Siegfried Schmauder
Leon Mishnaevsky Jr.

Micromechanics and Nanosimulation of Metals and Composites

Advanced Methods and Theoretical Concepts

Springer

Micromechanics and Nanosimulation
of Metals and Composites

Siegfried Schmauder · Leon Mishnaevsky Jr.

Micromechanics and Nanosimulation of Metals and Composites

Advanced Methods and Theoretical Concepts

Springer

Professor Dr. Siegfried Schmauder
Institute for Materials Testing,
Materials Science and Strength
of Materials (IMWF)
University of Stuttgart
Pfaffenwaldring 32
D-70569 Stuttgart
Germany
siegfried.schmauder@imwf.uni-stuttgart.de

Dr.-Ing. habil. Leon Mishnaevsky Jr.
Senior Scientist
Risø.DTU National Laboratory
for Sustainable Energy
Technical University of Denmark
AFM-228
DK-4000 Roskilde
Denmark
leon.mishnaevsky@risoe.dk

ISBN: 978-3-540-78677-1 e-ISBN: 978-3-540-78678-8

Library of Congress Control Number: 2008936029

Cover design: eStudio Calamar S.L.

Printed on acid-free paper

9 8 7 6 5 4 3 2 1

springer.com

Contents

Preface

The strength of metallic materials determines the usability and reliability of all the machines, tools and equipment around us. Yet, the question about which mechanisms control the strength and damage resistance of materials and how they can be optimised remains largely unanswered. How do real, heterogeneous materials deform and fail? Why can a small modification of the microstructure increase the strength and damage resistance of materials manifold? How can the strength of heterogeneous materials be predicted?

The purpose of this book is to present different experimental and computational analysis methods of micromechanics of damage and strength of materials and to demonstrate their applications to various micromechanical problems. This book summarizes at a glance some of the publications of the Computational Mechanics Group at the IMWF/MPA Stuttgart, dealing with atomistic, micro- and mesomechanical modelling and experimental analysis of strength and damage of metallic materials.

In chapter 1, the micromechanisms of damage and fracture in different groups of materials are investigated experimentally, using direct observations and inverse analysis. The interaction of microstructural elements with the evolving damage is studied in these experiments. Chapter 2 presents different approaches to the micromechanical simulation of composite materials: embedded unit cells, multiphase finite elements and multiparticle unit cells. Examples of the application of these models to the analysis of deformation and damage in different materials are given. Chapter 3 deals with the methods of numerical modelling of damage evolution and crack growth in heterogeneous materials. Different methods of damage evolution modelling, in particular in materials with ductile (aluminium, cobalt) and brittle matrices, are applied to investigate the interrelations between microstructures and strength of these materials. Chapter 4 provides an insight into several methods of micromechanical computational modelling of materials with interpenetrating phases using graded materials. It defines the matricity model and demonstrates its application to the analysis of different materials. Multilayer models of graded materials, functionally graded finite elements, multiparticle unit cells with graded particle distribution and voxel based method of the 3D FE mesh generation are described in this chapter as well as models of graded materials used for milling applications.

Chapter 5 deals with methods of atomistics and dislocation modelling of the material behaviour and damage.

Siegfried Schmauder Leon Mishnaevsky Jr.

Stuttgart, 13 August 2008 Roskilde, 13 August 2008

Acknowledgements

The investigations, described in this book, have been carried out in the framework of many research projects, funded by EU, ECSC (European Commission of Coal and Steel), DFG (Deutsche Forschungsgemeinschaft), Humboldt Foundation, and other funding bodies. In particular, the support by the German Bundesministerium für Bildung, Wissenschaft, Forschung und Technologie (BMBF) under grant No 1501029 and in connection with the COST-512 Program through contract 03K8004, by the European Commission via the Brite-Euram Project 8109 “Design of new tool materials with a structural gradient for milling application” and ECSC-Project 8834 “Influence of micromechanical mechanisms on strength and damage of tool steels under static and cyclic loading”, from Deutsche Forschungsgemeinschaft through the Sonderforschungsbereich 381 “Charakterisierung des Schädigungsverlaufes in Faserverbundwerkstoffen mittels zerstörungsfreier Prüfung”, through the projects 436RUS 17/68/04, Schm 746/16-1, Schm 746/25-1, Schm 746/12-1 and Schm 746/12-2 (Schwerpunktprogramm Gradientenwerkstoffe), RI 339/15-1, FI 686/1-1, Heisenberg fellowship “Werkstoffoptimierung auf dem Mesoniveau mittels numerischer Experimente unter Berücksichtigung von Effekten heterogener, komplexer und hierarchischer Phasenanordnungen” (MI 666-4/1) and other projects are gratefully acknowledged.

