

Micromechanical modeling of γ -TiAl based alloys

Von der Fakultät für Georessourcen und Materialtechnik
der Rheinisch-Westfälischen Technischen Hochschule Aachen

zur Erlangung des akademischen Grades eines
Doktors der Ingenieurwissenschaften genehmigte

Dissertation

vorgelegt von Dipl.-Ing.

Claudio Renato Zambaldi

aus München

Berichter: Professor Dr.-Ing. Dierk Raabe
Univ.-Prof. Dr. rer. nat. Dr. h. c. Günter Gottstein

Tag der mündlichen Prüfung: 14. Juni 2010

Diese Dissertation ist auf den Internetseiten der Hochschulbibliothek online verfügbar.

Berichte aus der Materialwissenschaft

Claudio Zambaldi

Micromechanical modeling of γ -TiAl based alloys

Shaker Verlag
Aachen 2010

Bibliografische Information der Deutschen Nationalbibliothek

Die Deutsche Nationalbibliothek verzeichnet diese Publikation in der Deutschen Nationalbibliografie; detaillierte bibliografische Daten sind im Internet über <http://dnb.d-nb.de> abrufbar.

Zugl.: D 82 (Diss. RWTH Aachen University, 2010)

Copyright Shaker Verlag 2010

Alle Rechte, auch das des auszugsweisen Nachdruckes, der auszugsweisen oder vollständigen Wiedergabe, der Speicherung in Datenverarbeitungsanlagen und der Übersetzung, vorbehalten.

Printed in Germany.

ISBN 978-3-8322-9717-6

ISSN 1618-5722

Shaker Verlag GmbH • Postfach 101818 • 52018 Aachen

Telefon: 02407 / 95 96 - 0 • Telefax: 02407 / 95 96 - 9

Internet: www.shaker.de • E-Mail: info@shaker.de

Meinen Eltern

Mira, esto de las cosas elásticas es muy raro, yo lo siento en todas partes. Todo es elástico, chico. Las cosas que parecen duras tienen una elasticidad . . . Piensa, concentrándose.

— . . . una elasticidad retardada— agrega sorprendentemente.

“Sieh mal, das mit den elastischen Dingen ist sehr seltsam, ich spüre das überall. Alles ist elastisch, Junge. Selbst die Dinge die hart zu sein scheinen, besitzen Elastizität . . .”

Er denkt angestrengt nach.

“ . . . eine verlangsamte Elastizität”, fügt er überraschend hinzu.

Julio Cortázar
El perseguidor (Der Verfolger), 1958

Acknowledgment

This work was carried out in the department of Microstructure Physics and Metal Forming at the Max-Planck-Institut für Eisenforschung in Düsseldorf. Prof. Dr.-Ing. D. Raabe, head of the department and director of the institute, is thanked for his continuous support during the preparation of this thesis. Valuable and inspiring discussions together with a high amount of scientific freedom have made possible the present results.

Prof. Dr. rer. nat. G. Gottstein is acknowledged for acting as the co-advisor for my examination and for providing valuable comments on a draft of this thesis.

Dr. rer. nat. F. Roters is thanked for decisive discussions about the intricacies of crystal plasticity modeling and simulation. His comments have often set me on the right track towards the solution.

Dr. habil. S. Zaefferer is gratefully acknowledged for his original idea of the fit-rank indexing and the fruitful collaboration that followed from it. Without his support on the arising issues, the microstructural characterization efforts would have hardly worked out in the way they did. Also, Dr. S. Wright (EDAX-TSL) is thanked for the excellent collaboration and discussions on the EBSD optimization and the incorporation of the improved indexing algorithm as part of the EDAX-TSL OIM software package.

I am indebted to Prof. K. Maruyama for hosting me at his laboratory at Tohoku University (Sendai) during a JSPS fellowship from October to December 2007. Further, I would like to thank Prof. K. Yoshimi, Dr. M. Tsunekane, and Dr. H. Ghassemi-Arkmaki for their assistance during that time and for making the visit successful and an enjoyable experience. Prof. K. Kishida is thanked for discussion time and for showing me the laboratories at Kyoto University during the Ti-2007 conference.

Many thanks to my present and former colleagues at the Institute, Prof. S. Nikolov, Prof. C.-S. Han, Dr. D. Ponge, Dr. M. Palm, Dr. F. Stein, Dr. N. Zaafarani, Dr. A. Ma, Dr. P. Romano, Dr. A. Bastos da Silva Fanta, Dr. H. Sato, Dr. H. Fabritius, Dr. P. Eisenlohr, Dr. D. Tjahjanto, S. Voss, D. Steinmetz, H. Knoll, D. Ma, B. Liu, L. Hantcherli, and Dr. K. Balasundaram for valuable discussions and their manifold support. Prof. S. Hild and C. Senöz are thanked for their help with the AFM measurements. Prof. S. Kobayashi deserves special mentioning because of his help and advice during the beginning of the work. Furthermore, I would like to thank Prof. T. R. Bieler for many helpful discussions during his sabbatical year at the institute. All colleagues in the department are thanked for creating a friendly and stimulating atmosphere.

