Teilprojekt C11

Untersuchung der Eigenschaften von Übergangsmetalloxid-Oberflächen mittels streifender Ionen-Streuung

H. Winter, D. Blauth, M. Busch, J. Lienemann, K. Maass,
R. Mitdank, A. Schüller, J. Seifert, S. Wethekam
Institut für Physik der Humboldt-Universität zu Berlin
Physik der Grenzflächen und dünnen Schichten

UP1: Structure of Monolayer Silica Films on Mo(112) — **Teilprojekt B1**, **Teilprojekt C5**

UP2: Investigation of SBA15 via Rutherford Backscattering (RBS) and NEXAFS (Mitdank)

UP3: Structure of Titania Films on Mo(112) — **Teilprojekt B7**

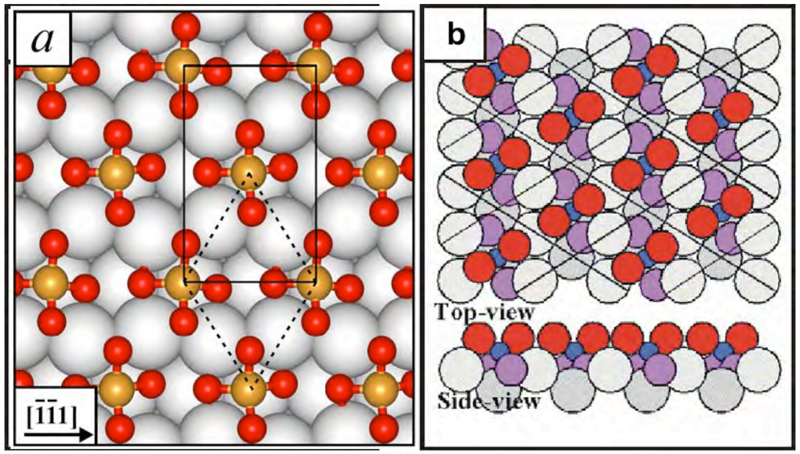
Struktur von Mo(112)/SiO: „Goodman vs Sfb546“

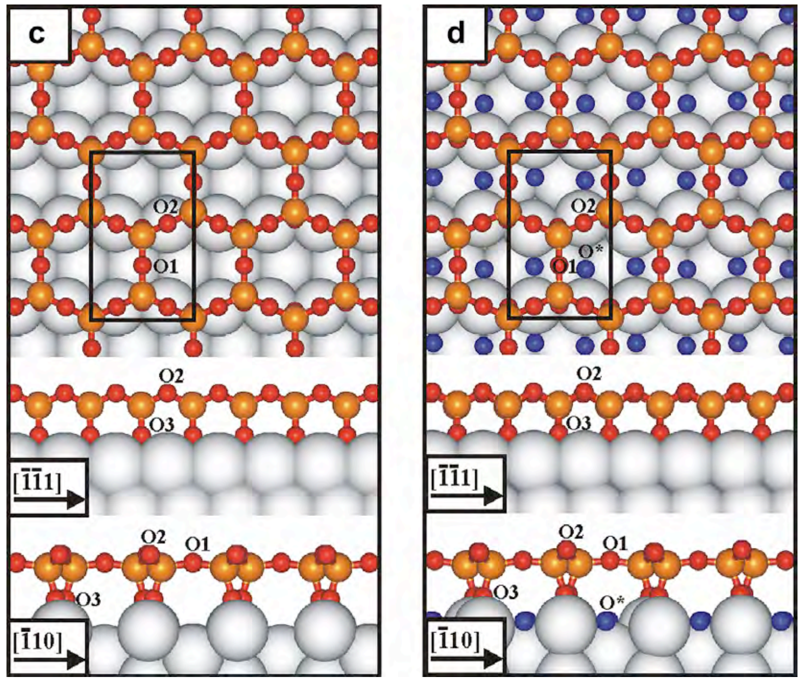
Goodman et al.
„[SiO_4] cluster model“

Teilprojekt
B1

Sierka et al.
„2D-network model“

Teilprojekt
C5





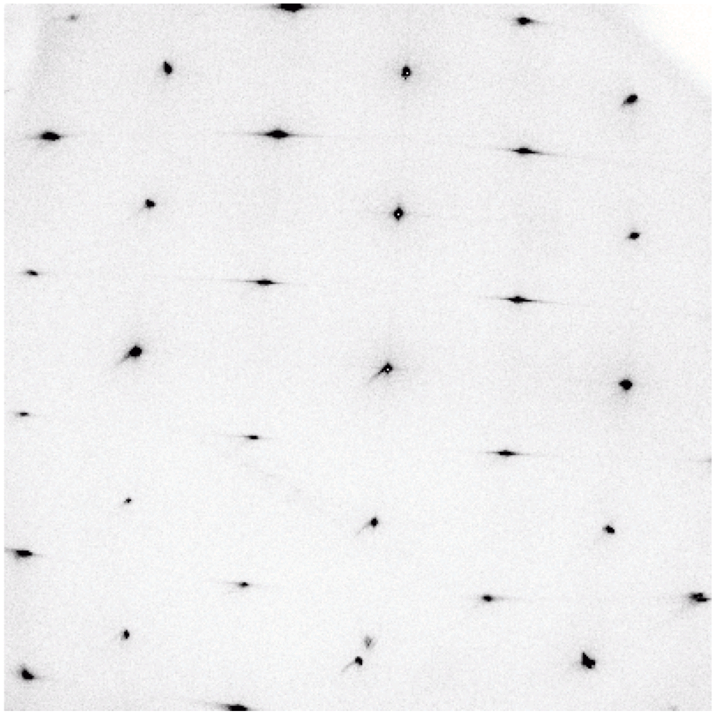
M. Chen, A.K. Santra and D.W. Goodman, Phys. Rev. B 69 (2004) 155404
M. Chen and D.W. Goodman, Surf. Sci. 600 (2006) L255

T.K. Todorova et al., Phys. Rev. B 73 (2006) 165414
J. Weissenrieder et al., Phys. Rev. Lett. 95 (2005) 076103
M. Sierka et al., Chem. Phys. Lett. 424 (2006) 115

siehe auch:
Finanzierungsantrag 2008-2011

SiO on Mo(112) – well defined ML-film

a)



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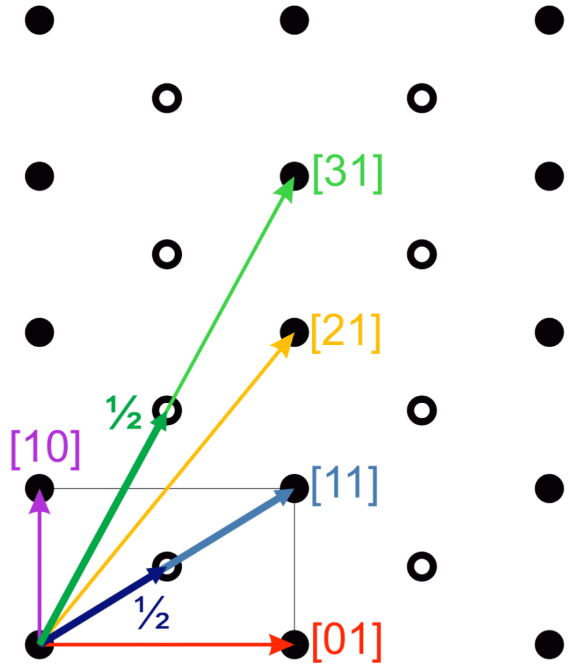
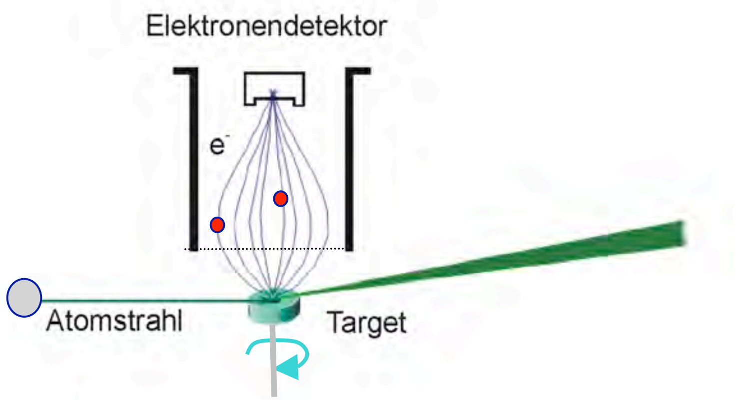
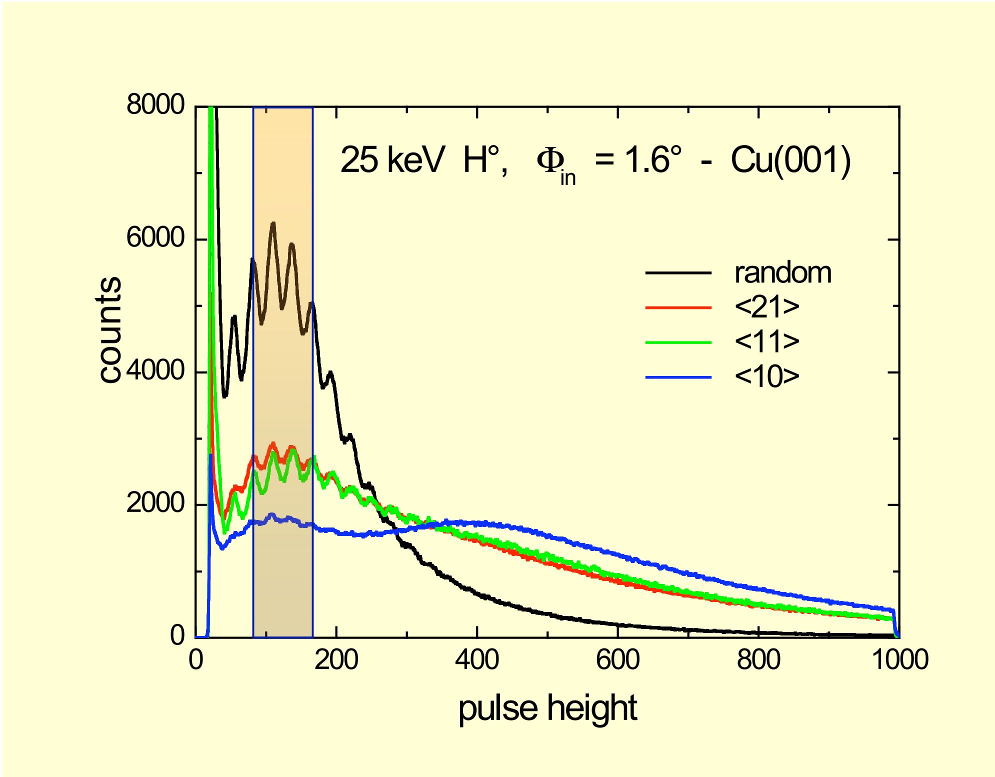


