

Strength Prediction of Particulate Reinforced Metal Matrix Composites

Von der Fakultät für Maschinenwesen der Rheinisch-Westfälischen Technischen
Hochschule Aachen zur Erlangung des akademischen Grades eines Doktors der
Ingenieurwissenschaften genehmigte Dissertation

vorgelegt von

Geng Chen

Berichter: Univ.-Prof. Dr.-Ing. C. Broeckmann

Berichter: Univ.-Prof. Dr.-Ing. Dr. h. c. (UA) D. Weichert

Tag der mündlichen Prüfung: 15. Juli 2016

Diese Dissertation ist auf den Internetseiten der Universitätsbibliothek online verfügbar

Werkstoffanwendungen im Maschinenbau
hrsg. von Prof. Dr.-Ing. Christoph Broeckmann

Band 12

Geng Chen

**Strength Prediction of Particulate Reinforced
Metal Matrix Composites**

Shaker Verlag
Aachen 2016

Bibliographic information published by the Deutsche Nationalbibliothek

The Deutsche Nationalbibliothek lists this publication in the Deutsche Nationalbibliografie; detailed bibliographic data are available in the Internet at <http://dnb.d-nb.de>.

Zugl.: D 82 (Diss. RWTH Aachen University, 2016)

Copyright Shaker Verlag 2016

All rights reserved. No part of this publication may be reproduced, stored in a retrieval system, or transmitted, in any form or by any means, electronic, mechanical, photocopying, recording or otherwise, without the prior permission of the publishers.

Printed in Germany.

ISBN 978-3-8440-4725-7

ISSN 2195-2981

Shaker Verlag GmbH • P.O. BOX 101818 • D-52018 Aachen

Phone: 0049/2407/9596-0 • Telefax: 0049/2407/9596-9

Internet: www.shaker.de • e-mail: info@shaker.de

Abstract

Particulate reinforced metal matrix composite (PRMMC) are made by dispersing reinforcement particles into a metal matrix and sintering. By optimizing the process parameters and the composition of the material, the major advantages of ceramics and metals can be combined and resulting in a material with high hardness, high wear resistance and sufficient toughness. When used as a structural material, failure of the PRMMCs are often caused by material deterioration accumulated over a large number of load cycles. As composed of two phases, PRMMCs can be regarded as mechanical systems on the mesoscale, therefore their overall responses are greatly influenced by the alignment of the reinforcement phase and the underlying material morphology. Understanding how the microstructure contributes to the global material behavior, above all the macroscopic strengths, is one of the central tasks of the thesis.

In the present study, a numerically based methodology for determining the load bearing capacity of PRMMCs under both monotonic and cyclic loadings is presented. To evaluate the influence of the composite structure on the global behavior of PRMMCs, a multi scale approach which combines the shakedown analysis with homogenization was used. To take into account the randomness associated with the composite structure of the material, statistical methods have been applied to interpret the results. To prepare a sufficient number of representative volume element (RVE) models for the statistical study, a computational tool was developed to automate the generation of RVE samples.

The general work flow of the established numerical approach can be summarized as follows: first, a large number of RVE was constructed as finite element models from either real or artificial material microstructures using the aforementioned in-house code. Next, lower and upper bound limit and shakedown problems were carried out by means of the interior-point method. Finally, results were converted to their corresponding macro quantities and evaluated statistically. With this approach a representative PRMMC material, WC/Co, was studied.

Based on the established numerical work flow, ultimate strength and endurance limit of the material were predicted. The relationship between them and other material parameters, such as the effective Young's modulus and the binder content was examined. The study investigated how the predicted strength is influenced by the RVE size and the size of reinforcement particles. The study also exposed the change of the feasible load domain, when the kinematic hardening of the binder phase is considered or when

multiple independently varied loads are applied simultaneously. In addition to that, the study built predictive models and used them to explain, what are the decisive factors that determine the endurance limit of the overall composite material.

Zusammenfassung

Partikelverstärkten Metall-Matrix Verbundwerkstoffen (PRMMC's) werden durch Dispergieren von Verstärkungspartikeln in einer Metallmatrix und anschließendes Sintern hergestellt. Durch Optimierung der Verfahrensparameter und Zusammensetzung der beiden Phasen können die Vorteile von Keramik und Metallen kombiniert werden und Dies führt zu einem Material mit hervorragenden Härte, Verschleißfestigkeit und ausreichender Zähigkeit. Bei Einsatz PRMMC als Strukturmaterial, wird dessen Versagen oft durch allmähliche Degradation infolge zyklischer Belastung verursacht. Da PRMMC's aus mindestens zwei Phasen bestehen, können diese als mesoskopische mechanische Systeme angesehen werden. Daher ist ihr gesamtes mechanisches Verhalten stark von der Ausrichtung der Verstärkungsphase und der vorliegenden Gefügemorphologie abhängig. Deshalb besteht die zentrale Aufgabe innerhalb dieser Arbeit darin, zu verstehen, wie die Ausprägung der Mikrostruktur zum globalen Materialverhalten beiträgt. Der Fokus wird dabei auf die Beeinflussung der makroskopischen Festigkeit gelegt.

