Werkstoffphysik, FB 12.1, Bau 2, D-6600 Saarbrücken, F.R.G.

FISCHMEISTER, H.- MPI für Metallforschung, Inst. für Werkstoffwissenschaften, Seestrasse 92, D-7000 Stuttgart 1, F.R.G.

FLORJANCIC, Jr., M.- Fa. SEL AG, Postfach 40 07 49, D-7000 Stuttgart 40, F.R.G.

FOULKES, W.M.C.- Inst. of Theoretical Sc., University of Oregon, Eugene, Oregon 97403, U.S.A.

FRACZKIEWICZ, A.- Ecole Nationale Supérieure des Mines, 158 Cours Fauriel, 42023 St Etienne, France.

GEROLD, V.- MPI für Metallforschung, Inst. für Werkstoffwissenschaften, D-7000 Stuttgart 1, F.R.G.

GIBSON, J.M.- AT&T Bell Laboratories, Room 1E234, 600 Mountain Avenue, Murray Hill, NJ 07974, U.S.A.

GLEITER, H.- Universität des Saarlandes, Werkstoffphysik, FB 12.1, Bau 2, D-6600 Saarbrücken, F.R.G.

GOTTHARDT, R.- EPFL/IGA, CH-1015 Lausanne, Switzerland.

GRABSKI, M.W.- Politechnika Warszawska, Institute of Materials Science and Engineering, Narbutta 85, 02-524 Warsaw, Poland.

GRIMMER, H.K.- EIR, Abt. Metallurgie, CH-5303 Würenlingen, Switzerland.

GROVENOR, C.R.- Department of Metallurgy, Oxford University, Oxford OX1 3RQ, U.K.

GUDLADT, H.-J.- MPI für Metallforschung, Inst. für Werkstoffwissenschaften, Seestrasse 92, D-7000 Stuttgart 1, F.R.G.

GUST, W.- MPI für Metallforschung, Inst. für Werkstoffwissenschaften, Seestrasse 92, D-7000 Stuttgart 1, F.R.G.

HAGEGE, S.- Equipe Matériaux Microsctructure, ISRMa-Université de Caen, 14032 Caen, France.

HAHN, H.- Universität des Saarlandes, Werkstoffphysik, FB 12.1, Bau 2, D-6600 Saarbrücken, F.R.G.

HAHN, W.- Universität des Saarlandes, Werkstoffphysik, FB 12.1, Bau 2, D-6600 Saarbrücken, F.R.G.

HAYDOCK, R.- Inst. of Theoretical Sc., University of Oregon, Eugene, Oregon 97403, U.S.A.

HERZIG, C.- Inst. für Metallforschung, Domagkstrasse 75, D-4400 Münster, F.R.G.

HOEL, R.H.- MPI für Metallforschung, Inst. für Werkstoffwissenschaften, Seestrasse 92, D-7000 Stuttgart 1, F.R.G.

HOFMANN, H.- MPI für Metallforschung, PML, Heisenbergstrasse 5, D-7000 Stuttgart 80, F.R.G.

HOFMANN-AMTENBRINK, M.- MPI für Metallforschung, PML, Heisenbergstrasse 5, D-7000 Stuttgart 80, F.R.G.

HOFMANN, S.- MPI für Metallforschung, Inst. für Werkstoffwissenschaften, Seestrasse 92, D-7000 Stuttgart 1, F.R.G.

ICHINOSE, H.- Institute of Industrial Science, University of Tokyo, 22-1 Roppongi, 7 Chome, Minato-ku, Tokyo 106, Japan.

IGNAT, M.- ENSEEG, B.P. 75, 38402 Grenoble, France.

ISHIDA, Y.- Institute of Industrial Science, University of Tokyo, 22-1 Roppongi, 7 Chome, Minato-ku, Tokyo 106, Japan.

KALONJI, G.- Department of Materials Science and Engineering, Massachusetts Institute of Technology, Cambridge, MA 02139, U.S.A.

KAYSSER, W.- MPI für Metallforschung, PML, Heisenbergstrasse 5, D-7000 Stuttgart 80, F.R.G.

KING, W.E.- Materials Science and Technology Division, Argonne National Lab., Argonne, IL 60439, U.S.A.

KLOMP, J.T.- Philips Research Labs., P.O. Box 80000, 5600 J.A. Eindhoven, The Netherlands.

LANCIN, M.- CNRS - LPM, 1, place A. Briand, 92360 Meudon Bellevue, France.

LARTIGUE, S.- Laboratoire de Métallurgie Physique, 36 de Latour Mauboury, 75007 Paris, France.