LEED shows c(2x2)

Anzahl emittierter Elektronen





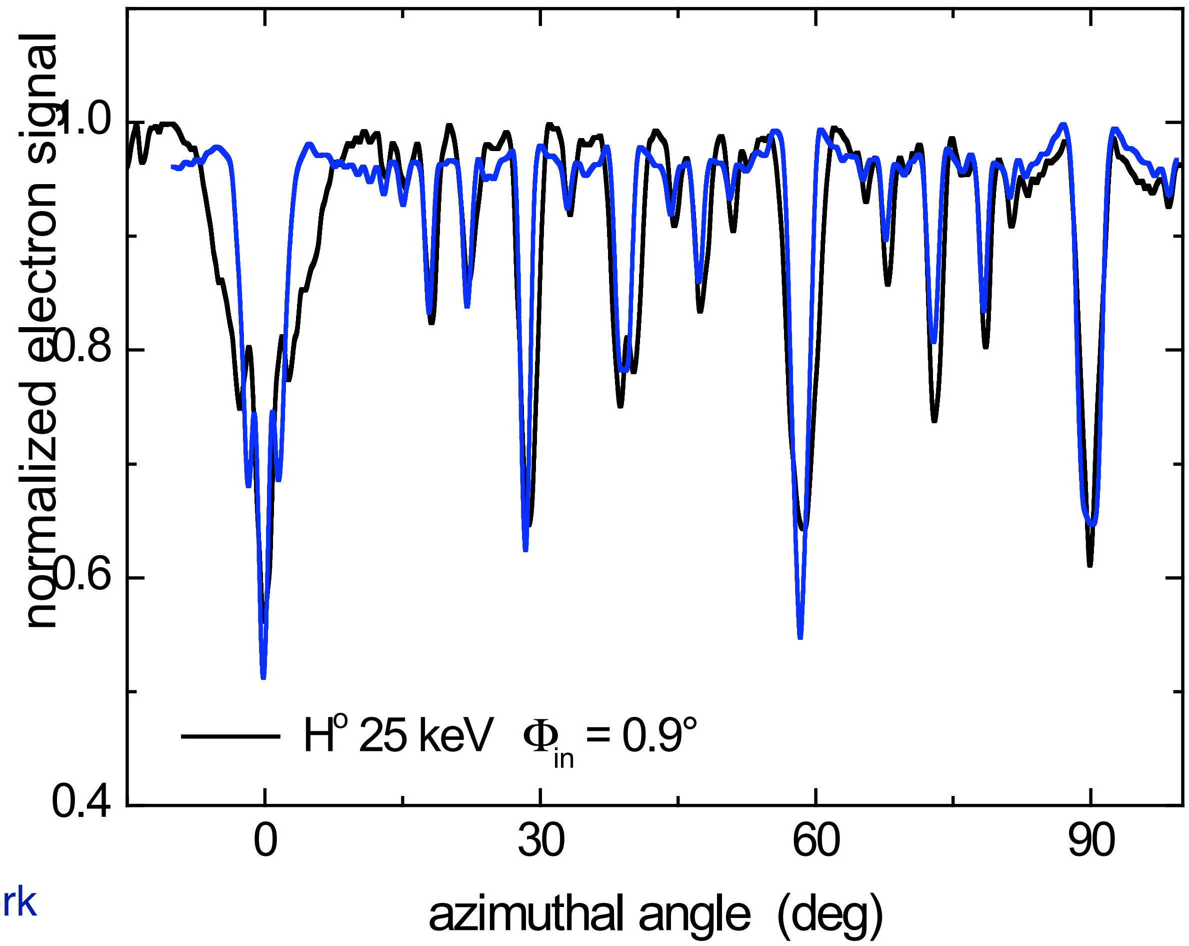
Aumayr et al.
Appl. Surf. Sci. 47 (1991) 139

(„Vienna detector")

- Selektion kleiner n_e: extreme Sensitivität auf oberste Lage
- sehr kleine Ströme (sub-fA): Keine Schädigung der Probe
- Methode auch anwendbar für Isolatoren
- effíziente Normierung der Daten auf Gesamtsignal