In der vorliegenden Studie wird eine numerische Methodik zur Festigkeitsvorhersage von PRMMC's unter monotoner und zyklischer Belastung vorgestellt. Um den Einfluss des Mikrogefüges auf das globale Verhalten von PRMMCs zu bewerten, wurde ein Multiskalenansatz präsentiert, der die Homogenisierung mit der Einspielanalyse kombiniert. Zur Berücksichtigung der Zufälligkeit in der Werkstoffmikrostruktur, wurden statistische Methoden angewendet, um die numerischen Ergebnisse zu interpretieren. Ein Rechenwerkzeug zur automatischen Erzeugung von repräsentativen Volumenelement (RVE) Modelle wurde entwickelt, um eine ausreichende Anzahl von Gefügemodellen für die statistische Untersuchung bereitzustellen.

Der allgemeine Arbeitsablauf des o. g. etablierten numerischen Ansatzes lässt sich wie folgt zusammenfassen: Zuerst wurden durch das o. g. eigene Programm eine große Anzahl von RVE's als Finite-Elemente-Modelle, auf Basis von künstlichen oder realen Materialgefügen, konstruiert. Als nächstes wurden die von Traglast- und Einspielanalyse generalisierten Optimierungsprobleme mit der Innenpunktmethod gelöst. Schließlich wurden die Ergebnisse zu ihrer entsprechenden makrogröße umgerechnet und statistisch ausgewertet. Mit diesem etablierten numerischen Verfahren wurde ein repräsentatives PRMMC Material, WC/Co, untersucht.

Basierend auf dem o. g. numerischen Verfahren wurden die Endfestigkeit und Dauerfestigkeit des Materials vorhergesagt. Die Beziehung zwischen diesen Größen und

anderen Materialparametern, wie beispielsweise dem effektiven Elastizitätsmodul und dem Bindemittelgehalt, wurde untersucht. Die Studie zeigte, wie die vorhergesagten Festigkeiten von der Größe des RVEs und der Größe der Verstärkungspartikel beeinflusst werden. Weiterhin wurde dargestellt, welche Veränderungen der zulässige Lastraum erfährt, wenn die kinematische Verfestigung der Binderphase betrachtet oder mehrere variierende und unabhängige Lasten gleichzeitig angelegt werden. Darüber hinaus wurde in der Studie durch die statistischen Vorhersagemodelle hergeleitet, welche entscheidenden Einflussfaktoren die Dauerfestigkeit von PRMMC bestimmen.

Acknowledgements

This thesis was created during my work as research assistant at two institutes of RWTH Aachen University: many ideas in the work are formed during my stay at the Institute of General Mechanics (IAM) and they continue to develop and finally become established during my stay at the Institute for Materials Applications in Mechanical Engineering (IWM). This work will never be accomplished without the help and support of many people, to whom I am indebted and would like to express my deepest gratitude.

First I am grateful to Prof. Dr.-Ing. Dr. h. c. Dieter Weichert for giving me the opportunity to start the work at his institute; for introducing me to the fascinating field of the direct method; and for his consistent encouragement, patient guidance, and inspirational scholarly inputs which accompanied me throughout the entire research work. Next I would like to greatly acknowledge and thank Prof. Dr.-Ing. Christoph Broeckmann for designing the research plan which allows me to work on this multidisciplinary field and receive supervision from both institutes; for supporting me in realizing the ideas in this work; and for many insightful comments and invaluable discussions which significantly improve both quality and depth of this thesis. Besides my advisors, I would like to appreciate Prof. Dr.-Ing. Dr.-Ing. E. h. Dr. h. c. Dr. h. c. Fritz Klocke for chairing my examination board.

I am grateful to my friend, former supervisor, and colleague Dipl.-Ing. Alexander Bezdol for providing me with the opportunity to work as his student assistant and for supporting me to overcome whatever challenges that I have ever faced. Without his help which spans over the entire duration of my master and Ph.D. phase, I couldn't have imagined that I could complete this task.

