



Universiteit
Leiden
The Netherlands

Exploring structure dependencies of gas-surface interactions with curved single crystals

Auras, S.V.

Citation

Auras, S. V. (2021, March 11). *Exploring structure dependencies of gas-surface interactions with curved single crystals*. Retrieved from <https://hdl.handle.net/1887/3151627>

Version: Publisher's Version

License: [Licence agreement concerning inclusion of doctoral thesis in the Institutional Repository of the University of Leiden](#)

Downloaded from: <https://hdl.handle.net/1887/3151627>

Note: To cite this publication please use the final published version (if applicable).

Cover Page



Universiteit Leiden



The handle <https://hdl.handle.net/1887/3151627> holds various files of this Leiden University dissertation.

Author: Auras, S.V.

Title: Exploring structure dependencies of gas-surface interactions with curved single crystals

Issue Date: 2021-03-11

Exploring structure dependencies of gas-surface interactions with curved single crystals

Proefschrift

ter verkrijging van
de graad van Doctor aan de Universiteit Leiden,
op gezag van Rector Magnificus Prof. Dr. ir. H. Bijl,
volgens besluit van het College voor Promoties
te verdedigen op donderdag 11 maart 2021
klokke 11:15 uur

door

Sabine Veronika Auras

Geboren te Munchen, Duitsland in 1991

Promotiecommissie

Promotor: Dr. L. B. F. Juurlink
Prof. dr. M. T. M. Koper

Overige leden: Prof. dr. S. J. van der Molen
Prof. dr. M. A. Stöhr
Prof. dr. A. W. Kleijn
Prof. dr. E. J. Baerends
Dr. I. M. N. Groot
Prof. dr. H. S. Overkleeft

ISBN: 978-94-642-3153-3

Cover: Sabine Auras

An electronic version of this thesis can be found at
<https://openaccess.leidenuniv.nl/>.

Printed by ProefschriftMaken with financial support from Scienta Omicron
Copyright © 2021 Sabine Auras

Meinen wundervollen Eltern gewidmet

CONTENTS

1	Introduction	1
1.1	Chemical reactions and the effect of catalysts	1
1.2	Heterogeneous catalysis	3
1.3	Surface science approach	4
1.4	Experimental techniques in this thesis	7
1.4.1	Low-energy electron diffraction	7
1.4.2	Scanning tunneling microscopy	7
1.4.3	Auger electron spectroscopy	7
1.4.4	King-and-Wells method	8
1.4.5	Temperature-programmed desorption.	9
1.5	Scope of this thesis	10
	References	11
2	Recent advances in the use of curved single crystal surfaces	13
2.1	Introduction	14
2.2	Brief historical overview	15
2.3	Surface structures on curved surfaces of single crystals	18
2.4	Currently used crystal shapes	24
2.5	Notation for curved crystals.	26
2.6	Considerations regarding experimental applications of curved crystals	27
2.6.1	Terrace widths and step densities on curved surfaces	28
2.6.2	Diffraction of regularly stepped surfaces along the curvature	30
2.7	Recent advances	32
2.7.1	Structure and electronic states of clean metal surfaces.	32
2.7.2	Adsorption and desorption from curved surfaces	37
2.7.3	Chemical reactions at curved surfaces	40
2.7.4	Magnetic, electronic, and chemical properties of films grown on curved crystals	45

2.8 Conclusion	49
References	50
3 Surface structure characterization of a curved Pt crystal	59
3.1 Introduction	60
3.2 Crystallographic orientation	61
3.3 Surface cleanliness and average terrace width	63
3.4 Terrace width distributions	65
3.4.1 Step-step interactions and their impact on terrace width dis- tributions	65
3.4.2 Results of terrace width analysis	66
3.4.3 Summary	70
3.5 Determining the step chirality	70
3.6 Structure of the kinked step edges.	72
3.6.1 Microscopic reconstructions along the kinked step	72
3.6.2 Statistical analysis of the kinked step structure.	72
3.6.3 Summary	75
References	75
4 Scaling Pt-catalyzed hydrogen dissociation on corrugated surfaces	81
4.1 Introduction	82
4.2 Experimental	83
4.3 Results and Discussion	84
4.4 Conclusion	91
References	92
5 Chiral Surface Characterisation and Reactivity toward H-D Exchange	95
5.1 Introduction	96
5.2 Experimental	98
5.3 Results and Discussions.	101
5.3.1 STM analysis of intentional and non-intentional defects.	101
5.3.2 D ₂ dissociation and HD formation on the curved crystal.	104
5.4 Outlook and Conclusion	108
References	108
6 It's not just the defects - a curved crystal study of H₂O desorption from Ag	115
6.1 Introduction	116
6.2 Experimental	117

6.3 Results	120
6.3.1 Surface structure investigation.	120
6.3.2 Temperature Programmed Desorption.	121
6.4 Discussion	125
6.5 Conclusions.	128
References	129
7 Outlook	133
7.1 Exploring reactive sites towards CO ₂ dissociation.	134
7.2 Determining adsorption sites and structures by low-temperature STM.	139
7.3 Introducing curved crystals of bimetallic alloys	144
7.4 Possible future applications of curved crystals	147
References	148
8 Summary	151
9 Samenvatting	157
A Supplementary Information for Chapter 3	163
A.1 Histograms of facet distributions in kinked steps	163
B Supplementary Information for Chapter 4	167
B.1 Initial sticking probabilities at step sites	167
B.2 Coordination at the lower step edge.	168
B.3 Structural analysis of the kinked {210} steps.	168
C Supplementary Information for Chapter 5	171
C.1 Terrace width analysis.	171
D Analysis procedure for determining steps in STM images	173
D.1 Procedure 1	173
D.2 Procedure 2	174
D.3 Procedure 3	176
D.4 Procedure 4	177
D.5 Procedure 5	178
D.6 Procedure 6	184
List of Publications	187
Curriculum Vitae	189