Some materials from previous publications of the authors, and other publications are reproduced here with kind permissions from Elsevier, Institute of Physics (IOP), Annual Reviews, EDP Sciences, Kluwer/Springer, Hanser and Sage publishers.

The authors want to express their gratitude to Dr. R. Balokhonov (Tomsk, ISPMS), Dr. P. Binkele (IMWF), Dr. M. Dong (Eberspächer), Dr. S. Hönle (Bosch), Dr. P. Kizler (MPA), Dr. C. Kohnle, Dr. C. Kohler (IMWF), Dr. N. Lippmann (Bosch), Dr. W. Lutz (Bosch), Dr. O. Minchev, Dr. J. Rohde, Dr. V. Romanova (Tomsk, ISPMS), Dr. E. Soppa (MPA), and Dr. U. Weber (MPA/IMWF), as well as all their colleagues and former colleagues who contributed to our works.

The author L.M. gratefully acknowledges the valuable comments and suggestions by Lennart Mischnaewski.

The authors are grateful to Mrs. G. Amberg for her help during the preparation of the manuscript.

Siegfried Schmauder — Leon Mishnaevsky Jr.

Stuttgart, 13 August 2008 — Roskilde, 13 August 2008

References

This book includes (fully or partially) the following publications of authors and their colleagues:

Chapter 1.

X. Ge, S. Schmauder, "Micromechanism of Fracture in Al/SiC Composites", J. Mat. Sci. 30, pp. 173-178 (1995).

L.L. Mishnaevsky Jr., N. Lippmann, S. Schmauder, P. Gumbsch, "In-situ Observation of Damage Evolution and Fracture in AlSi7Mg0.3 Cast Alloys", Eng. Fract. Mech. 63, pp. 395-411 (1999).

L. Mishnaevsky Jr., N. Lippmann, S. Schmauder, "Micromechanisms and Modelling of Crack Initiation and Growth in Tool Steels: Role of Primary Carbides", Zeitschrift f. Metallkunde 94, pp. 676-681 (2003).

Chapter 2.

S. Schmauder, "Computational Mechanics", Annual Rev. Mater. Res. 2002.32, pp. 437-465 (2002).

M. Dong, S. Schmauder, "Modeling of Metal Matrix Composites by a Self-Consistent Embedded Cell Model", Acta metall. mater. 44, pp. 2465-2478 (1996).

N. Lippmann, Th. Steinkopff, S. Schmauder, P. Gumbsch, "3D-Finite-Element-Modelling of Microstructures with the Method of Multiphase Elements", Computational Materials Science 9, pp. 28-35 (1997).

L. Mishnaevsky Jr., M. Dong, S. Hönle, S. Schmauder, "Computational Mesomechanics of Particle-Reinforced Composites", Computational Materials Science 16, pp. 133-143 (1999).

L. Mishnaevsky Jr., "Three-dimensional Numerical Testing of Microstructures of Particle Reinforced Composites", Acta Materialia 52/14, pp. 4177-4188 (2004).

V.A. Romanova, E. Soppa, S. Schmauder, R.R. Balokhonov, "Mesomechanical analysis of the elasto-plastic behavior of a 3D composite-structure under tension", Computational Mechanics 36, pp. 475-483 (2005).

Chapter 3.

S. Schmauder, "Crack Growth in Multiphase Materials", Encyclopedia of Materials: Science and Technology, Elsevier Science Ltd., pp. 1735-1741 (2001).

J. Wulf, S. Schmauder, H. Fischmeister, "Finite Element Modelling of Crack Propagation in Ductile Fracture", Computational Materials Science 1, pp. 297-301 (1993).

S. Aoki, Y. Moriya, K. Kishimoto, S. Schmauder, "Finite Element Fracture Analysis of WC-Co Alloys", Engineering Fracture Mechanics 55, pp. 275-287 (1996).

S. Hönle, S. Schmauder, “Micromechanical Simulation of Crack Growth in WC/Co Using Embedded Unit Cells”, Computational Materials Science 13, pp. 56-60 (1998).

L. Mishnaevsky Jr., N. Lippmann, S. Schmauder, “Computational modeling of crack propagation in real microstructures of steels and virtual testing of artificially designed materials”, International Journal of Fracture 120, pp. 581-600 (2003).

L. Mishnaevsky Jr., U. Weber, S. Schmauder, “Numerical analysis of the effect of microstructures of particle-reinforced metallic materials on the crack growth and fracture resistance”, International Journal of Fracture 125, pp. 33-50 (2004).