I would like to thank all colleagues from both institutes with whom I have been worked with. I would like to thank Dr. Bengt Hallstedt for reviewing some chapters of this thesis, and Dipl.-Ing. Wolfgang Kayser for correcting the German translation. My special thanks go to members of the shakedown group at IAM and micromechanics group at IWM which include, but are not limited to, following individuals: Dr.-Ing. Abdelkader Hachemi, Dr.-Ing. Jaan Simon, Dr.-Ing. Min Chen, Ph.D. Konstantinos Nikolaou, Dr.-Ing. Utku Ahmet Özden, Dr.-Ing. Atilim Eser, M.Sc. Stanley van Kempen, and M.Sc. Keng Jiang. I would like to thank for their assistance and the pleasant working environment that they created.

Last but not least, I would like to take this opportunity to express my gratitude to my

parents for their selfless love and unconditioned support. Also, I would like to thank my fiancée, Nan Ma, for her understanding of my decision to study abroad and to pursue a doctoral degree. I feel very blessed to have her in my life.

Table of Contents

List of Figures	xii
List of Tables	xiii
Nomenclature	xv
1 Introduction	1
1.1 Overview	1
1.2 Motivations and objectives of the thesis	10
1.3 Organization of the thesis	11
2 Static and Kinematic Direct Methods	13
2.1 Fundamentals of theory of plasticity	13
2.1.1 Compatibility and equilibrium	13
2.1.2 Definition of the yield surface	14
2.1.3 Normality hypothesis and consistency condition	16
2.1.4 Tresca and von Mises yield conditions	17
2.1.5 Perfectly plastic material models	19
2.1.6 Hardening and subsequent yield surface	20
2.1.7 Drucker's postulate	22
2.2 Shakedown of elastic-perfect plastic materials	24
2.2.1 Cyclic inelastic material behavior	24
2.2.2 Static theorem for elastic-perfectly plastic materials	26
2.2.3 Kinematic theorem for elastic-perfectly plastic materials	32
2.3 Shakedown of hardening materials	35
2.3.1 Two-surface model and dissipation function	35
2.3.2 Static theorem for bounded linearly kinematic hardening materials	39
2.3.3 Kinematic theorem for bounded linearly kinematic hardening materials	39
3 Micromechanics of Random Composites	41
3.1 Analytical and numerical homogenization methods	41
3.2 Elasto-plastic homogenization	43
3.3 Random composite and statistical RVE	46
3.4 Shakedown of composite materials	49

4	Numerical Formulation and Solution	51
4.1	Finite element discretization	51
4.2	Numerical static problem	54
4.2.1	Finite element formulation of the static problem	54
4.2.2	Reformulation of the lower bound problem	55
4.2.3	Considering kinematic hardening	56
4.3	Numerical kinematic problem	57
4.3.1	Finite element formulation of the kinematic problem	57
4.3.2	Reformulation of the upper bound problem	60
4.4	Duality theorem	62
4.5	Algorithms for nonlinear programming	63
4.5.1	Interior point method implementation in IPOPT	64
4.5.2	Generating linearized KKT system	70
4.5.3	Linear algebra packages for solving the reduced KKT system	73
4.5.4	Second order cone programming	74
4.6	High dimensional load space	74
5	Models for Results Interpretation	79
5.1	Fundamentals of probability	79
5.2	Descriptive statistical measures	83
5.3	Statistical inference	85
5.4	Conditional probability and Bayes' theorem	88
5.5	Regression models	91
5.5.1	Linear regression	93
5.5.2	Classification and logistic regression	95
6	Numerical Results and Discussion	99
6.1	Workflow of the numerical study	99
6.2	Details of RVE models	103
6.2.1	Automatic modeling of 2D RVE samples	103
6.2.2	2.5D RVE models	105
6.2.3	Influence of the boundary condition	109
6.2.4	Influence of the yield limit of the reinforcement phase	112
6.2.5	Description of RVE sample groups	114
6.2.6	Description of statistical indicators	115
6.3	Validation of the numerical work flow	116
6.4	Influence of the RVE size	123
6.5	Influence of the binder content	129
6.6	Influence of the particle size	134
6.7	Influence of the binder hardening	140
6.8	Strength under combined stresses	148
6.9	Statistical learning and predictive models	152
6.9.1	Selecting features for the predictive models	152
6.9.2	Predictive models on endurance limit	154

7	Conclusions and Outlook	163
	References	165
A	Reformulation of the static problem	191
A.1	Perfect plastic materials	191
A.2	Materials with kinematic hardening	197
B	Proof of the duality theorem	199
C	Filter method in IPOPT	205