LAVAL, J.-Y.- Laboratoire des Microstructures, E.S.P.C.I., 10 Rue Vauquelin, 75231 Paris Cedex 05, France.

ŁOJKOWSKI, W.- UNIPRESS, High Pressure Research Center, 01-142 Warsaw, Poland.

LÖSCH, K.- MPI für Metallforschung, Inst. für Werkstoffwissenschaften, Seestrasse 92, D-7000 Stuttgart 1, F.R.G.

LOUIE, S.G.- Department of Physics, University of California, Berkeley, CA 94720, U.S.A.

MADER, W.- MPI für Metallforschung, Inst. für Werkstoffwissenschaften, Seestrasse 92, D-7000 Stuttgart 1, F.R.G.

MARTIN, J.-L.- Institut Génie Atomique, EPFL, CH-1015 Lausanne, Switzerland.

MAURER, R.- Universität des Saarlandes, Werkstoffphysik, FB12.1, Bau 2, D-6600 Saarbrücken, F.R.G.

MAURICE, J.L.- Laboratoire d'Etude et de Synthèse des Microsctructures, ERA 912, CNRS-ESPCI, 10, Rue Vauquelin, 75231 Paris Cedex 05, France.

MAYER, S.- MPI für Metallforschung, Inst. für Werkstoffwissenschaften, Seestrasse 92, D-7000 Stuttgart 1, F.R.G.

MECARTNEY, M.L.- MPI für Metallforschung, Inst. für Werkstoffwissenschaften, Seestrasse 92, D-7000 Stuttgart 1, F.R.G.

MERKLE, K.L.- Materials Science and Technology Division, Argonne National Lab., Argonne, IL 60439, U.S.A.

MOLINARI, E.- MPI für Festkörperforschung, Heisenbergstrasse 1, D-7000 Stuttgart 80, F.R.G.

MULDER, C.A.M.- Philips Research Labs., 5600 J.A. Eindhoven, The Netherlands.

NECKER, G.- MPI für Metallforschung, Inst. für Werkstoffwissenschaften, Seestrasse 92, D-7000 Stuttgart 1, F.R.G.

NEUMANN, P.- MPI für Eisenforschung, Postfach 140260, D-4000 Düsseldorf, F.R.G.

OEI, Y.-S.- Laboratory of Metallurgy, Delft Univ. of Technology, P.O. Box 5025, 2600 G.A. Delft, The Natherlands.

OPPOLZER, H.- Siemens, AG, Otto-Hahn-Ring 6, D-8000 München 83, F.R.G.

PAXTON, T.- Dept. of Metallurgy and Science of Materials, Oxford University, Parks Road, Oxford OX1 3PH, U.K.

PETZOW, G.- MPI für Metallforschung, PML, Heisenbergstrasse 5, D-7000 Stuttgart 1, F.R.G.

PIERAGGI, B.- ENSCT, Laboratoire Met. Physique, 118, Route de Narbonne, 31077 Toulouse Cedex, France.

POND, R.C.- Department of Metallurgy, University of Liverpool, P.O. Box 147, Liverpool L69 3BX, U.K.

PRIESTER, L.- Laboratoire Met. Physique, 29, Rue Boussingault, 75013 Paris, France.

RADNÓCZI, G.- Res. Inst. for Technical Physics of the Hungarian Academy of Sciences, P.O. Box 76, 1325 Budapest, Hungary.

RAJ, R.- Department of Materials Science and Engineering, Bard Hall, Cornell University, Ithaca, NY 14853, U.S.A.

RATKE, L.- MPI für Metallforschung, Inst. für Werkstoffwissenschaften, Seestrasse 92, D-7000 Stuttgart 1, F.R.G.

REVCOLEVSCHI, A.-Laboratoire de Chimie Appliquée, Bât. 414, Université de Paris, 91405 Orsay Cedex, France.

REY, C.- Laboratoire PMTM, Avenue J.B. Clément, 93430 Villetaneuse, France.

ROCHER, A.M.- Laboratoire d'Optique Electron., 29, Rue J. Marvig, 31400 Toulouse, France.

ROLL, U.- MPI für Metallforschung, Inst. für Werkstoffwissenschaften, Seestrasse 92, D-7000 Stuttgart 1, F.R.G.

RÖSLER, H.-J.- MPI für Metallforschung, Inst. für Werkstoffwissenschaften, Seestrasse 92, D-7000 Stuttgart 1, F.R.G.

RÜHLE, M.- MPI für Metallforschung, Inst. für Werkstoffwissenschaften, Seestrasse 92, D-7000 Stuttgart 1, F.R.G.