The experimental work was supported by G. Bialkowski, H. Bögershausen, K. Angenendt, M. Nellesen, E. Bartsch, M. Adamek, and H. Faul and I would like

to thank all of them for their assistance. C. Regner and P. Siegmund are acknowledged for the fast and reliable service when it came to ordering books and scientific articles. A. Kuhl and B. Beckschäfer are thanked for their valuable support regarding the used computer infrastructure.

The largest part of the present work was performed within the European Union FP6 IMPRESS integrated project. The financial support and the excellent project management is acknowledged. It was fun to be part of such a successful international project. From the project members I would like to thank U. Hecht, Dr. G. Behr and Dr. W. Löser, C. Gugushev, Dr. D. Hu, Prof. I. Egry, and Prof. J. Lapin for valuable discussions as well as for providing sample material. Prof. H. Fecht and Dr. N. Deyneka are thanked for providing the initial nanoindentation data.

Prof. F. Appel is thanked for a very helpful discussion during a visit at GKSS at the beginning of the project. Dr. V. Kouznetsova and Dr. L. Delannay are acknowledged for valuable hints on the implementation of periodic boundary conditions.

Without free software such as JabRef, Gwyddion, the mtex toolbox and others, generously made accessible by its creators, many tasks that were accomplished during the course of work, would have taken significantly more effort.

Contents

Acknowledgment	9
I Introduction, literature review, and state of the art	17
1 General introduction and research objectives	19
1.1 Introduction	19
1.1.1 Present and future applications of titanium aluminides	19
1.1.2 Related literature	20
1.1.3 Timeline of titanium aluminide alloy development	20
1.2 Motivation	20
1.3 Research objectives	21
1.4 Outline of this thesis	22
2 Microstructures of γ-TiAl based alloys	23
2.1 Introduction	23
2.2 The Ti-Al phase diagram	23
2.3 Crystallographic phases in γ -TiAl based alloys	24
2.4 Metallurgy of titanium aluminides	26
2.5 Phase transformation in titanium aluminides	27
2.6 Blackburn orientation relationship between γ - and α_2 -phase	28
2.7 The domain structure of γ -TiAl	28
2.8 Formation of lamellar microstructures during slow cooling	30
2.8.1 Polycrystalline fully lamellar (FL) microstructures	33
2.8.2 Polysynthetically-twinned (PST) crystals	34
2.9 Massive transformation during rapid cooling	34

3	Micromechanics of titanium aluminides	37
3.1	Introduction	37
3.2	Linear elasticity	37
3.2.1	Elastic behavior of γ -TiAl	38
3.2.2	Elastic behavior of α_2 -Ti ₃ Al	40
3.3	Inelastic deformation of γ -TiAl	40
3.3.1	Deformation of γ -TiAl by dislocation glide	40
3.3.2	Deformation of γ -TiAl by twinning	43
3.4	Deformation systems of hexagonal ordered α_2 -Ti ₃ Al	44
3.5	Non-Schmid effect on dislocation glide	47
3.6	Kinematic constraints and Hall-Petch effect	47
3.6.1	Anisotropic yield strength of PST material	47
3.6.2	Hall-Petch effect in γ -TiAl based alloys	49
3.6.3	Pre-yielding and pre-yield cracking	52
4	Review of crystal plasticity models of γ-TiAl based alloys	53
4.1	Introduction	53
4.2	The 2D-CPFEM model of Lee, Ahzi, Kad, Dao, Asaro	53
4.3	The CPFEM model of Parteder, Schlögl, Marketz, Fischer, Clemens	53
4.4	The self-consistent crystal plasticity model of Lebensohn et al.	55
4.5	The CPFEM model of Werwer, Cornec and others	55
4.6	The CPFEM model of Grujicic, Zhang, Cao and Batchu	55
4.7	The CPFEM model of Brockman et al.	56
4.8	The CPFEM model of Heripré, Roos et al.	56
4.9	The CPFEM model of Bieler et al.	56
4.10	Conclusion	56
5	Instrumented Indentation	59
5.1	Basics of Indentation	59
5.1.1	Hardness testing and intermetallics	59
5.1.2	Instrumented indentation and nanoindentation	60
5.1.3	Identification of constitutive parameters by instrumented indentation	62
5.2	Indenter geometries	63
5.2.1	Berkovich geometry	63
5.2.2	Spherical and sphero-conical indenters	64
5.2.3	Tip geometry imperfections	65
5.3	Indentation response of single crystals	65
5.3.1	Studies on ionic crystals, and metals with different crystal structures	65
5.3.2	Indentation pile-up as the finger print of single crystal plasticity	66
5.3.3	Incipient plasticity during single crystal indentation	68
5.4	Continuum simulation of indentation	69
5.5	Nanoindentation studies on Ti-Al	70

