
Grain boundary-dislocation interaction:
A local investigation via micron-sized
bicrystals

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Contents

Acknowledgments	iii
List of Tables	v
List of Figures	vii
Abstract	xi
Zusammenfassung	xiii
1. Introduction	1
2. Literature review	3
2.1. Grain boundary-dislocations interaction	3
2.2. Bicrystals in the literature	5
2.2.1. Macroscopic bicrystals	5
2.2.2. Microscopic bicrystals	9
2.3. Criteria on slip transmission	10
2.4. Mesoscopic bicrystals	12
3. Experimental procedure	15
3.1. Sample preparation	15
3.1.1. Macroscopic sample preparation	15
3.1.2. Microscopic sample preparation	19
3.2. Characterization of microscopic samples	28
3.2.1. FIB-Pillars	28
3.2.2. FIB-Litho-Pillars	28
3.3. Micromechanical examinations	31
3.3.1. Positioning of micropillars under the flat-ended tip	31
3.3.2. Loading procedure	32
3.4. Microstructural examinations	36
3.4.1. Micropillar microstructure	36
3.4.2. Micropillar free surface	39
4. Molecular Dynamics Simulation	41
5. Results and Discussion	43
5.1. Results of micromechanical tests	43

Contents

5.1.1.	Large pillars	45
5.1.2.	Medium pillars	48
5.1.3.	Small pillars	53
5.2.	Discussion of micromechanical test results	60
5.2.1.	FIB damage effect	60
5.2.2.	Stress-strain curve analysis	62
5.2.3.	Correlation between grain boundary effect and size	65
5.2.4.	Slip line analysis	68
5.2.5.	Slip Transmission	73
5.2.6.	Consideration of elastic anisotropy	78
5.2.7.	Consideration of source properties	79
5.2.8.	Consideration of size effect hypothesis	81
5.3.	Results of MD Simulation	86
5.4.	Discussion on MD simulation results	88
5.5.	Preliminary conclusion	90
5.6.	Results of microstructural tests	92
5.6.1.	Homogeneous medium with easy glide behavior	92
5.6.2.	Homogeneous medium with the presence of non-planar dislocations	92
5.6.3.	Inhomogeneous medium with the presence of a grain boundary	96
5.7.	Discussion on microstructural test results	102
5.7.1.	Homogeneous medium with easy glide behavior	102
5.7.2.	Homogeneous medium with the presence of non-planar dislocations	103
5.7.3.	Inhomogeneous medium with the presence of a grain boundary	103
6.	Conclusion and Outlook	107
6.1.	Conclusion	107
6.2.	Outlook	108
6.2.1.	Determination of the grain boundary strength	108
6.2.2.	In-situ compression tests	109
6.2.3.	Hydrogen embrittlement	109
A.	Compatibility conditions	111
B.	Prime criteria on slip transmission	113
C.	Orientation characterization in OIM software	115
D.	Investigation of FIB damage by nanoindentation	119
E.	Strain rate sensitivity of bicrystalline micropillars	123
F.	Finite Element Simulation	125

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List of Tables

3.1. Sample and surface preparation parameters	17
3.2. The considered grain boundary parameters	19
3.3. Lithography parameters in this study.	24
3.4. Electrochemical wet etching process parameters.	25
3.5. Two $5\mu\text{m}$ diameter micropillars, each fabricated with a different technique, are compared in terms of time and beam current intensity.	27
3.6. Crystallographic orientation, Schmidt factor and elastic modulus of the grains included the single and bicrystalline pillars.	30
5.1. Yield stresses of bicrystalline and single-crystalline micropillars of $5\mu\text{m}$ diameter.	45
5.2. Yield stresses of bicrystalline and single-crystalline micropillars with diameter 3 to $2\mu\text{m}$	49
5.3. Yield stresses of bicrystalline and single-crystalline micropillars of $1.4\mu\text{m}$ diameter	53
5.4. Yield stresses of bicrystalline and single-crystalline micropillars of $1\mu\text{m}$ diameter.	56
5.5. The thickness of damaged layer on the free surface of the micropillars with different damage levels.	62
5.6. Incoming slip system in grain A and potential outgoing slip systems in grain B, Schmid factor, angle α between the intersection lines of the slip planes and the grain boundary line on the bicrystal top surface as well as the angle θ between the incoming slip plane in grain A (slip system 1) and potential slip planes in the grain boundary plane (slip systems 2, 3 and 4).	72
5.7. Stress distribution of the component crystals.	78
5.8. Applied shear stresses on the primary slip systems in the component crystals of the bicrystal using Equations 5.9 and 5.10.	79
5.9. The bicrystal and single crystal diameters with the relationship $r = R/\sqrt{2}$	84
5.10. Four bicrystals analyzed for grain boundary-induced lattice rotation in details.	96
D.1. Parameters varied for the nanoindentation of FIB-damaged layers.	120