SASS, S.L.- Department of Materials Science and Engineering, Bard Hall, Cornell University, Ithaca, NY 14853, U.S.A.

SAWHILL, H.T.- Department of Materials Science and Engineering, Massachusetts Institute of Technology, Room 13-4077, Cambridge, MA 02139, U.S.A.

SCHAPINK, W.F.- Laboratory of Metallurgy, Delft Univ. of Technology, 2628 AG Delft, The Netherlands.

SCHLÜTER, M.- AT&T Bell Laboratories, 600 Mountain Avenue, Murray Hill, NJ 07974, U.S.A.

SCHMAUDER, S.K.- MPI für Metallforschung, Inst. für Werkstoffwissenschaften, Seestrasse 92, D-7000 Stuttgart 1, F.R.G.

SCHMÜCKLE, F.- BBC Forschungszentrum, CH-5400 Baden, Switzerland.

SCHULZE, K.K.- MPI für Metallforschung, PML, Heisenbergstrasse 5, D-7000 Stuttgart 1, F.R.G.

SEIDMAN, S.- Hebrew University of Jerusalem, Givat Ram, Campus, Bergman Bldg., School of Applied Science, 91904 Jerusalem, Israel.

SMITH, J.R.- Physics Department, General Motors Res. Lab., Warren, MI 48090-9055, U.S.A.

SOLENTHALER, C.- Sulzer AG, CH-8401 Winterthur, Switzerland.

SUGA, T.- The University of Tokyo, Faculty of Engineering, Department of Precision Machinery Eng., Hongo 3-7, Bunkyo-ku, 113 Tokyo, Japan.

SUTTON, A.P.- Department of Metallurgy and Science of Materials, Oxford University, Parks Road, Oxford OX1 3PH, U.K.

TASKER, P.- Theoretical Physics Division, AERE Harwell, Didcot, Oxon OX11 ORA, U.K.

TAYLOR, R.- Physics Division, National Research Council of Canada, Ottawa K1A OR6, Canada.

TURWITT, M.- MPI für Metallforschung, Inst. für Werkstoffwissenschaften, Seestrasse 92, D-7000 Stuttgart 1, F.R.G.

VAUDIN, M.- Department of Materials Science and Engineering, Bard Hall, Cornell University, Ithaca, NY 14853, U.S.A.

VEHOFF, H.- MPI für Eisenforschung, Postfach 140260, D-4000 Düsseldorf, F.R.G.

VERWEIJ, A.D.- Philips Res. Lab. SAQ-p421, 5600 MD Eindhoven, The Netherlands.

VIGNAUD, C.- Laboratoire de Physique des Liquides et Electrochimie, Université Pierre et Marie Curie, 75230 Paris Cedex, France.

VITEK, J.- Oak Ridge National Lab., Oak Ridge, TN 37831, U.S.A.

VITEK, V.- University of Pennsylvania, Department of Materials Science and Engineering /K1, Philadelphia, PA 19104, U.S.A.

WARRINGTON, D.H.- 1 Haddon Drive, Bakewell, Derbyshire DE4 1BD, U.K.

WATANABE, T.- Department of Materials Science, Faculty of Eng., Tohoku University, Sendai 980, Japan.

WOLF, D.- Materials Science and Technology Division, Argonne Nat. Laboratory, Argonne, IL 60439, U.S.A.

WUNDERLICH, W.- MPI für Metallforschung, Inst. für Werkstoffwissenschaften, Seestrasse 92, D-7000 Stuttgart 1, F.R.G.

ZHU, X.- Universität des Saarlandes, Werkstoffphysik, FB 12.1, Bau 2, D-6600 Saarbrücken, F.R.G.

