Engineering Materials and Processes

Series Editor

Professor Brian Derby, Professor of Materials Science
Manchester Materials Science Centre, Grosvenor Street, Manchester, M1 7HS, UK

Other titles published in this series

Fusion Bonding of Polymer Composites
C. Ageorges and L. Ye

Composite Materials
D.D.L. Chung

Titanium
G. Lütjering and J.C. Williams

Corrosion of Metals
H. Kaesche

Corrosion and Protection
E. Bardal

Intelligent Macromolecules for Smart Devices
L. Dai

Microstructure of Steels and Cast Irons
M. Durand-Charre

Phase Diagrams and Heterogeneous Equilibria
B. Predel, M. Hoch and M. Pool

Computational Mechanics of Composite Materials
M. Kamiński

Gallium Nitride Processing for Electronics, Sensors and Spintronics
S.J. Pearton, C.R. Abernathy and F. Ren

Materials for Information Technology
E. Zschech, C. Whelan and T. Mikolajick

Fuel Cell Technology
N. Sammes

Casting: An Analytical Approach
A. Reikher and M.R. Barkhudarov

Computational Quantum Mechanics for Materials Engineers
L. Vitos

Modelling of Powder Die Compaction
P.R. Brewin, O. Coube, P. Doremus and J.H. Tweed

Silver Metallization
D. Adams, T.L. Alford and J.W. Mayer

Microbiologically Influenced Corrosion
R. Javaherdashti

Modeling of Metal Forming and Machining Processes
P.M. Dixit and U.S. Dixit

Electromechanical Properties in Composites Based on Ferroelectrics
V.Yu. Topolov and C.R. Bowen

Charged Semiconductor Defects
E.G. Seebauer and M.C. Kratzer

Modelling Stochastic Fibrous Materials with Mathematica®
W.W. Sampson

Ferroelectrics in Microwave Devices, Circuits and Systems
S. Gevorgian

Porous Semiconductors
F. Kochergin and H. Föll

Chemical Vapour Deposition
C.-T. Yan and Y. Xu

Composite Materials
D.D.L. Chung

Jaroslav Pokluda · Pavel Šandera

Micromechanisms of Fracture and Fatigue

In a Multiscale Context

Springer

Prof. Jaroslav Pokluda
Prof. Pavel Šandera

Brno University of Technology
Faculty of Mechanical Engineering
Technicka 2
61669 Brno
Czech Republic

pokluda@fme.vutbr.cz
sandera@fme.vutbr.cz

ISSN 1619-0181
ISBN 978-1-84996-265-0 e-ISBN 978-1-84996-266-7
DOI 10.1007/978-1-84996-266-7

British Library Cataloguing in Publication Data
A catalogue record for this book is available from the British Library

Library of Congress Control Number: 2010928264

Cover design: eStudioCalamar, Figueres/Berlin

Printed on acid-free paper

Springer is part of Springer Science+Business Media (www.springer.com)

There are only a few things that may improve when getting older. One of these is a grasp on the rules of Nature.

Preface

Classical concepts and numerical methods of mechanical engineering such as, for example, fracture mechanics and finite element analysis focus on macroscale problems where the microstructure is incorporated by using averaging constitutive laws. On the other hand, the domain of materials science and solid state physics focuses on investigation of atomic bonds, lattice defects, microstructural elements and their interactions at nano, micro and meso scales. However, a recent development in fracture and fatigue research clearly indicates that the most promising and effective concepts are based on coupling engineering mechanics with materials science within so-called multiscale fracture models. The objective of these approaches is to bridge the enormous gap between time and space scales and, therefore, they constitute a great challenge in the sense of scientific knowledge. Moreover, they still drive at psychological barriers of conservative mechanical engineers and/or material scientists. Therefore, an overwhelming majority of books about fracture and fatigue were written from the point of view of either mechanical engineers or material scientists. To our knowledge, a pioneering attempt to produce a successful integrated concept of fracture was made by Kelly and Macmillan [1]. Since that time, however, many new methods and concepts have been developed which should be incorporated into advanced multiscale models of fracture and fatigue.

