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

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**Title:** Exploring structure dependencies of gas-surface interactions with curved single crystals
**Issue Date:** 2021-03-11
SUPPLEMENTARY INFORMATION FOR CHAPTER 3: SURFACE STRUCTURE CHARACTERIZATION OF A CURVED Pt CRYSTAL WITH HIGHLY KINKED STEPS

A.1. Histograms of facet distributions in kinked steps
Figure A.1: a)–m) STM images and distributions of segment lengths along the kinked step edges. Kink densities and Gaussian fits are used in figure 3.9.
Figure A.1: a)–m) STM images and distributions of segment lengths along the kinked step edges. Kink densities and Gaussian fits are used in figure 3.9.
Figure A.1: a–m) STM images and distributions of segment lengths along the kinked step edges. Kink densities and Gaussian fits are used in figure 3.9.
B.1. Initial sticking probabilities at step sites

The slope $\Sigma_0$, as obtained from the linear fits of $S_0$ at different positions of the curved crystal, has a unit of nm due to the x-axis (step density) being in units of nm$^{-1}$.

$$S_0(SD) = S_0^{(111)} + \Sigma_0[\text{nm}] \cdot SD[\text{nm}^{-1}] \quad (B.1)$$

An alternative way to quantify the additional reactivity caused by steps is to consider the fraction of the surface area occupied by steps ($f_{\text{step}}$), instead of mere step density:

$$S_0 = S_0^{(111)} \cdot (1 - f_{\text{step}}) + S_{\text{step}}^0 \cdot f_{\text{step}} \quad (B.2)$$

Obtaining a unitless $S_{\text{step}}^0$ may feel more intuitive when comparing reactivities of the step edge with reactivities of the (111) terrace. However, determining a value $f_{\text{step}}$ requires an assumption on the size of a step within the unit cell. Defining it as one atom row at the upper step edge will give a different step size for kinked steps (0.277 nm) than A- and B-type steps (0.240 nm), due to their orientation on the (111) terrace. Considering the upper edge and lower cusp of each step type will yield different step sizes for each type. The same step density may thus correspond to three different values for $f_{\text{step}}$, resulting in a weighing of $S_{\text{step}}^0$ purely based on atom arrangement.

We therefore consider the weighing of reactivity by step density in equation B.1 a more appropriate approach when comparing different step types. The unit, nm, in
turn can be interpreted as length over which the step is reactive, i.e. a 'chemical step size'. The implications of $\Sigma_0$ as a physical length are further discussed in the main text.

The decreasing fraction of (111) terraces on the stepped surfaces, $(1 - f_{step})$ is neglected there, due to the inherently small value of $S_0^{(111)}$.

**B.2. Coordination at the Lower Step Edge**

For atoms at the lower edges, $CN$ and $\overline{CN}$ values for the three step types vary slightly, as listed in table B.1. The coordination number in the lower plane of the A-type step is lower than both the B-type step and any combined contribution of inner and outer kinks. The A-type should thus be most reactive. If only outer kinks contribute to reactivity, the $\{210\}$ steps should react similarly to the A-type. The B-type should be least reactive.

<table>
<thead>
<tr>
<th></th>
<th>upper edge</th>
<th>lower edge</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>A</td>
<td>B</td>
</tr>
<tr>
<td>$CN$</td>
<td>7</td>
<td>7</td>
</tr>
<tr>
<td>$\overline{CN}$</td>
<td>5.50</td>
<td>5.50</td>
</tr>
</tbody>
</table>

Table B.1: Coordination numbers ($CN$) and generalized coordination numbers ($\overline{CN}$) of atoms at the upper and lower edge of the three step types in this study.

**B.3. Structural Analysis of the Kinked $\{210\}$ Steps**

Table B.2 lists kink atoms (K) and step atoms (A or B) in fully-kinked (a) and longer segments (b,c,d...). In the ultimate case of step faceting, a single $\{210\}$ step would break into very large segments of the A- and B-type. This reconstruction of the $\{210\}$ step has a combined total length of 1.16 times that of a straight line connecting the first and last atom of the edge. These ideas form the basis for a model that extracts the average chemical reactivity of inner and outer kinks. We take into account the length and composition of possible step sections, the measured reactivity for A- and B-type steps, and the distribution of A- and B-sections in $\{210\}$ steps as obtained by STM.