C. Kohnle, O. Mintchev, S. Schmauder, “Elastic and Plastic Fracture Energies of Metal/Ceramic Joints”, Computational Materials Science 25, pp. 272-277 (2002).

Chapter 4.

P. Leßle, M. Dong, S. Schmauder, “Self-Consistent Matricity Model to Simulate the Mechanical Behaviour of Interpenetrating Microstructures”, Computational Materials Science 15, pp. 455-465 (1999).

S. Schmauder, U. Weber, “Modelling of Functionally Graded Materials by Numerical Homogenization”, Arch. Appl. Mech. 71, pp. 182-192 (2001).

J. Rohde, S. Schmauder, G. Bao, “Mesoscopic Modelling of Gradient Zones in Hardmetals”, Computational Materials Science 7, pp. 63-67 (1996).

L. Mishnaevsky Jr., “Functionally gradient metal matrix composites: numerical analysis of the microstructure-strength relationships”, Composites Sci. & Technology 66/11-12, pp. 1873-1887 (2006).

L. Mishnaevsky Jr., “Automatic voxel based generation of 3D microstructural FE models and its application to the damage analysis of composites”, Materials Science & Engineering A407/1-2, pp. 11-23 (2005).

S. Schmauder, A. Melander, P.E. McHugh, J. Rohde, S. Hönle, Or. Mintchev, A. Thuvander, H. Thoors, D. Quinn, P. Connolly, “New Tool Materials with a Structural Gradient for Milling Applications”, J. Phys. IV France 9, pp. Pr9-147 - Pr9-156 (1999).

Chapter 5.

M. Ludwig, D. Farkas, D. Pedraza, S. Schmauder, “Embedded Atom Potential for Fe-Cu Interactions and Simulations of Precipitate-Matrix Interfaces”, Modelling and Simulation in Materials Science and Engineering 6, pp. 19-28 (1998).

S.Y. Hu, M. Ludwig, P. Kizler, S. Schmauder “Atomistic Simulations of Deformation and Fracture of α-Fe”, Modelling and Simulation in Materials Science and Engineering 6, pp. 567-586 (1998).

L. Farrissey, M. Ludwig, P.E. McHugh, S. Schmauder, “An Atomistic Study of Void Growth in Single Crystalline Copper”, Computational Materials Science 18, pp. 102-117 (2000).

S. Nedelecu, P. Kizler, S. Schmauder, N. Moldovan, “Atomic Scale Modelling of Edge Dislocation Movement in the α-Fe-Cu System”, Modelling and Simulation in Materials Science and Engineering 8, pp. 181-191 (2000).

Y. Furuya, H. Noguchi and S. Schmauder, “Molecular Dynamics Study on Low Temperature Brittleness in Tungsten Single Crystals”, International Journal of Fracture 107, pp. 139-158 (2001).

S. Schmauder, P. Binkele, “Atomistic Computer Simulation of the Formation of Cu-Precipitates in Steels”, Computational Materials Science 24, pp. 42-53 (2002).

C. Kohler, P. Kizler, S. Schmauder, “Atomistic simulation of the pinning of edge dislocations in Ni by Ni_3Al precipitates”, Mat. Sci. and Engng. A400-401, pp. 481-484 (2005).

Chapter 1: Micromechanical Experiments

The purpose of this chapter is to analyse the micromechanisms of damage and fracture in heterogeneous materials, metals and composites, using direct observations of the damage evolution at the microlevel, combined with the macroscopic and/or computational analysis of the damage evolution.

In section 1.1, a SEM study of the micromechanism of fracture in SiC particle-reinforced 6061 aluminium composites is presented. The results lead to a better understanding of the micromechanism of particle breakage and interface debonding, and the special role of the particle effects in these composites.

In section 1.2, the mechanisms of damage initiation, evolution and crack growth in AlSi cast alloys are studied by in-situ tensile testing in a scanning electron microscope. It is shown that microcracks in these alloys are predominantly formed in the Si particles. Shear bands are seen to precede the breaking of the Si particles and the dislocation pile-up mechanism can thus be confirmed as the dominant damage initiating process in the matrix. Both micro- and macrocrack coalescence have been observed in the course of the experiments. The effect of the microstructure of the AlSi7Mg cast alloys on damage nucleation, crack formation and compliance reduction is analysed.

In section 1.3, micromechanisms of damage initiation and crack growth in high speed and cold work steels are investigated using scanning electron microscopy *in situ* experiments. The role of primary carbides in initiation and growth of cracks in tool steels is clarified. It is shown that initial microcracks in the steels are formed in primary carbides and then join together. A hierarchical finite element model of damage initiation, which included a macroscopic model of the deformation of the specimen under real experimental conditions and a mesomechanical model of damage in real microstructures of steels, was developed. Using the hierarchical model, the conditions of local failure in the steels have been obtained.