This book was written as an overview of scientific results achieved by the authors during about 40 years of their research. However, another strong motivation was to support advanced trends in fracture and fatigue which lead to the development of multiscale concepts for securing the integrity of engineering components and structures. This second aim has always prevailed over the first. Therefore, the book is composed in a compact manner and provides a rather comprehensive survey of fracture micromechanisms and related multiscale models. Although these models were predominantly proposed by the authors of this book, many passages devoted to models that were published by other authors are included in order to ensure a consistent presentation of the subject. A prevailing part of the book reflects the joint work of authors

at the Brno University of Technology. However, several results and models originate from the research of the first author, performed at the Military Institute of Material Science and Technology from 1973 to 1985. The opportunity to present these results is much appreciated since, for obvious reasons, they were not allowed to be published in international scientific journals at that time.

The book addresses students at graduate and postgraduate levels, lecturers, materials scientists and mechanical engineers, as well as materials physicists and chemists. Any kind of criticism or advice that can help to improve the text will be very welcome.

Many results presented in this book were achieved either in the frame of international scientific collaboration or appeared as a consequence of stimulating discussions with colleagues from foreign universities and research institutes. Our very special thanks go to Prof. R. Pippan from the Institute of Materials Science, Austrian Academy of Sciences, in Leoben, Austria, Prof. V. Vitek from the University of Pennsylvania in Philadelphia, Pennsylvania, USA and Prof. Y. Murakami from the Kyushu University in Fukuoka, Japan, for our stimulating discussions during our long-term collaboration. Our warm thanks go to Dr. A. Doig from the Military Academy in Shrivenham, England, and Dr. R. Gröger from the Los Alamos National Laboratory, USA, for their fruitful comments on the scientific content and English language of this book. We are also deeply indebted to Prof. O. Kolednik, Prof. J. Janovec, Prof. M. Jenko, Prof. Y. Kondo, Dr. G. Chai, Prof. Y. Kitamura, Prof. C. Laird, Prof. S. Stanzel-Tschegg, Dr. M. Sauzay, Prof. M. Zehetbauer, Prof. A. Krasowski, Prof. E. Macha, Prof. A. Shaniavsky and Prof. L. Tóth for helpful and friendly discussions associated with joint publications and/or scientific meetings and visits.

There are also a number of Czech colleagues who directly or indirectly contributed to this book. Let us first mention a long-term collaboration, fruitful discussions and extended joint work with Prof. M. Šob from the Masaryk University in Brno and Prof. P. Lejček from the Institute of Physics, Academy of Sciences of the Czech Republic in Prague. Furthermore, Dr. P. Lukáš from the Institute of Physics of Materials, Academy of Sciences of the Czech Republic in Brno and Dr. F. Kroupa (†) from the Institute of Plasma Physics, Academy of Sciences of the Czech Republic in Prague have helped us very much particularly during the first periods of our research activities. We are also grateful to Prof. J. Švejcar, Dr. I. Saxl (†), Prof. I. Dlouhý, Prof. B. Vlach, Prof. M. Kotoul, Dr. P. Ponížil, Prof. K. Stránský, Prof. I. Dvořák, Dr. J. Siegl, Dr. L. Obdržálek, Prof. J. Zeman, Prof. L. Kunz, Prof. Z. Knésl, Prof. P. Lukáč, Dr. A. Machová, Dr. V. Paidar, Prof. V. Navrátil, Prof. J. Polák, Dr. M. Holzmann, Prof. J. Kohout, Prof. R. Foret, Dr. P. Staněk, Dr. A. Buchal, Dr. K. Obrtlík, Prof. M. Šlesár (†), Prof. M. Bílý, Dr. V. Oliva and Dr. H. Lauschmann for helpful discussions associated with joint publications and/or scientific meetings.