The STM images in figure 4.3b)–e) gives us distributions of segment lengths in averages stretches of step edges. We use those distributions and the atomic compositions of segments laid out in table B.2 and displayed in figure 4.3a) to calculate the number of kink atoms ($N_K$), as well as intermittent atoms in longer segments of A- or B-type orientation ($N_A$ and $N_B$):

$$N_A = 0 \cdot a_A + 1 \cdot b_A + 2 \cdot c_A + \cdots$$  (B.3)
B.3. Structural Analysis of the Kinked \{210\} Steps

<table>
<thead>
<tr>
<th>segment</th>
<th>atoms in segment</th>
<th>{001}-oriented</th>
<th>{110}-oriented</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>K</td>
<td>A</td>
</tr>
<tr>
<td>a</td>
<td>2</td>
<td>1</td>
<td>0</td>
</tr>
<tr>
<td>b</td>
<td>4</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>c</td>
<td>6</td>
<td>1</td>
<td>2</td>
</tr>
<tr>
<td>d</td>
<td>8</td>
<td>1</td>
<td>3</td>
</tr>
<tr>
<td>...</td>
<td>...</td>
<td>...</td>
<td>...</td>
</tr>
</tbody>
</table>

Table B.2: Composition of atoms found in kinked steps with various segment lengths, as displayed in figure 4.3a) of the main text. Atoms at the top of the step edge can be considered either a direct kink atom (K), or a step atom. Depending on the orientation of the segment, step atoms are either A-type (A) or B-type (B).

\[
N_B = 0 \cdot a_B + 1 \cdot b_B + 2 \cdot c_B + \cdots \quad (B.4)
\]

\[
N_K = a_A + b_A + b_B + c_A + c_B + \cdots \quad (B.5)
\]

Here \(a_A\) is the fractional occurrence of bin a of the \{001\} histogram, \(b_A\) is the fractional occurrence of segments in bin b of the \{001\} histogram, \(a_B\) is the fractional occurrence of segments in bin a of the \{110\} histogram, etc...

Table B.3 lists the results, as well as kink densities and \(\Sigma_0\), as described in the main text.

<table>
<thead>
<tr>
<th>image in fig.4.3</th>
<th>(N_A)</th>
<th>(N_B)</th>
<th>(N_K)</th>
<th>(N)</th>
<th>(N_K/N)</th>
<th>(\Sigma_0^K)</th>
</tr>
</thead>
<tbody>
<tr>
<td>b)</td>
<td>152.201</td>
<td>122.222</td>
<td>200</td>
<td>474.423</td>
<td>0.422</td>
<td>0.747</td>
</tr>
<tr>
<td>c)</td>
<td>139.734</td>
<td>161.9</td>
<td>200</td>
<td>501.634</td>
<td>0.399</td>
<td>0.734</td>
</tr>
<tr>
<td>d)</td>
<td>73.6264</td>
<td>106.522</td>
<td>200</td>
<td>380.1484</td>
<td>0.526</td>
<td>0.667</td>
</tr>
<tr>
<td>e)</td>
<td>163.158</td>
<td>127.016</td>
<td>200</td>
<td>490.174</td>
<td>0.408</td>
<td>0.758</td>
</tr>
</tbody>
</table>

Table B.3: Numbers of atoms found in kinked steps with various segment lengths, as displayed in figure 4.3a), averaged to 100 segments in \{001\} orientation and 100 segments in \{110\} orientation. Atoms are considered either a kink atom (K), or an atom resembling those in type A steps (A) and type B steps (B).
C.1. Terrace Width Analysis

Figure C.1a) shows the averaged terrace widths for each image, 300 µm on either side of the apex. Blue data with error bars represent each image’s average terrace width and standard deviation. The red dots are, for each image, the local maximum terrace width which, together with the standard deviation, provide an idea of the terrace width distribution across the crystal. The black traced lines are the expected terrace widths as described by equation 5.1. We observe a close match with the expected terrace width except for in the ~40 µm around the apex. This is more clearly visible in the zoomed-in section of the figure.