1.1 Micromechanisms of fracture in Al/SiC composites[1]

Engineering materials with a discontinuous second phase as a toughener [1] or reinforcement [2] have been widely studied in materials science and engineering. Investigations of the fracture characteristics of SiC particle-reinforced aluminium have shown that particle addition usually lowers the fracture toughness [3-5]. Reported fracture toughness' values for unreinforced aluminium alloys are in the range of 25-75 MPa $m^{1/2}$, while the composites have plane strain toughness values of 7-25 MPa $m^{1/2}$ [6, 7]. Many researchers have shown that the effect of microstructure on the fracture toughness is significantly affected by the details of the matrix microstructure, interface characteristics, and degree of clustering in the materials [8-9]. However, SEM fractography has revealed that the fracture surface consists of microvoids, corresponding to ductile fracture with dimples [10]. The sources of these dimples have been attributed to fracture of SiC particles [11], inclusions and precipitates or decohesion from the matrix as well as matrix failure [12, 13]. An attempt to explain these special failure characteristics of Al/SiC composite materials, which behave macroscopically brittle, but microscopically ductile, were the main purpose of this work. The fracture toughness tests on the composites were carefully designed with single-edge notched sheet (SENS) [14] specimens in the SEM. Both qualitative observations of void nucleation and quantitative measurements of crack profiles were made to assess the specific role of the particle-reinforcement mechanism in the composites. The microstructure analysis is proposed to understand and explain the particle effects during the crack initiation and propagation in these composites.

1.1.1 Experimental procedure

The composites used consisted of particle-reinforced aluminium alloy 6061 manufactured by extruding mixtures of aluminium powder and SiC particles. The volume fractions of particles in the composites were 0%, 10% and 20%. The mechanical properties of these composites are shown in Table 1.1. Distributions of measured SiC particle diameters are shown in Fig. 1.1a and b.

The SENS sample was designed according to the requirements of the SEM machine. The dimensions of the sample are shown in Fig. 1.2. The test was carried out in a Jeol JSM-35 scanning microscope. The machine automatically records the applied load versus displacement curves, and the monitor is used to examine the tip of the notch to understand the notch deformation, as well as nucleation, growth and coalescence of voids during loading. A record of the process is made by a video recorder.

---

[1] Reprinted from X. Ge, S. Schmauder, "Micromechanism of Fracture in Al/SiC Composites", J. Mat. Sci. 30, pp. 173-178 (1995) with kind permission from Springer

1.1.2 Results of Experiments and Analysis

Qualitative observations of void nucleation

General observations were made on the tip and root of the notch during the loading process. Voids nucleated in the middle of the notch root, as observed in the SEM, at K_0 / K_1 equal to 0.68, 0.784, and 0.85 for 0%, 10% and 20% SiC volume fraction composites, respectively, where K_1, is the stress intensity factor of the sample calculated according to Brown and Srawley [15] and K_0 is the fracture toughness. Measured data of K_0 and K_1 are shown in Table 1.2.

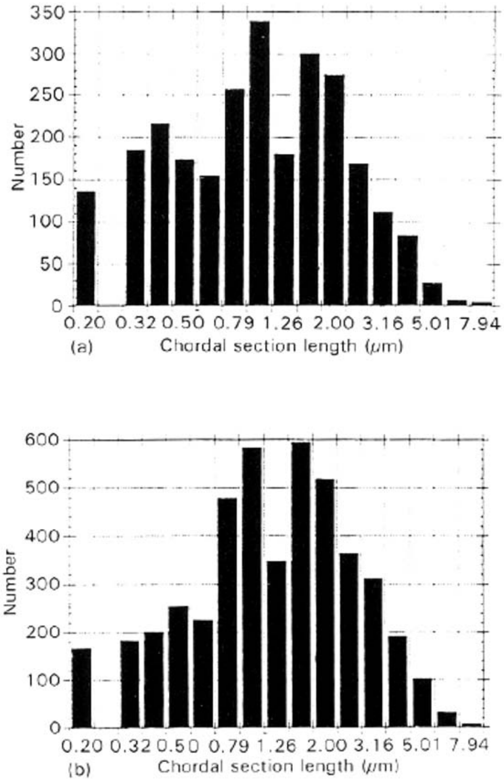

Fig. 1.1 Distributions of particle diameters. (a) 10% Al/SiC, (b) 20% Al/SiC (courtesy J. Wulf).