CONTENTS

## CALCULATIONS ON THE STRUCTURES OF INTERNAL INTERFACES



## RELATION BETWEEN CALCULATED AND EXPERIMENTALLY OBSERVED STRUCTURES OF INTERNAL INTERFACES



## NEW DIRECTIONS FOR CALCULATIONS

**RELATION BETWEEN STRUCTURES AND PROPERTIES OF INTERNAL INTERFACES**



**SEGREGATION AND DIFFUSION AT INTERNAL INTERFACES**

**RELATION BETWEEN STRUCTURES AND MECHANICAL PROPERTIES OF INTERNAL INTERFACES**

# INTRODUCTORY OVERVIEW

JOURNAL DE PHYSIQUE
Colloque C4, supplément au n°4, Tome 46, avril 1985 

# STRUCTURE AND PROPERTIES OF HIGH ANGLE GRAIN BOUNDARIES

H.F. Fischmeister

*Max-Planck-Institut für Metallforschung, D-7000 Stuttgart 1, F.R.G.*

Résumé - Dans cet article de revue sont présentés la crystallographie des bicristaux, les conceptes de coincidence, les mécanismes de relaxation, les principes et résultats essentiels de modélisation sur ordinateur ainsi que la description des joints de grains à large angle de désorientation par des séries périodique de dislocations ou des séquences ordonnées de certains polyhèdres de coordination. Les relations de structure aux propriétés des joints de grains sont exposées à la lumière des modèles existants en insistant plus particulièrement sur la ségrégation d'impuretés au niveau des joints ainsi que ses effets sur leur structure comme observé dans les simulations sur ordinateur.

Abstract - This is a tutorial review covering the crystallography of bicrystals, coincidence concepts, relaxation mechanisms, principles and main results of computer modelling, and the description of high angle grain boundaries in terms of periodic arrays of either dislocations or ordered sequences of coordination polyhedra in the boundaries. Structure - property relations in grain boundaries are reviewed in the light of existing models, with special emphasis on the segregation of impurities at grain boundaries and its effects on boundary structure as indicated by computer modelling.

## 1. INTRODUCTION

With few exceptions, metals and ceramics are used in polycrystalline form. Boundaries between grains, or between different phases, often play a decisive role in determining the material's properties. For example, the toughness and strength of steels has been drastically improved since the 1950's by rigorous control of grain size, of the chemistry of grain boundaries and of nonmetallic inclusions in the metal.

HOMOPHASE BOUNDARIES are interfaces between regions of identical crystal structure; they include grain boundaries, twin boundaries, and domain boundaries. Stacking faults are commonly included in this category although they can be viewed as thin lamellae of a different (but related) crystal structure.

HETEROPHASE BOUNDARIES are interfaces between regions of different crystal structure which may, but need not, have different chemical

composition. Examples of the first kind would be boundaries between coexisting allotropic modifications, for instance between grains of the tetragonal and the monoclinic phase of $ZrO_2$. Examples of the second kind are virtually omnipresent in technical alloys and ceramics, for instance the boundaries between austenite and ferrite in a 'duplex' stainless steel, or the surfaces of the non-metallic inclusions mentioned above. In both cases, with compositional difference and without, the regions adjoining the interface belong to different phases in the classical thermodynamic sense; therefore the simpler term PHASE BOUNDARIES is often used for them.

Control of grain boundary chemistry by doping, scavenging, selective precipitation or suppression of second phases has become standard practice, and so has the manipulation of grain boundary mobility and shape by pinning, or by directional solidification or annealing. A highly sophisticated practice of grain boundary engineering is in common use today for superalloys, certain high-technology ceramics, but also for such deceptively 'simple' materials as steels, whose design limits would be drastically lower without the benefit of boundary engineering. - Yet, only part of this engineering knowledge has a firm ground in science. In particular, understanding in terms of atomistic structure has lagged far behind the art of engineering manipulation for most types of internal boundaries.

For low-angle grain boundaries, a dislocation model was proposed by Taylor /1/ as early as 1934. Its verification by etch pit observations as well as the prediction of the influence of misorientation upon interfacial energy /2/ and boundary diffusivity /3/ were early triumphs of the evolving understanding of real crystal properties in terms of lattice dislocations.

For high-angle boundaries, the development of structural models has been slower and more tortuous. Theory and experimental techniques for constructing and testing detailed models have only recently become available, triggering a wave of exciting developments which are the main subject of this review.

Heterophase boundaries are more complicated still. Only quite recently have the first steps been taken towards an understanding of their structures, in particular for metal-ceramic boundaries. In contrast to grain boundaries, engineering control of phase boundaries has yet to be developed, and one could still hope that rapid progress might enable science to take the lead in this development.

The present paper will review the state of the subject with emphasis on recent ideas; experimental results and techniques will be discussed only in relation to theoretical concepts. For background, and for comprehensive summaries of experimental results, reviews and conference books are available /4-13/. The following section will introduce the special crystallographic nomenclature developed for boundaries, and discuss the geometry of unrelaxed bicrystals. Sections 3 and 4 deal with relaxation processes and their study by computer modelling, and section 5 reviews a priori ideas concerning the relation between the structure of grain boundaries and their properties. Finally, section 6 reviews computer modelling results concerning grain boundary segregation, where particularly detailed ideas have been developed very recently. No systematic treatment is attempted for heterophase boundaries, but important contributions to this subject are referenced.