We are deeply grateful to our friends and colleagues from the Department of Materials Micromechanics and Applied Acoustics, especially to Dr. M. Černý, who was our partner and consultant in most topics of the first chapter. We have also very much appreciated the help of Dr. J. Horníková and Dr. K. Slámečka with experimental and theoretical investigations in mixed-mode fracture and fatigue as well as with the design and preparation of many figures. Finally, we would like to thank Anthony Doyle from Springer UK, who has offered us the opportunity to write this book.

Brno, *Jaroslav Pokluda*
December 2009 *Pavel Šandera*

Contents

0 Introduction 1

1 Deformation and Fracture of Perfect Crystals 9
1.1 Ideal Strength of Solids 10
1.1.1 From Classics to Recent Concepts 11
1.1.2 Calculation Principles 16
1.1.3 Simple Loading Modes 26
1.1.4 Multiaxial Loading 36
1.1.5 Nanocomposites 46
1.1.6 Influence of Crystal Defects and Temperature 52
1.2 Intrinsic Brittleness and Ductility 54
1.2.1 Fundamentals 55
1.2.2 Calibration of Crystals 59
1.3 Multiscale Model of Nanoindentation Test 63
1.3.1 Description of Submodels 64
1.3.2 Simulation of Pop-in Effects 66

2 Brittle and Ductile Fracture 69
2.1 Brittle Fracture 73
2.1.1 Geometrically Induced Crack Tip Shielding 74
2.1.2 Pyramidal Model of Tortuous Crack Front 78
2.1.3 Fracture Toughness of Particle Reinforced Glass Composite 80
2.2 Quasi-brittle Fracture 88
2.2.1 Statistical Approach to Geometrical Shielding Based on Size Ratio Effect 90
2.2.2 Anomalous Fracture Behaviour of Ultra-high-strength Steels 93
2.2.3 Mixed Intergranular and Cleavage Fracture of Phosphorus-doped Fe-2.3%V Alloy 98
2.3 Ductile Fracture 108

2.3.1 Kinetics of Plastic Deformation During Uniaxial Ductile Fracture: Modelling and Experiment 111
2.3.2 Fracture Strain 116
2.3.3 Assessment of Fracture Toughness from Basic Mechanical Characteristics 121

3 Fatigue Fracture 125
3.1 Quantitative Fractography 126
3.1.1 Topological Analysis 127
3.1.2 Morphological Patterns in Fatigue 135
3.2 Opening Loading Mode 139
3.2.1 Discrete Dislocation Models of Mechanical Hysteresis . 141
3.2.2 Nucleation and Growth of Short Cracks 150
3.2.3 Discrete Dislocation Models of Mode I Growth of Long Cracks 155
3.2.4 Crack Closure Mechanisms 164
3.2.5 Unified Model of Crack-tip Shielding 175
3.2.6 Applications of the Unified Model 179
3.2.7 Influence of Shielding on Crack Growth Rate 185
3.3 Shear and Mixed-mode Loading 188
3.3.1 Models of Shear-mode Crack Growth 189
3.3.2 Propagation of Cracks under Cyclic Torsion 194
3.3.3 Propagation of Cracks under Cyclic Shear 203
3.3.4 Crack Growth and Fatigue Life under Combined Bending-torsion Loading 217
3.3.5 Formation of Fish-eye Cracks under Combined Bending-torsion Loading 227
3.4 Failure Analysis 237
3.4.1 Theoretical Background 238
3.4.2 Case Study 240

4 Final Reflections 243
4.1 Useful Results 243
4.2 Open Tasks 246

Appendixes

A *Ab initio* Computational Methods 249
A.1 TB-LMTO-ASA Code 251
A.2 Wien 95 – w2k Codes 252
A.3 VASP Code 253

B Mixed-mode Criteria of Crack Stability 255
B.1 Energy Criterion 255
B.2 Criterion of Linear Damage Accumulation 256

B.3 Criterion of Minimal Deformation Energy 256
B.4 Criterion of Maximal Principal Stress 257

C Plastic Flow Rate Inside the Neck 259
C.1 Ideal Model 259
C.2 Real Model 261

List of Reprinted Figures 265

References 269

Index 283