Teilprojekt **B1** Teilprojekt **C5**

Struktur von Mo(112) / SiO

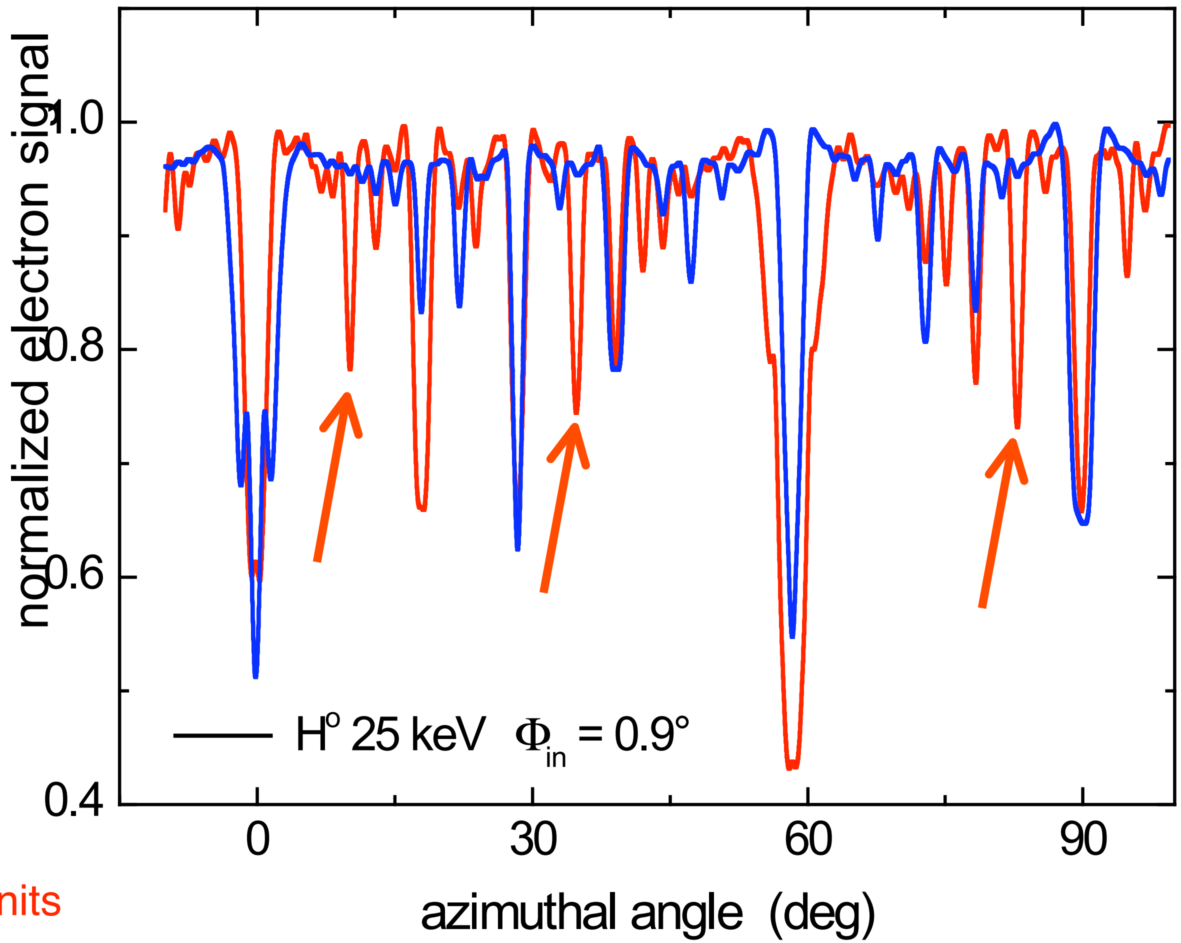


simulation 2D network

Teilprojekt **B1**

Teilprojekt **C5**

Struktur von Mo(112) / SiO



simulation 2D network

simulation with SiO_4 units

Structure of Mo(112)/SiO: „2D network vs. SiO_4 units“

PRL 103, 017601 (2009) PHYSICAL REVIEW LETTERS week ending 3 JULY 2009

Evidence for 2D-Network Structure of Monolayer Silica Film on Mo(112)

J. Seifert, D. Blauth, and H. Winter*

Institut für Physik, Humboldt Universität zu Berlin, Brook-Taylor-Str. 6, D-12489 Berlin-Adlershof, Germany

(Received 26 March 2009; published 1 July 2009)

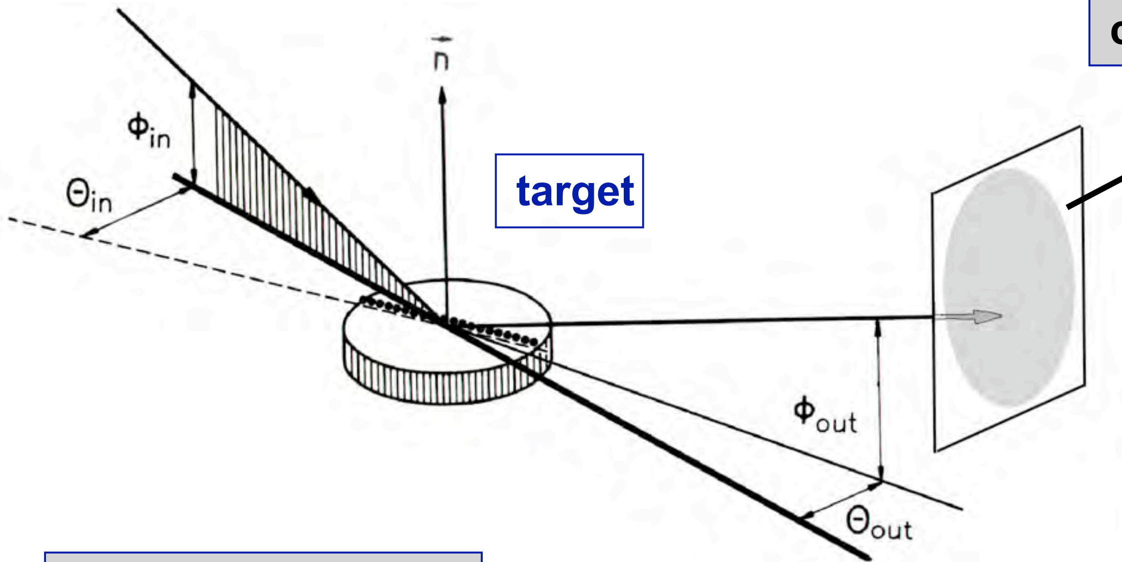
The structure of a monolayer silica film on a Mo(112) surface is investigated by grazing scattering of 25 keV H^0 atoms. By detection of the number of projectile induced emitted electrons as function of azimuthal angle of rotation of the target surface, the geometrical structure of atoms forming the topmost layer of the silica film is determined via ion beam triangulation. From our data we find evidence for the arrangement of surface atoms in terms of a two-dimensional Si-O-Si network model.

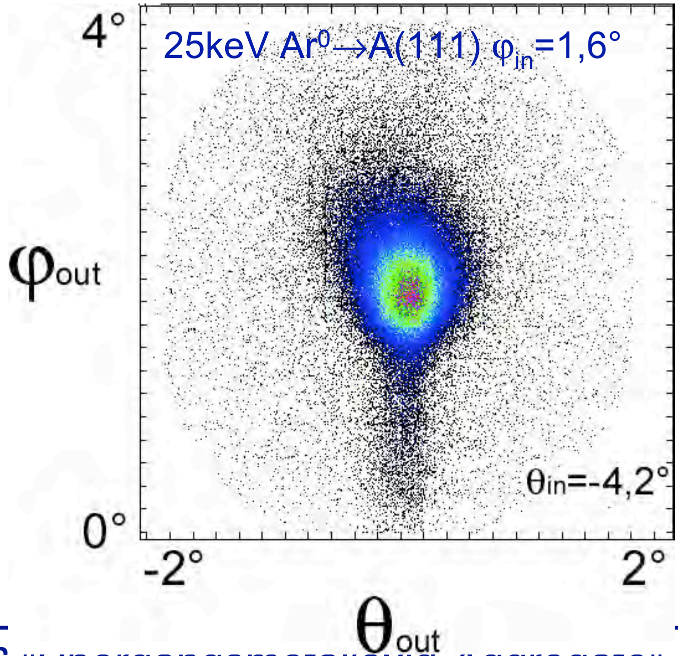
DOI: 10.1103/PhysRevLett.103.017601 PACS numbers: 79.20.Rf, 68.55.−a, 68.60.−p, 81.15.−z

sketch of the experiment

position sensitive channelplate detector

target





atomic beam
(no image charge)