By taking the inverse of the terrace widths, we expect to see a linearly increasing step density where the slope is determined by the radius of curvature and interatomic distance. Beyond 400 µm on the (-Y) side of the crystal, terrace width distribution was low enough to simply divide the number of steps in an image by the distance between the first and last step. This data, along with the inverse of the terrace widths previously shown, is plotted in figure C.1b). We can see that all along the imaged regions of the crystal, the step density increases linearly with distance from the apex respecting the expected defect density.
Figure C.1: a) Terrace widths as a function of distance from the apex for 330 nm on either side of the apex. Blue data points indicate the average terrace widths including the standard deviation per STM image and red data points are the maximum terrace widths per image. A subfigure in the top right shows a zoom around the center of the graph where the averages start to deviate from the expected TW curve (in black). b) Step densities as a function of position on the crystal. Black line represents the expected step density taken from the inverse of equation 5.1.
STM analysis procedure to determine outlines of steps in STM images with IGOR Pro

D.1. Procedure 1

One pixel wide line profiles in vertical direction are created across the entire STM image.

Function alllineprofiles(i,j,name,x)

variable i //first line profile
variable j //last line profile
variable x //number of pixels in image
wave name
make/n=2 xxx,yyy
wave xxx ; wave yyy
string srcwave ; string xwave ; string ywave
Display

For (i=i; i<j+1;i +=1)
xxx=i,i ; yyy=0,(x-1)
string num=num2str(i) ; string profile="Prof"+num
ImageLineProfile srcwave=name, xwave=xxx, ywave=yyy, width=3
duplicate W_; ImageLineProfile $profile
D.2. PROCEDURE 2

Step edges are found along the horizontal direction, across all line profiles.

Function limitprofiles(i,j,k,x,name,A,B,n)

variable i //first x
variable j //last x that you take a lineprofile of
variable A //first point of y values in which to find the step
variable B //last point of y values in which to find the step
variable n //how manyth step in image
variable k //imagesize (nm)
variable x //number of pixels in image

string st="step"+num2str(n)
make/n=(j+1) $st
wave step=$st

For (i=i; i<j+1;i +=1)
string num=num2str(i) ; string profile="Prof"+num
wave pro=$profile
string profiledif="Prof"+num+"_dif"
wave dif=$profiledif
wavestats/Q/R=(A,B) dif
step[i]=V_maxRowLoc
EndFor

step[0]=step[1]; step[j]=step[j-1]
string stnm="step"+num2str(n)+"_nm"
duplicate/O step $stnm
wave step_nm=$stnm
step_nm=step/x*k

string stx="stepX_nm"
duplicate/O step $stx
wave stepX=$stx
stepX=p/(j+1)*k

AppendToGraph step vs W_LineProfileY
ModifyGraph mode=4,marker=19

If(n==2)
ModifyGraph rgb(step2)=(65280,21760,0)
elseif(n==3)
ModifyGraph rgb(step3)=(65280,43520,0)
elseif(n==4)
ModifyGraph rgb(step4)=(26112,52224,0)
elseif(n==5)
ModifyGraph rgb(step5)=(0,39168,0)
elseif(n==6)
ModifyGraph rgb(step6)=(0,39168,39168)
elseif(n==7)
ModifyGraph rgb(step7)=(0,9472,39168)
elseif(n==8)
ModifyGraph rgb(step8)=(19712,0,39168)
elseif(n==9)
ModifyGraph rgb(step9)=(52224,0,41728)
elseif(n==11)
ModifyGraph rgb(step11)=(65280,21760,0)
D.3. PROCEDURE 3

The terrace widths in between step edges are determined.