II Microstructural and mechanical characterization, and crystal plasticity modeling of γ-TiAl and γ-TiAl based alloys	73
Introduction to the results of this thesis	75
6 EBSD characterization of γ-TiAl order domains	77
6.1 Introduction and motivation	77
6.2 Discrimination of γ -TiAl order variants by superlattice reflections . .	77
6.3 Limitations of conventional EBSD analysis of γ -TiAl	79
6.4 Enhanced accuracy EBSD pattern analysis	82
6.4.1 Pattern center calibration	82
6.4.2 Accurate Kikuchi band detection	83
6.4.3 Accurate and robust indexing and the fit-rank indexing method	86
6.5 Experimental details	86
6.6 Results and discussion	87
6.6.1 Validation of the proposed fit-rank method	87
6.6.2 Orientation mapping of the order domain structure	91
6.6.3 Further improvement of the algorithm	93
6.7 Conclusions	95
7 Crystal plasticity modeling of γ-TiAl	97
7.1 Motivation	97
7.2 The finite strain elasto-viscoplastic crystal plasticity formulation . . .	97
7.2.1 Continuum mechanics	98
7.2.2 The constitutive model	99
7.2.3 Time-integration of the phenomenological crystal plasticity law	101
7.2.4 Numerical approximation of the material point tangent stiffness	103
7.3 Implementation of ordinary and super dislocation glide systems of γ -TiAl	103
7.4 Implementation of twinning on four true twinning systems of γ -TiAl .	104
7.5 Incorporation of the single crystal constitutive law into the finite element method	104
7.6 Validation of the CPFEM implementation of the deformation modes .	105
7.7 Discussion of appropriate hardening parameters of single phase γ -TiAl	111
7.8 Conclusion	112

8	Single crystal indentation of γ-TiAl – experiments and CPFEM modeling	113
8.1	Introduction	113
8.2	Indentation experiments	113
8.2.1	Experimental methods	113
8.2.2	Results of indentation experiments	114
8.2.3	Experimentally measured pile-up topographies of γ -TiAl . . .	117
8.2.4	Discussion of the nanoindentation results	123
8.3	CPFEM simulation of nanoindentation in γ -TiAl	123
8.3.1	A finite element model of single crystal indentation	123
8.3.2	Influence of friction on simulated pile-up profiles	124
8.3.3	Establishing the model and the constitutive parameters	125
8.3.4	Computational costs of three-dimensional indentation simulation	128
8.4	A method for a combined experimental and simulation study of single crystal indentation	128
8.4.1	An in-plane orientation convention for the unique representa- tion of pile-up profiles	129
8.4.2	Simulation results for 51 orientations in the unit triangle . . .	131
8.4.3	Detailed results for high symmetry orientations	132
8.4.4	Comparison of experimental and simulated pile-up topographies	133
8.5	Discussion of the developed nanoindentation method	134
8.5.1	Relation between surface deformation and plastic anisotropy .	134
8.5.2	Possible applications of the developed method	138
8.5.3	Discussion of the influence of indenter shape	138
8.5.4	Analysis of deformation mechanisms	139
8.5.5	The advantage of relying only on high precision measures . .	140
8.5.6	Other advantages of the presented method	140
8.5.7	Preliminary estimate on the anisotropic hardness of γ -TiAl . .	140
8.6	Conclusions	142
9	A homogenized constitutive law for two-phase γ/α_2 microstructures	143
9.1	Introduction	143
9.2	Rationalization of the selection of incorporated slip systems	143
9.3	Application of the homogenized material law to the anisotropic plas- ticity of PST-crystals	147
9.4	Application of the homogenized law to two different microstructures .	148
9.5	Discussion	153
9.6	Conclusions	155

III Summary, outlook, and backmatter	157
10 Summary and main conclusions	159
11 Outlook	161
A Literature on titanium aluminides	163
A.1 Proceedings	163
A.2 Journal issues	163
B Crystallographic orientations	165
B.1 Bunge Euler angles	165
B.2 Generation of near-equidistant orientations	165
B.3 Orientation representation of the hexagonal phase	167
C Periodic boundary conditions	169
Abstract	171
Zusammenfassung (German abstract)	173
Bibliography	177
Curriculum vitae	201