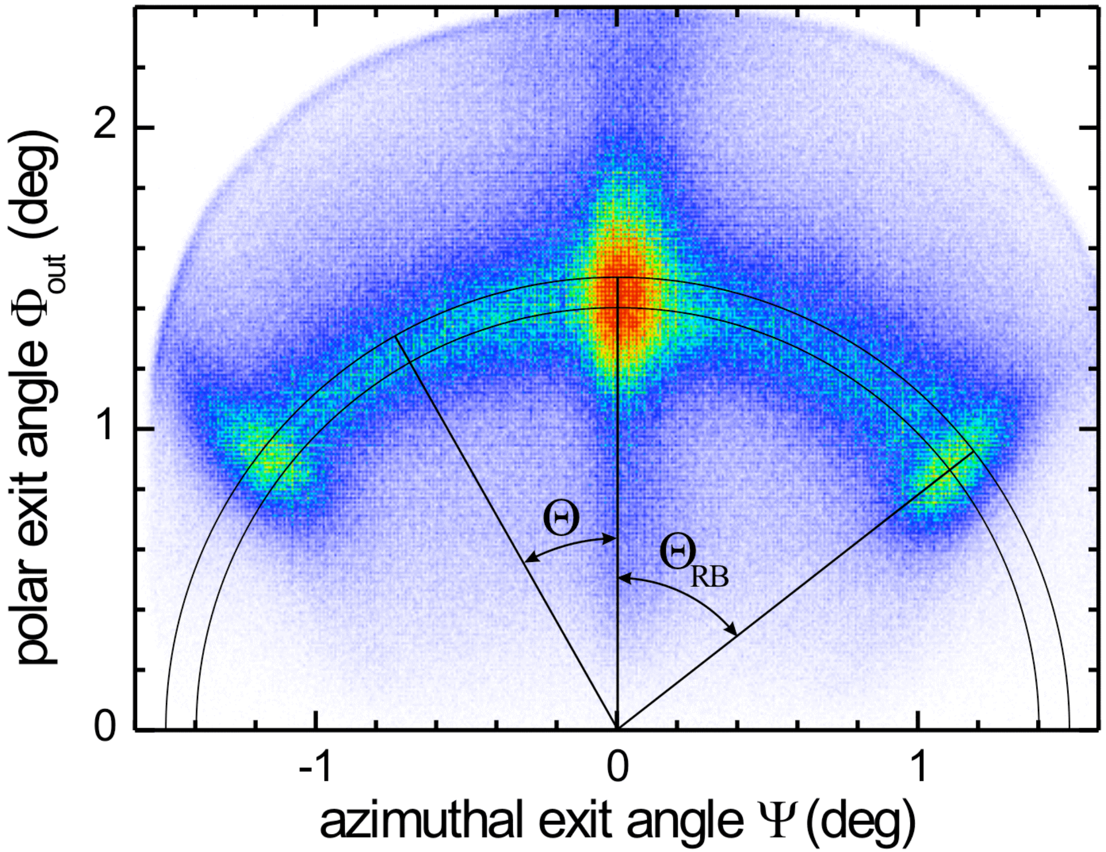
$E_z = E_0 \sin^2\phi_{in}$

ϕ_{in} = 0,5° - 2,5°

E_0 = 1keV - 100keV

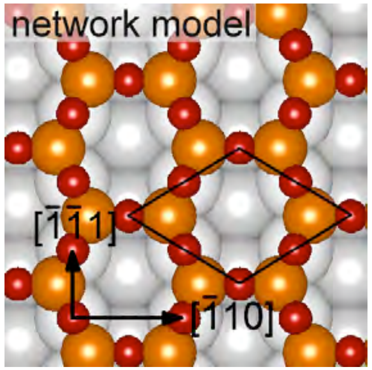
E_z = 1eV - 100eVD

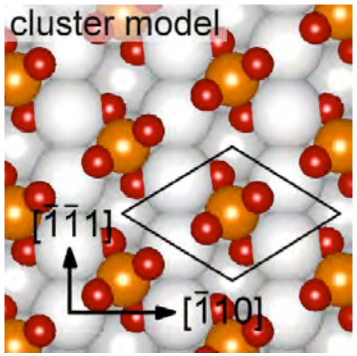
(classical) rainbow scattering from Mo(112)/SiO under axial surface channeling conditions

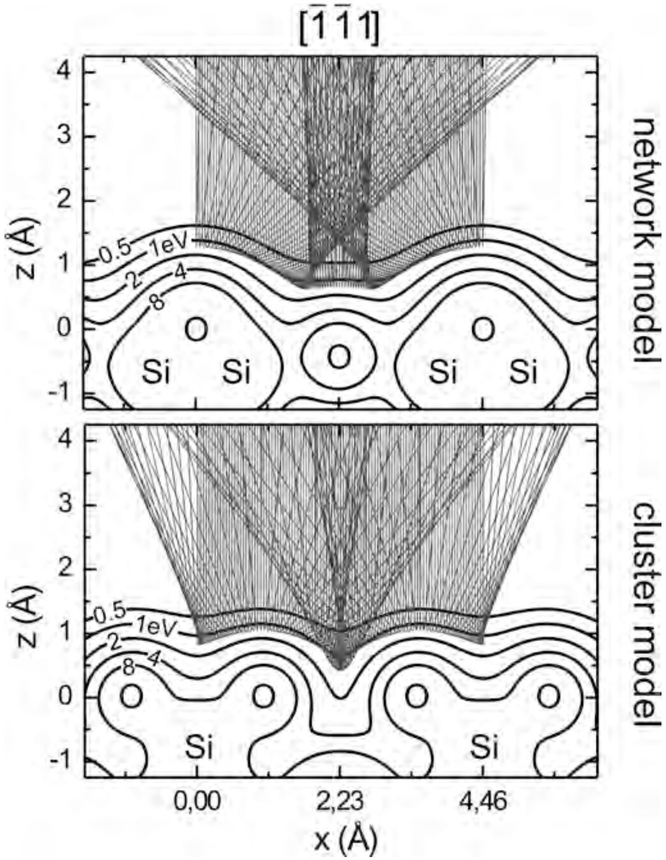


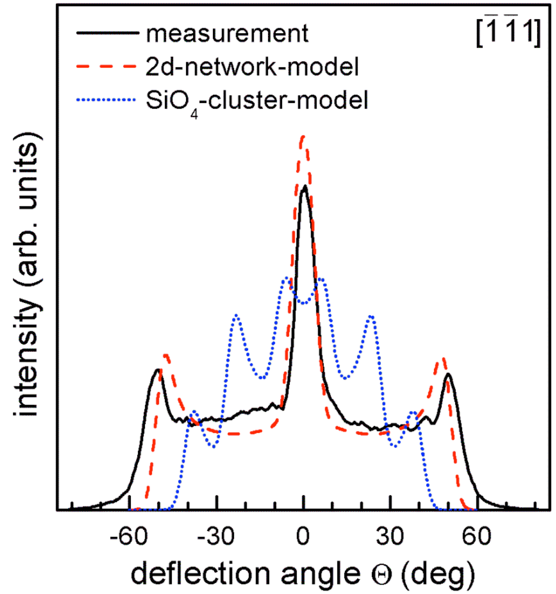
trajectories and angular distributions

2 keV He° → Mo(112)/SiO_2 Φ_{in} = 1.5°



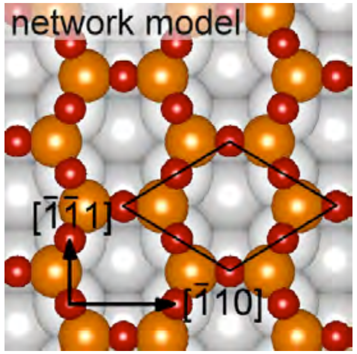


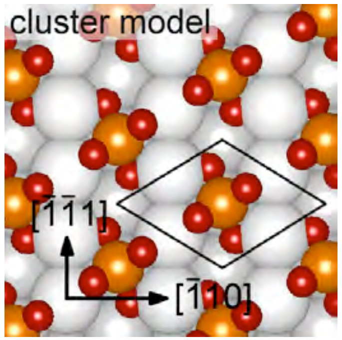


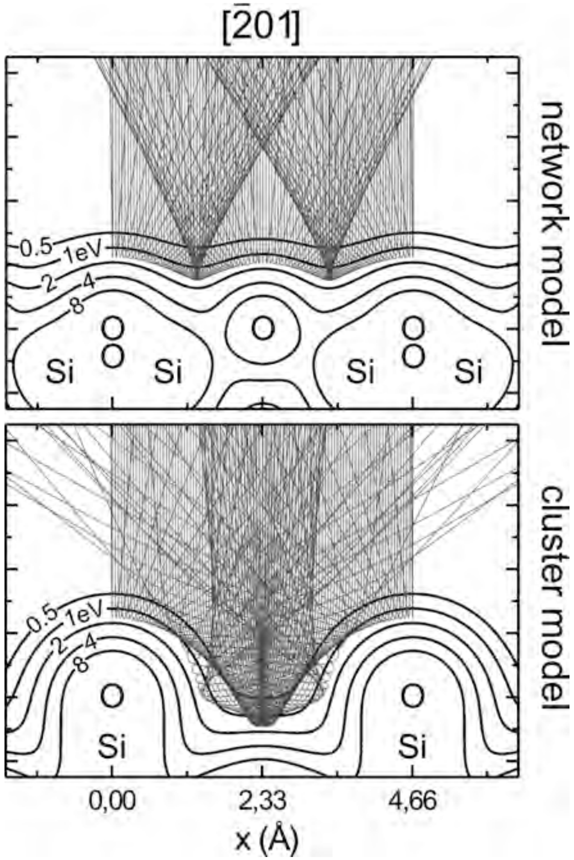


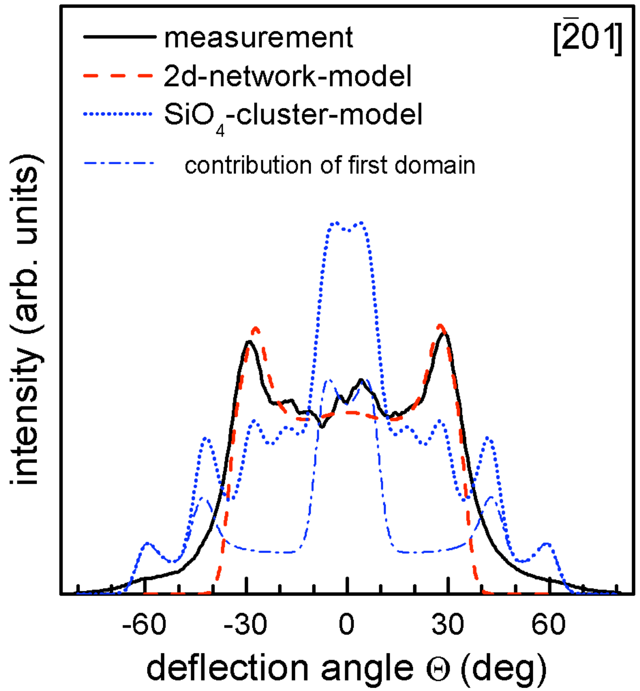
trajectories and angular distributions

2 keV $He^{o} \rightarrow Mo(112)/SiO_2 \quad \Phi_{in} = 1.5°$









(classical) rainbow scattering from Mo(112)/SiO under axial surface channeling conditions