List of Tables

List of Figures

2.1.	Nanoindentation of polycrystalline nickel with variable grain sizes used as a grain boundary effect test method	4
2.2.	The lower bound estimate of the total GND density distribution around the indent [Wilkinson <i>et al.</i> , 2010].	5
2.3.	The misorientation angle θ affects the flow stress curves of the bicrystals.	6
2.4.	A photomicrograph showing double glide in the vicinity of the grain boundary in a specimen with the misorientation of 85°	7
2.5.	Stress-strain curves of (100) bicrystals having 4° , 14° and 37° misorientation boundaries compared with the component single crystals [Miura and Saeki, 1978].	7
2.6.	Orientation images showing the successive progression of lattice orientation after 30 % compression [Field and Alankar, 2011].	8
2.7.	Slip transmission observed by the ex-situ and the in-situ TEM experiments	9
2.8.	TEM observations showing the mechanisms of slip transmission across a grain boundary.	10
2.9.	Schematic diagram showing the geometrical relationship between the incoming and outgoing slip planes and θ [Clark <i>et al.</i> , 1992].	11
3.1.	The special procedure developed for production of two-dimensional, structured samples.	16
3.2.	Nickel samples and the sample holders designed and employed in this work.	18
3.3.	Grain boundary characterization according to grain boundary type definitions.	20
3.4.	EBSM map of the polycrystalline bulk sample surface used to produce micropillars.	21
3.5.	Different views from the electron and the ion beams directions of a typical micropillar cut in a DB-FIB.	21
3.6.	The SEM image of a typical bicrystalline micropillar.	22
3.7.	SEM image of a pillar produced by electrochemical etching before and after FIB milling.	23
3.8.	Standard lithography procedure.	24
3.9.	Light microscopy image made by normal contrast of lithographically produced, structured specimen.	24
3.10.	SEM image of a pillar produced by electrochemical etching.	25

List of Figures

3.11.	The curves compare the two mentioned fabrication techniques: FIB-Pillars and FIB-Litho-Pillars. The ion current intensity used and the time consumed in FIB are considered.	26
3.12.	Crystallographic orientation of all the grains used for fabrication of micropillars studied.	28
3.13.	A schematic of the TriboIndenter™ and the bulk sample installed on the stage.	31
3.14.	The topography images of the pillar surface before and after centering the position of the micropillar.	32
3.15.	Schematical view of the flat-ended tip and the micropillar during the imaging process.	34
3.16.	Cyclic load function applied to the pillars at the beginning of the compression test.	34
3.17.	Stress-strain curves obtained from the open-loop/load-controlled and the displacement-controlled compression test. SEM image of a shape memory alloy micropillar and its hysteresis stress-strain curve.	35
3.18.	The film preparation out of a deformed bicrystalline micropillar.	37
3.19.	SEM images and corresponding OIM maps of the two sides of a thick film cut out of a deformed bicrystal.	38
3.20.	SEM images of micropillars fabricated with different levels of ion beam damage.	40
4.1.	The bicrystal generated in the MD software before deformation.	42
5.1.	Schematic profile of (a) single-crystalline and (b) bicrystalline micropillars displaying the average diameter and height used for calculations.	44
5.2.	Engineering stress-strain curves of bicrystals and single crystals of the same diameters ($5\mu\text{m}$).	46
5.3.	SE contrast SEM images of bicrystals and the single crystals of the same diameters ($5\mu\text{m}$) after compression tests.	47
5.4.	Engineering stress-strain curves of bicrystals and the single crystals of the same diameters (2 and $3\mu\text{m}$).	50
5.5.	SE contrast SEM images of a bicrystal and single crystals of the same range diameters (2 to $3\mu\text{m}$) after compression tests.	51
5.6.	Thompson tetrahedron	52
5.7.	Engineering stress-strain curves of bicrystals and single crystals of the same diameters ($1.4\mu\text{m}$).	54
5.8.	SE contrast SEM images of bicrystals and single crystals of the same diameters ($1.4\mu\text{m}$) after compression tests.	55
5.9.	Engineering stress-strain curves of bicrystals and single crystals of the same diameters ($1\mu\text{m}$).	57
5.10.	SE contrast SEM images of bicrystals of the same diameters ($1\mu\text{m}$) after compression tests.	58