Function maketerraces(j,k,x)

variable j //number of steps
variable k //imagesize (nm)
variable x//number of pixels in image
variable i ; variable a=0

For (i=1; i<j; i +=1)
string st="step"+num2str(i)
wave step=$st
string st2="step"+num2str(i+1)
wave step2=$st2
string ter="terrace"+num2str(i)
duplicate/O step $ter
wave terrace = $ter
terrace = step2-step
string termn="terrace"+num2str(i)+"_nm"
duplicate/O terrace $termn
wave terrace_nm = $termn
terrace_nm=terrace/x*k
wavestats/Q terrace_nm
a += V_avg
EndFor

print "avg terrace width [nm]" ; print a/(j-1)
End

**D.4. PROCEDURE 4**

Terrace width distribution histograms are created from the available terrace widths.
Function terracehist(j,k,x)

variable j //number of terraces
variable k //image size (nm)
variable x//number of pixels in image
variable l=k*2/0.277
variable i
display

For (i=1; i<j+1;i +=1)
string termn="terrace"+num2str(i)+"_nm"
wave terrace_nm = $termn
string hist="terrace"+num2str(i)+"_Hist"
string number=num2str(l)
D.5. Procedure 5

Segments along a step edge (in between kink sites) are determined and their length is determined.

Function makeblock(step,stepX)

wave step; wave stepX
variable x//image size
string st=nameofwave(step) // name of step wave
string stx=nameofwave(stepX) // name of x wave of step wave
duplicate/O step $st+"_dif" // name of x wave of step wave
wave step_dif = $st+"_dif"
Differentiate/METH=1 step/X=stepX/D=step_dif;
duplicate/O step_dif $st+"block"
wave block = $st+"block"

variable i ; variable j = numpnts(step) //number of points in wave

For (i=0; i<j; i +=1)
If(step_dif[i]>0.1)
block[i]=1
Elseif(step_dif[i]<-0.1)
block[i]=-1
else
block[i]=0
EndIf
EndFor

duplicate/O stepX $st+"blockpos"
wave position=$st+"blockpos"
duplicate/O block $st+"blockvalue"
wave value=$st+"blockvalue"
duplicate/O position $st+"blockpos_fw"
wave posfw=$st+"blockpos_fw"
duplicate/O block $st+"blockvalue_fw"
wave valuefw=$st+"blockvalue_fw"
duplicate/O position $st+"blockpos_bw"
wave posbw=$st+"blockpos_bw"
duplicate/O block $st+"blockvalue_bw"
wave valuebw=$st+"blockvalue_bw"

For (i=0; i<j; i +=1)
if(valuefw(i)==0)
deletepoints i,1,posfw ; deletepoints i,1, valuefw
i=i-1
EndIf
EndFor
For (i=numpnts(step); i>0; i -=1)
If(valuebw[i]==0)
deletepoints i,1,posbw ; deletepoints i,1,valuebw
EndIf
EndFor

For (i=1; i<numpnts(valuefw); i +=1)
if(valuefw(i)==valuefw[i-1])
deletepoints i,1,posfw ; deletepoints i,1, valuefw
i=i-1
EndIf
EndFor

For (i=1; i<numpnts(valuefw); i +=1)
if(posfw(i)-posfw(i-1)<0.12)
deletepoints i,1,posfw ; deletepoints i,1, valuefw
i=i-1
EndIf
EndFor

For (i=1; i<numpnts(valuefw); i +=1)
if(valuefw(i)==valuefw[i-1])
deletepoints i,1,posfw ; deletepoints i,1, valuefw
i=i-1
EndIf
EndFor

For (i=0; i<numpnts(valuebw); i +=1)
If(valuebw(i)==valuebw(i+1))
deletepoints i,1,posbw ; deletepoints i,1,valuebw
i=i-1
EndIf
EndFor
For (i=0; i<numpnts(valuebw) ;i +=1) 
If(posbw(i+1)-posbw(i)<0.12) 
deletepoints i,1,posbw ; deletepoints i,1,valuebw 
i=i-1 
EndIf 
EndFor

For (i=0; i<numpnts(valuebw) ;i +=1) 
If(valuebw(i)==valuebw(i+1)) 
deletepoints i,1,posbw ; deletepoints i,1,valuebw 
i=i-1 
EndIf 
EndFor

duplicate/O posfw $st+_facet_fw$
wave facetfw=$st+_facet_fw$
For (i=1; i<j;i +=1)
facetfw[i]=posfw[i]-posfw[i-1]
Endfor

duplicate/O posbw $st+_facet_bw$
wave facetbw=$st+_facet_bw$
For (i=0; i<j;i +=1)
facetbw[i]=posbw[i+1]-posbw[i]
Endfor