Surface Science 603 (2009) L109–L112

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Surface Science Letters

Structure of monolayer silica on Mo(1 1 2) investigated by rainbow scattering under axial surface channeling

J. Seifert, H. Winter*

Institut für Physik der Humboldt-Universität zu Berlin, Newtonstr. 15, D-12489 Berlin-Adlershof, Germany

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Keywords:
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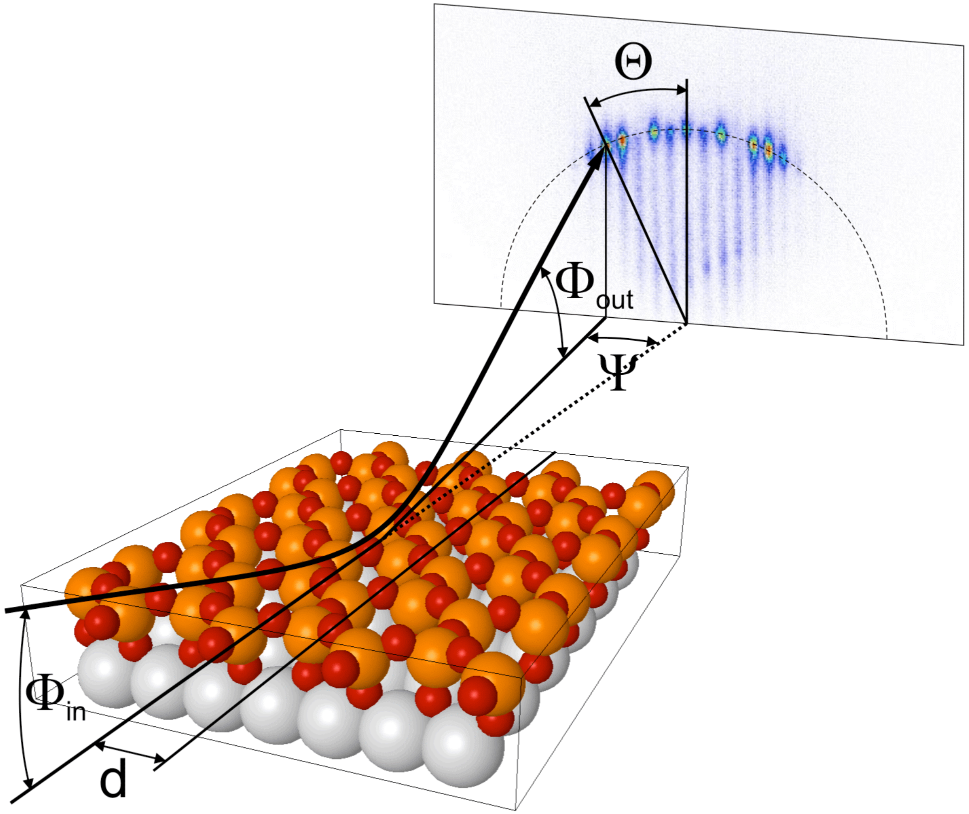
Oxide surface
Ion scattering
Surface structure

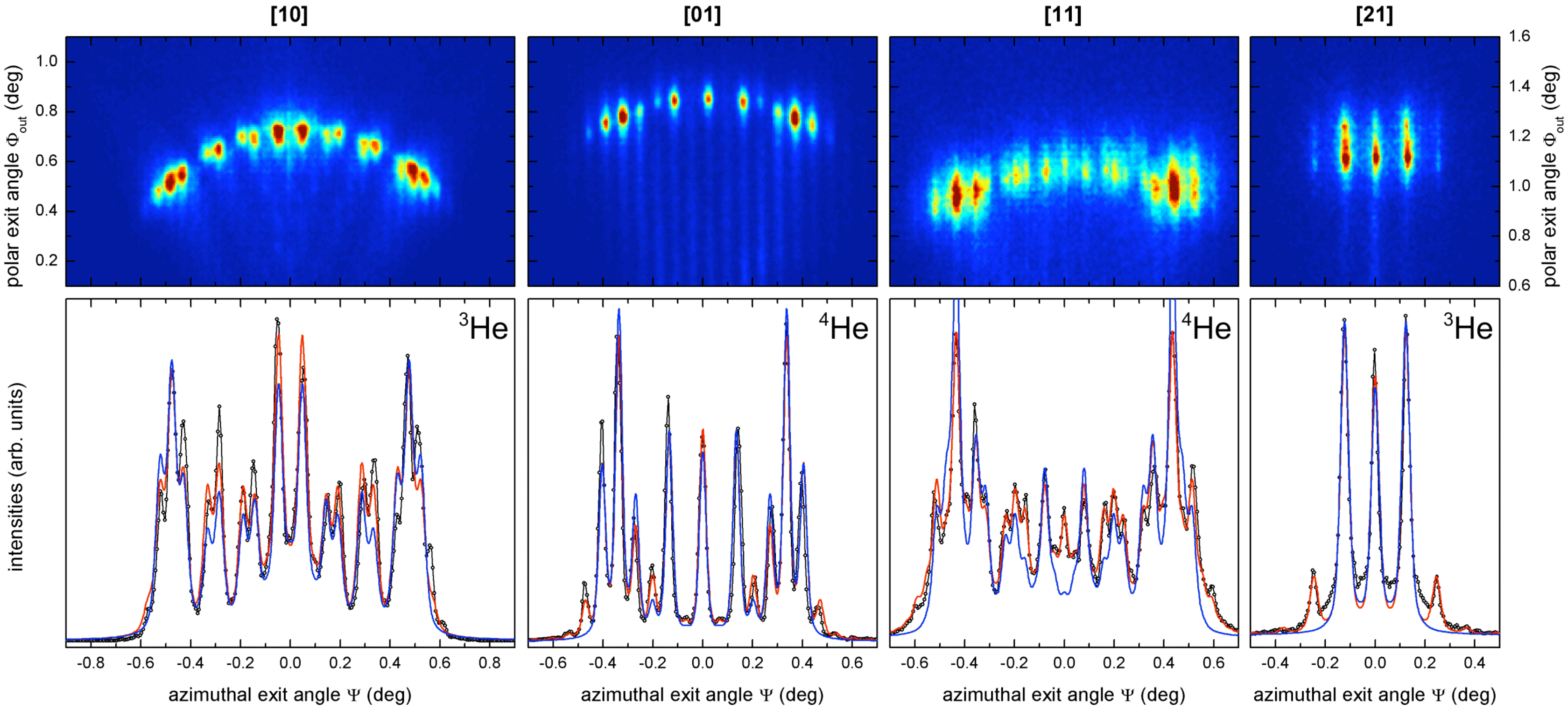
ABSTRACT

The structure of a monolayer crystalline silica film grown on a Mo(1 1 2) substrate is investigated via grazing scattering of fast atoms. For scattering along low indexed directions in the surface plane ("axial surface channeling") the corrugation of the interaction potential leads to an azimuthal out-of-plane scattering with an intensity enhancement for the maximum deflection angle, the so called "rainbow". From the comparison of the experimental angular distributions for scattered projectiles with classical trajectory simulations we obtain information on the arrangement of atoms in the topmost surface layer. Our work provides evidence for the structural model of a two-dimensional network for the silica film.