5.11. SE contrast SEM images of single crystals of the same diameters ($1\ \mu\text{m}$) after compression tests.	59
5.12. OIM maps and OGM analyses at the free surface of a Litho-Pillar, a FIB-Litho-Pillar, a FIB-Pillar and a micropillar heavily bombarded with the ion beam.	61
5.13. Engineering stress-strain curves of a bicrystals compared with the two corresponding single crystals for different specimen diameters.	64
5.14. Schematic drawing of the source distribution in specimens with different sizes.	65
5.15. Stress at 0.5 % strain vs. pillar diameter.	67
5.16. The intersection lines of the slip planes on the grain boundary plane and the intersection lines of the same slip planes on the pillar top surface are indicated.	70
5.17. The schematic view of four slip systems activated in a typical bicrystal in this study.	71
5.18. Activation of secondary slip systems at the grain boundary in a bicrystal with the presence of primary slip systems ($\times 150$) [Hook and Hirth, 1967a].	73
5.19. Activation of slip system 2 in different small bicrystalline micropillars. .	75
5.20. Activation of slip systems in a bicrystals with $5\ \mu\text{m}$ diameters.	76
5.21. Double-ended and single-ended pile-ups for two different positions of the Frank-Read source as proposed by Friedman and Chrzan [Friedman and Chrzan, 1998].	80
5.22. Single-ended pile-up for two different positions of the Frank-Read source: in the crystal interior and on the crystal surface.	80
5.23. Size effect of single-crystalline pillars with (a) single slip orientation and (b) multiple slip orientation.	82
5.24. Post-deformation SEM images of $1\ \mu\text{m}$ diameter single crystals oriented for $\approx (1\ 1\ 1)$	83
5.25. Schematic comparison of two micropillars the same size with and without the grain boundary.	84
5.26. The relation between radii of the assumed two single crystals and the corresponding bicrystal.	84
5.27. Bicrystals with diameter R are compared with the multiple slip oriented single crystals of diameter r , where $R = \sqrt{2} r$	85
5.28. Stress-strain curve obtained from the simulation of a bicrystal under compression testing.	86
5.29. Sectional views from Y and Z directions at different strains shown by points A, B and C in Figure 5.28.	87
5.30. Grain boundary atoms at initial state compared to the yield point. . . .	89
5.31. A magnified view of the deformed pillar shows the slip transmission. . .	89
5.32. MD simulation predicts the activation of identical slip systems as observed in experiments.	89
5.33. Misorientation analysis of the perfect shear.	93

List of Figures

5.34. Stepwise compression test of the single-crystalline pillar with double slip orientation.	94
5.35. Misorientation analysis of slip systems interaction.	95
5.36. Misorientation analysis of a bicrystalline micropillar of $5\text{ }\mu\text{m}$ diameter.	97
5.37. Misorientation analysis of a bicrystalline micropillar of $1\text{ }\mu\text{m}$ diameter.	98
5.38. Misorientation analysis of a bicrystalline micropillar of $1\text{ }\mu\text{m}$ diameter.	99
5.39. Misorientation analysis of a bicrystalline micropillar of $1\text{ }\mu\text{m}$ diameter.	101
5.40. Comparison of the misorientation changes between the large bicrystal and the single-crystalline micropillars single slip and with double slip orientations.	105
5.41. Comparison of the OGM analysis between the large bicrystal and the single-crystalline micropillars with single slip and with double slip orientations.	105
A.1. Bicrystal geometry employed in [Hook and Hirth, 1967a,b; Livingstone and Chalmers, 1957; Hauser and Chalmers, 1961].	111
B.1. Pictured transmission criteria proposed by Livingstone (a) and Shen (b) [Kashihara and Inoko, 2001].	114
C.1. The position of the crystal coordinate system of a typical grain relative to the sample coordinate system.	116
C.2. An example to show the Angle/Axis description.	117
D.1. Schematical drawing of the Ni sample surface sputtered by different ion currents and at incidence angles.	119
D.2. Nanoindentation results with varying loads on surfaces irradiated with different ion beam currents.	121
D.3. Topography images of the irradiated regions with the help of in-situ imaging capability of the nanoindentation system.	122
E.1. Some typical results of the strain rate sensitivity compression tests on bicrystalline micropillars of the same size.	124
F.1. Stress distribution in different pillar geometries. (a) A tapered pillar. (b) An ideal cylinder with no tapering.	126

Abstract

In this research work, an experimental method is developed at the mesoscopic scale to investigate the interaction of dislocations with a selected grain boundary and its strengthening effect as a function of the grain boundary type.

The local mechanical testing method is based on microcompression tests of Focused Ion Beam (FIB)-cut bicrystalline micropillars with the component crystals oriented for single slip and multiple slip. Orientations identical to the experiments are used to generate models of the bicrystalline micropillars with up to four million atoms (140 nm in diameter) in Molecular Dynamics (MD) simulations. The compression test of these bicrystals is followed by Electron Backscatter Diffraction (EBSD) measurements on the bicrystal cross sections to investigate crystal lattice rotation in correlation with the excess dislocation density.