duplicate/O facetfw $st+"_plusfacet_fw"
wave plusfw =$st+"_plusfacet_fw"
duplicate/O valuefw $st+"_plusvalue_fw"
wave plusvalfw = $st+"_plusvalue_fw"
duplicate/O facetfw $st+"_minusfacet_fw"
wave minusfw = $st+"_minusfacet_fw"
duplicate/O valuefw $st+"_minusvalue_fw"
wave minusvalfw = $st+"_minusvalue_fw"
For (i=0; i<j;i +=1)
If(plusvalfw[i]!=1)
deletepoints i,1,plusfw ; deletepoints i,1,plusvalfw
i=i-1
Endif
Endfor

For (i=0; i<j;i +=1)
If(plusfw[i]==0)
deletepoints i,1,plusfw ; deletepoints i,1,plusvalfw
i=i-1
Endif
Endfor

For (i=0; i<j;i +=1)
If(minusvalfw[i]!=-1)
deletepoints i,1,minusfw ; deletepoints i,1,minusvalfw
i=i-1
Endif
Endfor

For (i=0; i<j;i +=1)
If(minusfw[i]==0)
deletepoints i,1,minusfw ; deletepoints i,1,minusvalfw
i=i-1
Endif
Endfor

duplicate/O facetbw $st+"plusfacet_bw"
wave plusbw = $st+"plusfacet_bw"
duplicate/O valuebw $st+"plusvalue_bw"
wave plusvalbw = $st+"plusvalue_bw"
duplicate/O facetbw $st+"minusfacet_bw"
wave minusbw = $st+"minusfacet_bw"

duplicate/O valuebw $st+"minusvalue_bw"

wave minusvalbw = $st+"minusvalue_bw"

For (i=0; i<j;i +=1)

If(plusvalbw[i]!=1)

deletepoints i,1,plusbw ; deletepoints i,1,plusvalbw

i=i-1
Endif
Endfor

For (i=0; i<j;i +=1)

If(plusbw[i]==0)

deletepoints i,1,plusbw ; deletepoints i,1,plusvalbw

i=i-1
Endif
Endfor

For (i=0; i<j;i +=1)

If(minusvalbw[i]!=-1)

deletepoints i,1,minusbw ; deletepoints i,1,minusvalbw

i=i-1
Endif
Endfor

For (i=0; i<j;i +=1)

If(minusbw[i]==0)

deletepoints i,1,minusbw ; deletepoints i,1,minusvalbw

i=i-1
Endif
Endfor

Make/O/N=200/O $st+"_plus_hist_fw"

wave plh_fw=$st+"_plus_hist_fw"
D. ANALYSIS PROCEDURE FOR DETERMINING STEPS IN STM IMAGES

D.6. PROCEDURE 6

From this part of the code, distributions of segment lengths are determined separately for {001}- and {110}-oriented segments.

Function plotstephistograms(j)

variable j ; variable i

Display

For (i=1; i<j+1; i +=1)

string plus = "step"+num2str(i)+"_nm_plus_hist_avg"

string minus = "step"+num2str(i)+"_nm_minus_hist_avg"

wave plh_avg = $plus
wave mnh_avg = $minus
string l="L"+num2str(i) ; string b="B"+num2str(i) ; string m="L"+num2str(i+j) ; string t="T"+num2str(i)

AppendToGraph/L=$l/B=$b plh_avg
AppendToGraph/L=$m/T=$t mnh_avg

variable a = (i-1)/j ; variable c= (i/j)

ModifyGraph axisEnab($b)=a,c ; ModifyGraph axisEnab($t)=a,c
ModifyGraph axisEnab($l)=0,0.5 ; ModifyGraph axisEnab($m)=0.5,1
ModifyGraph freePos($l)=a,kwFraction ; ModifyGraph freePos($m)=a,kwFraction
ModifyGraph freePos($b)=0,$l ; ModifyGraph freePos($t)=0,kwFraction
ModifyGraph mode=5,hbFill=4 ; ModifyGraph standoff=0 ; ModifyGraph axisOnTop=1

string mna = "step_all_nm_min_hist"
string pla = "step_all_nm_plus_hist"