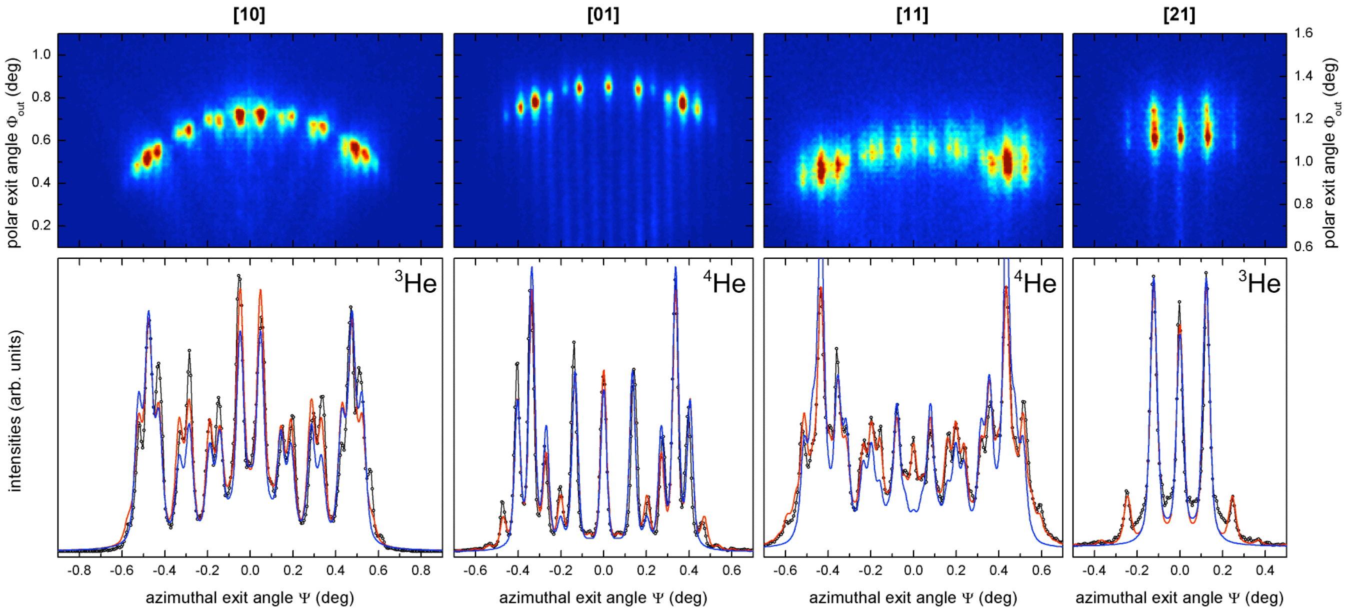
Fast Atom Diffraction (FAD) during scattering from Mo(112)/SiO under axial surface channeling conditions



Fast Atom Diffraction (FAD) during scattering from Mo(112)/SiO under axial surface channeling conditions



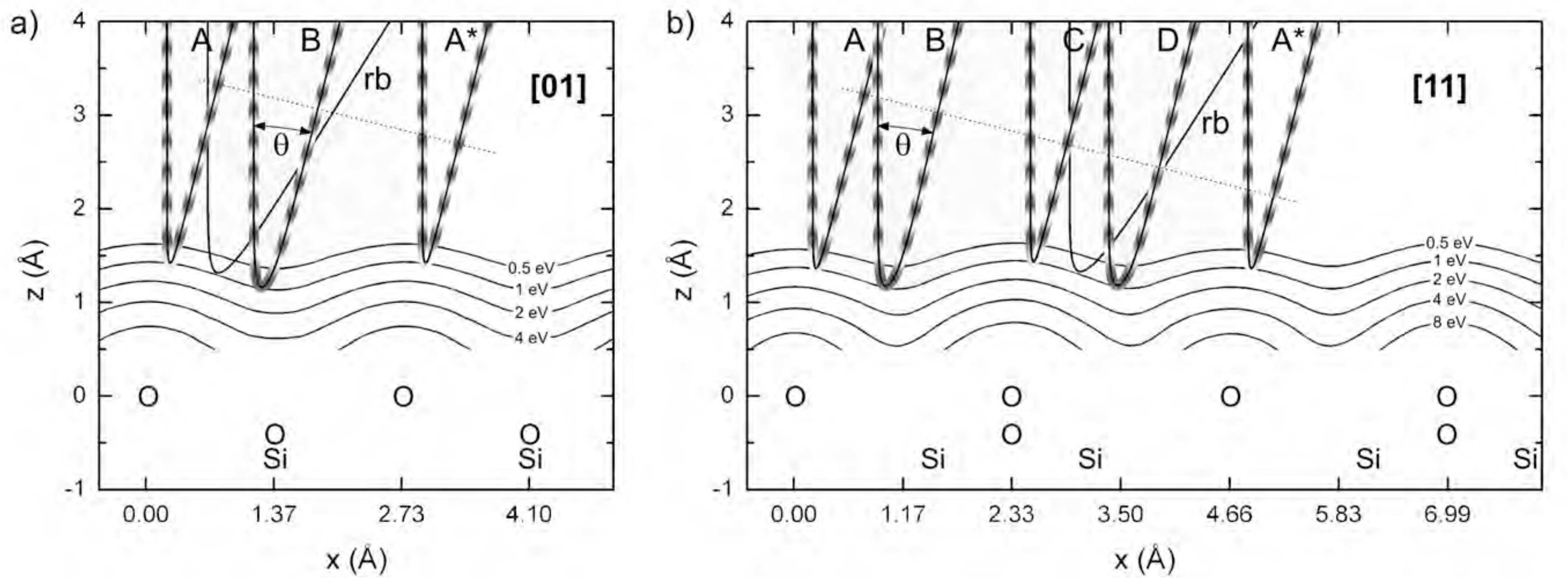
Mo(112)/SiO_2: splittings of Bragg peaks



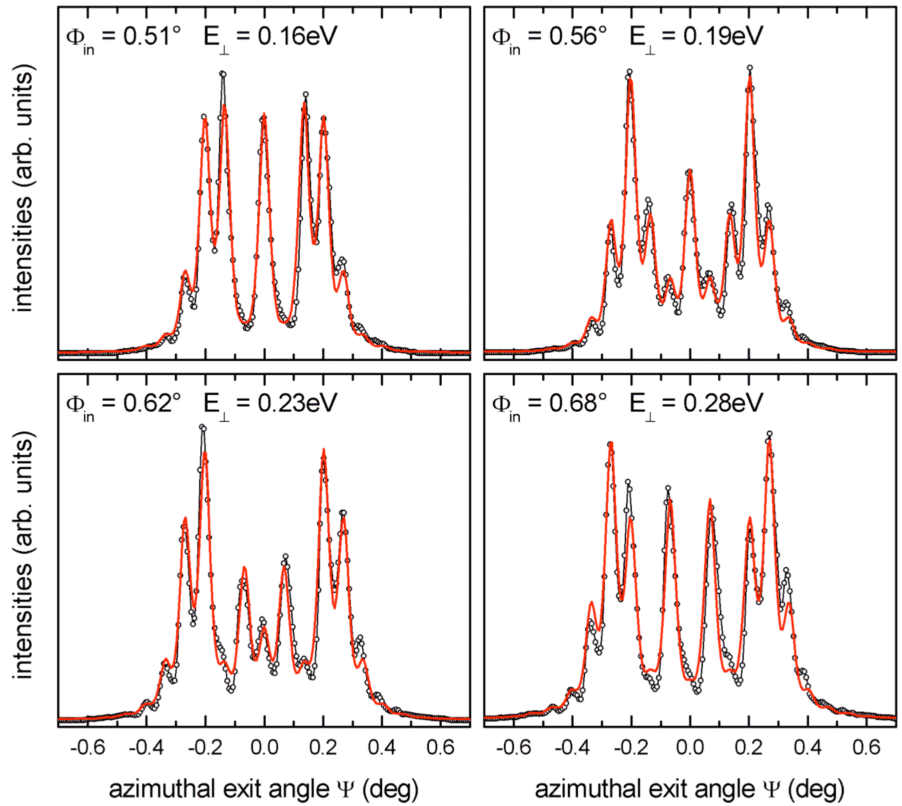
^{3}He, ^{4}He

d_{Mo} = 4.46 Å	d_{Mo} = 2.73 Å	d_{Mo} = 2.33 Å	d_{Mo} = 1.73 Å
d_{SiO} = 4.46 Å	d_{SiO} = 2.73 Å	d_{SiO} = 4.66 Å	d_{SiO} = 1.73 Å
(4.54 ± 0.08) Å	(2.74 ± 0.08) Å	(4.82 ± 0.05) Å	(1.76 ± 0.06) Å

Fast Atom Diffraction (FAD) during scattering from Mo(112)/SiO under axial surface channeling conditions



Fast Atom Diffraction (FAD) during scattering from Mo(112)/SiO under axial surface channeling conditions