The microscopic test specimens are fabricated using high-voltage ion beam currents, which leads to the interaction of the ions with the host material. This problem, referred to as “FIB damage”, was examined by high-resolution EBSD and nanoindentation techniques. The results show that FIB damage is a function of the ion beam current and the crystallographic orientation of the lattice, and that its main effect is the introduction of surface defects and the facilitation of dislocation nucleation.

Different sized bicrystals, from 1 to 5 μm in diameter, show different deformation behaviors. In bicrystals over 2 μm in diameter, identical flow stresses to single crystals with multiple slip orientation are obtained. These bicrystals resemble two single-crystalline micropillars connected in parallel and Taylor hardening is the responsible mechanism of deformation. Diameters below 2 μm , where the grain boundary-dislocation interaction plays a more crucial role than the dislocation-dislocation interaction, show a pronounced hardening effect of the grain boundary. Our EBSD measurements and the orientation analyses on the bicrystals with 1 μm diameters prove the increase of the misorientation in the vicinity of the grain boundary. In contrast, in a large bicrystalline micropillar with a 5 μm diameter, the orientation gradient is observed only in the bottom-up direction (parallel to the loading axis), which is a clear evidence of the independent deformation of the adjacent crystals. In agreement with the literature, lattice rotation is required for slip transmission and, thus, for compatible deformation of the bicrystals.

Zusammenfassung

Im Rahmen dieser Arbeit wurde eine experimentelle Methode entwickelt, um die Wechselwirkung zwischen Versetzungen und ausgewählten Korngrenzen, sowie ihre Verfestigungseffekte auf einer mesoskopischen Skala als Funktion des Korngrenzentyps zu untersuchen. Die lokale mechanische Testmethode basiert auf Mikro-Drucktests von Focused Ion Beam (FIB) geschnittenen bikristallinen Mikropillars, deren Einzelkristalle für Einfachgleitung sowie für Mehrfachgleitung orientiert sind.

Die gleichen Orientierungen werden benutzt, um Drucktests an bikristallinen Mikropillars mit bis zu vier Millionen Atomen mittels Molekular-Dynamik-(MD) Rechnungen zu simulieren. Im Anschluss an die Druckversuche wurden Electron BackScatter Diffraction (EBSD) Messungen auf der Querschnittsseite der Mikropillars durchgeführt, um die Gitterrotation des Kristalles in Korrelation mit Überschussversetzungen (excess dislocations) zu bestimmen.

Die Mikropillars wurden mit Ionenstrahlen hoher Beschleunigungs-Spannung hergestellt, was üblicherweise zu einer Wechselwirkung zwischen den Ionen und dem Probenmaterials führt. Dieses als “FIB Schädigungseffekt” bekannte Problem wurde durch hoch aufgelöste EBSD-Messungen und durch die Nanoindenter Messungen überprüft. Die Ergebnisse zeigen, dass die FIB Schädigung eine Funktion der Ionenstrahlstärke und der kristallographische Gitterorientierung ist und, dass ihr Haupteffekt die Erzeugung von Oberflächendefekten und dadurch eine erleichterte Versetzungsnukleation ist.

Unterschiedlich große Bikristalle von 1 bis $5\text{ }\mu\text{m}$ Durchmesser zeigen unterschiedliches Verformungsverhalten. In Bikristalle über $2\text{ }\mu\text{m}$ Durchmesser ist die Fließspannung gleich der Fließspannung einkristalliner Mikropillars, die für Mehrfachgleitung orientiert sind. Diese Bikristalle gleichen zwei einkristallinen “parallel geschalteten” Mikropillars wobei die Taylor Verfestigung die Verformung kontrolliert. Bikristalle unter $2\text{ }\mu\text{m}$ Durchmesser zeigen ausgeprägte Verfestigungseffekte der Korngrenze, wobei die Wechselwirkung zwischen Korngrenze und Versetzung eine wesentlich wichtigere Rolle als die Wechselwirkung der Versetzungen untereinander spielt.

Die EBSD Messungen an Bikristallen mit $1\text{ }\mu\text{m}$ Durchmesser und die darauf basierende Orientierungsanalyse weisen eine steigende Fehlorientierung in unmittelbarer Nähe der Korngrenze nach. Im Gegensatz dazu ist in einem großen Bikristall mit $5\text{ }\mu\text{m}$ Durchmesser der Orientierungsgradient nur in der “Bottom-Up”-Richtung (parallel zu der Belastungsrichtung) zu beobachten, was ein klarer Beweis für die unabhängige Verformung beider Einzelkristalle ist. In Übereinstimmung mit der Literatur konnte die Gleittransmission als Ursache für die Gitterrotation bestätigt werden und somit für die kompatible Verformung der Bikristalle als erforderlich identifiziert werden.

I would probably not say everything
I think, but definitely think all I say.

Gabriel Garcia Marquez