If(i==1)
duplicate/O mnh_avg $mna
wave mnall =$mna
duplicate/O plh_avg $pla
wave plall =$pla
Else
mnall += mnh_avg ; plall += plh_avg
Endif
Endfor

string plat="step_all_plus_hist_atoms"
string mnat="step_all_minus_hist_atoms"
duplicate/O mnall $mnat
wave mn_at=$mnat
duplicate/O plall $plat
wave pl_at=$plat
mn_at = mnall*p ; pl_at = plall*p
End
**LIST OF PUBLICATIONS**

**CHAPTER 2**
Recent advances in the use of curved single crystal surfaces


**CHAPTER 4**
Scaling Platinum-Catalyzed Hydrogen Dissociation on Corrugated Surfaces


**CHAPTER 5**
Chiral Surface Characterisation and Reactivity Toward H–D Exchange of a Curved Platinum Crystal


**CHAPTER 6**
It's not just the defects - a curved crystal study of H₂O desorption from Ag


*These authors contributed equally to the manuscript*
OTHER PUBLICATIONS

On the correlation of structure and catalytic performance of VPO catalysts

Step-type and step-density influences on CO adsorption probed by reflection absorption infrared spectroscopy using a curved Pt(111) surface

Site-specific reactivity of molecules with surface defects – the case of H\textsubscript{2} dissociation on Pt
Sabine Auras is a trained chemist, who received most of her education at the Ludwig-Maximilians University in Munich, Germany. After a broad undergraduate education (B.Sc. in Chemistry and Biochemistry, 2013), she developed an interest in physical chemistry during her Master studies (M.Sc. in Chemistry in 2015).

During an Erasmus stay at Leiden University in the Netherlands, Sabine had the opportunity to join the group of Dr. Ludo Juurlink for six months and studied the structure of a curved Ag(001) crystal. Subsequently, she returned to Germany to complete her M.Sc. degree. During her master thesis project, she investigated the correlations between structure and catalytic performance of VPO catalysts, under supervision of Dr. S. Böcklein and Dr. G. Mestl at Clariant AG. VPO is the industrial catalyst for the selective oxidation of maleic anhydride from \( n \)-butane, a reaction similar to ethylene oxidation.

Sabine started her Phd at Leiden University in December 2015, under supervision of Dr. Ludo Juurlink, where she studied the structure and reactivity of curved crystal surfaces with a variety of different techniques. Sabine explored the fundamental aspects of gas-surface dynamics, using multiple curved metal crystals (Ag, Pt, NiAl). A combination of surface structure techniques (LEED, AES, STM), spectroscopy (RAIRS) and mass spectrometry based techniques (TPD, TOF, King-and-Wells) have been the key to unraveling underlying structure dependencies in such reactions. A main focus of the PhD project has been the introduction of STM to the Juurlink group, by reviving an old VT-STM and initiating collaborations with STM-focused groups in Spain and the USA. Namely, Sabine had short-term stays abroad with the groups of Prof. Ortega (CFM, San Sebastian, Spain) and Prof. Killelea (Loyola University, Chicago, USA).

The results of her PhD work are presented in this thesis and resulted in several publications. Sabine also presented her work at various Dutch and international conferences, e.g. the Gordon Research Seminar and Conference on Chemical Reactions at Surfaces in 2017, the Gordon Research Seminar and Conference on Dynamics at Surfaces (2017 and 2019), several Dutch Scanning Probe Microscopy Days and HRSMC Symposia, the Reedijk Symposium (2017), and the AVS Prairie Chapter meeting (2017). In particular, she gave talks at the Gordon Research Seminar on Dynamics at Surfaces in 2019 and the HRSMC Symposium in 2019.

Sabine attended the NIOK course *Catalysis, An Integrated Approach* in 2017 and the HRSMC *Tulip School on Modern Advances in Spectroscopy* in 2018. She was also a
member of the HRSMC PhD platform. Throughout her time in Leiden, Sabine supervised and coached several Bachelor and Master students, and assisted teaching in the *algemene en anorganische chemie* and *practicum basisvaardigheden* courses of the *Molecular Science and Technology* B.Sc. programme of Leiden University and TU Delft.

Sabine will start her PostDoc at the Centro de Física de Materiales in Donostia, Spain in spring 2021.