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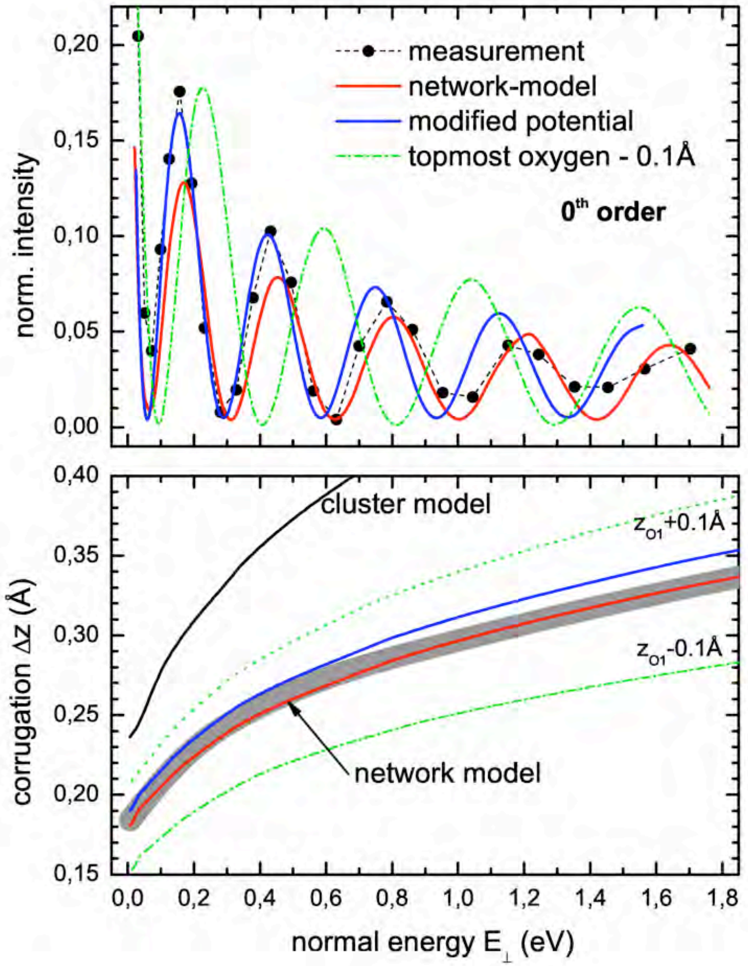
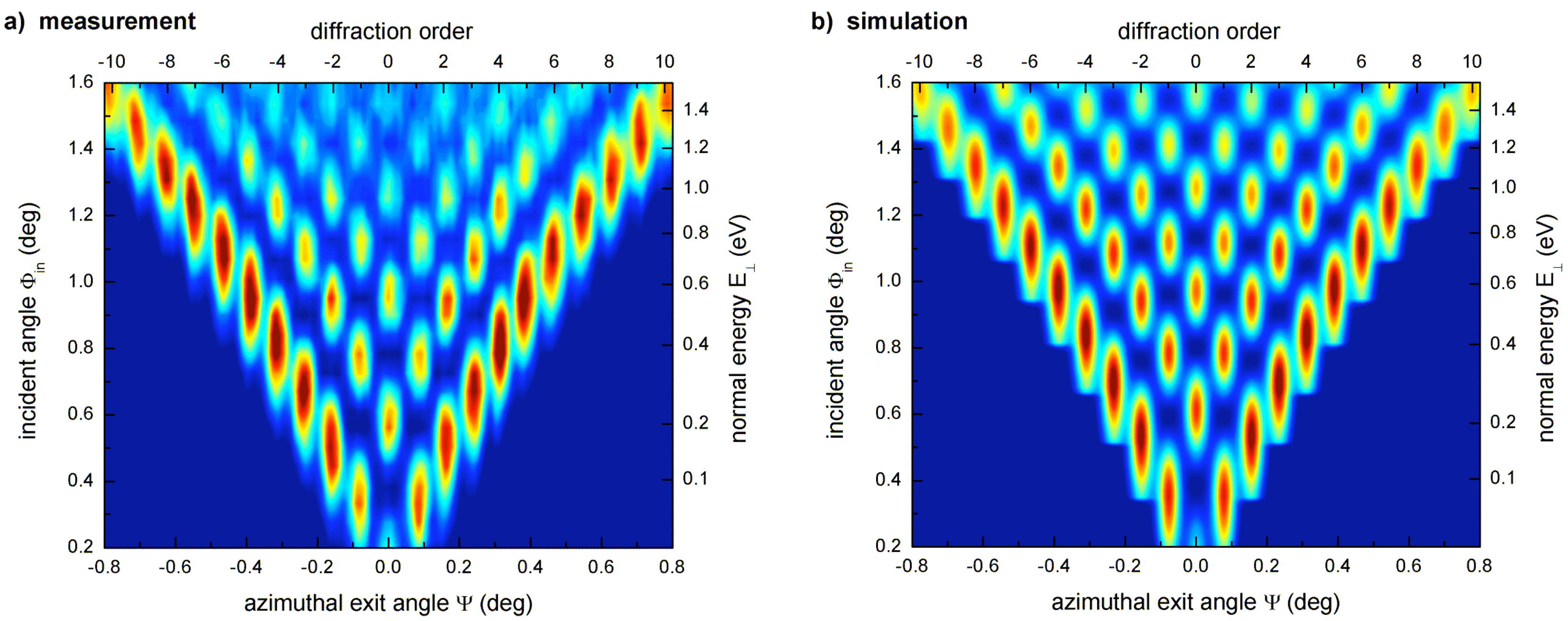


interaction potential from DFT calculations

(Wlodarczyk, Sierka)

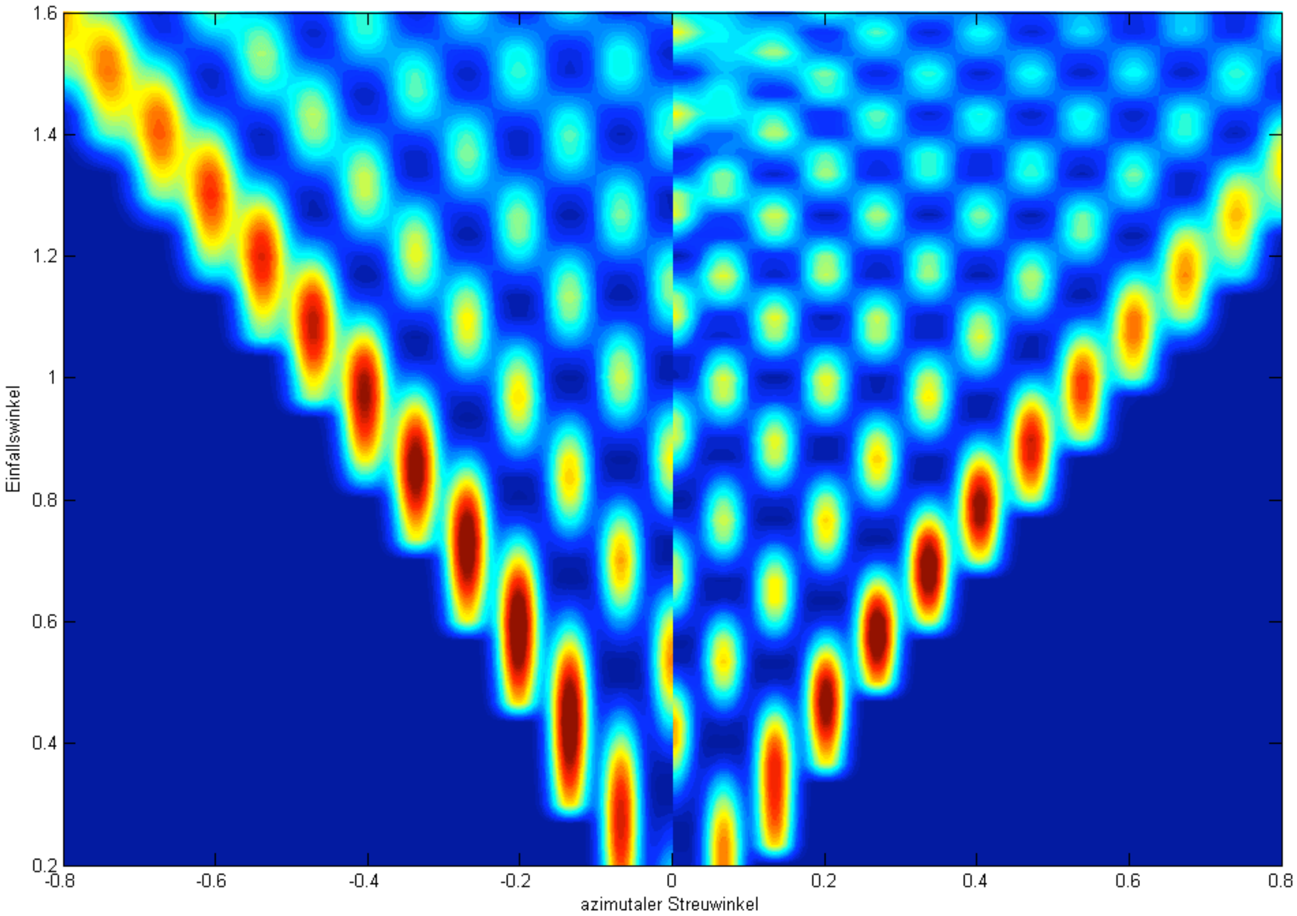
Fast Atom Diffraction (FAD) during scattering from Mo(112)/SiO under axial surface channeling conditions



interaction potential from DFT calculations

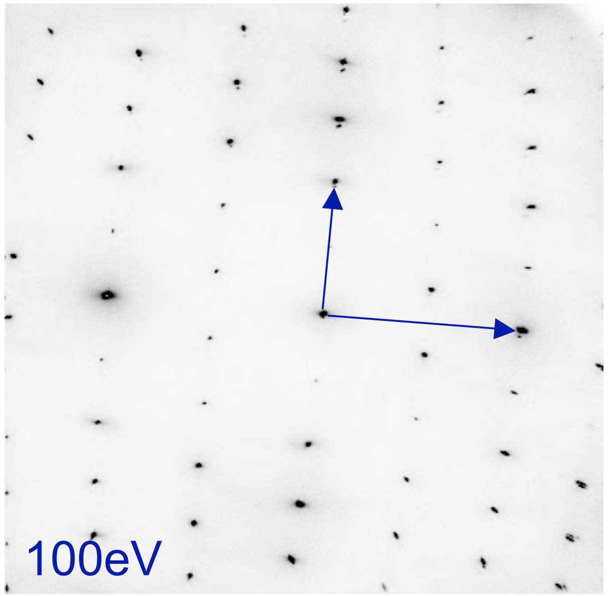
(Wlodarczyk, Sierka)

Structure of Mo(112)/SiO: „2D network vs. SiO_4 units"

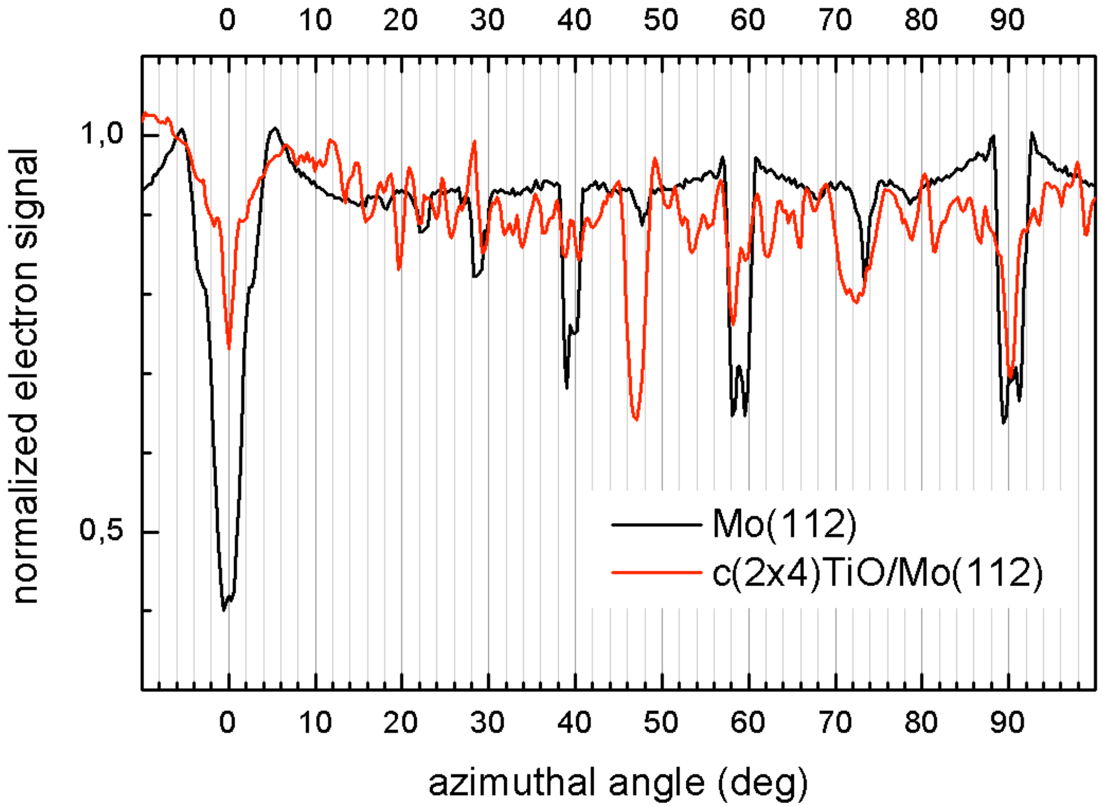


c(2x4)TiO/Mo(112)

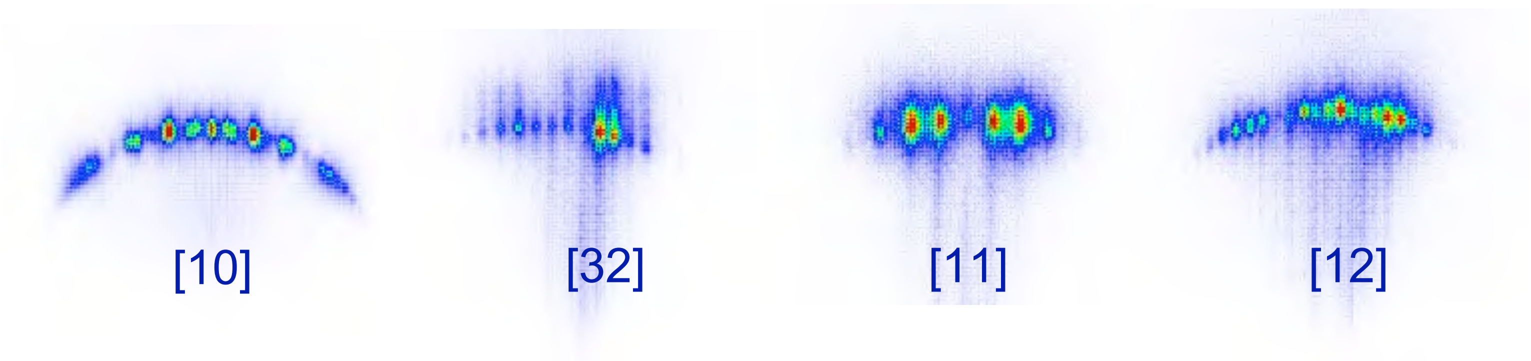
- growth of 2ML titanium at 1050K in $2*10^{-7}$mbar oxygen atmosphere on oxygen covered Mo(112)
- annealing for 5min at 1300K

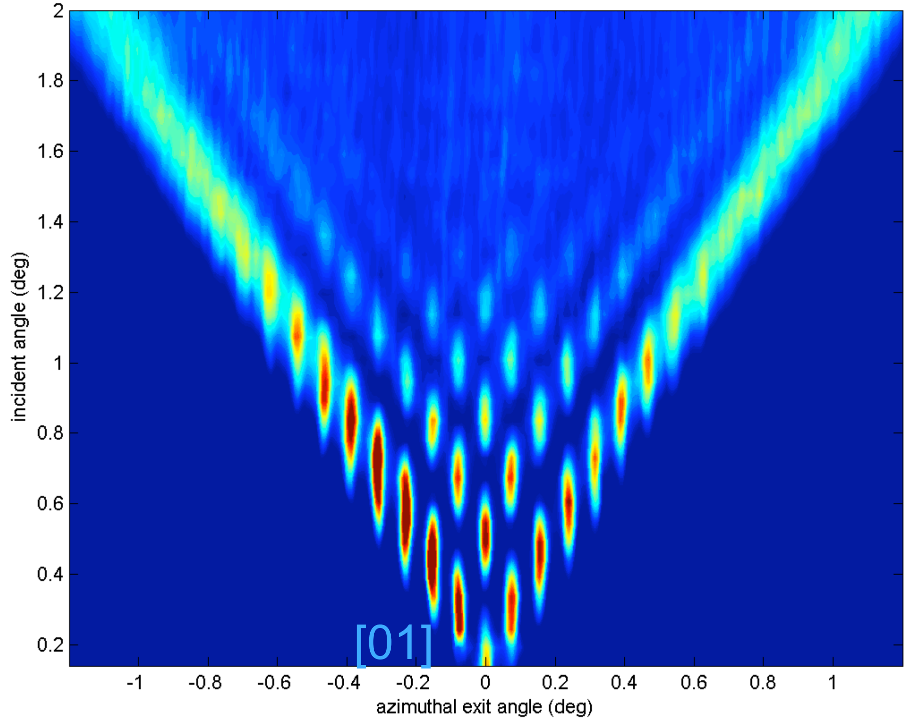


ion beam triangulation (IBT) with 25 keV H atoms



fast atom diffraction (FAD) with 1.5 keV He atoms





Publikationen TP C11 – Unterprojekt 1

- H. Winter, J. Seifert, D. Blauth, M. Busch, A. Schüller, S. Wethekam
  Structure of ultrathin oxide layers on metal surfaces from grazing scattering of fast atoms
  *Applied Surface Science **256** (2009) 365*

- J. Seifert, D. Blauth, H. Winter
  Evidence for 2D-network structure for monolayer silica film on Mo(112)
  *Physical Review Letters **103** (2009) 017601*

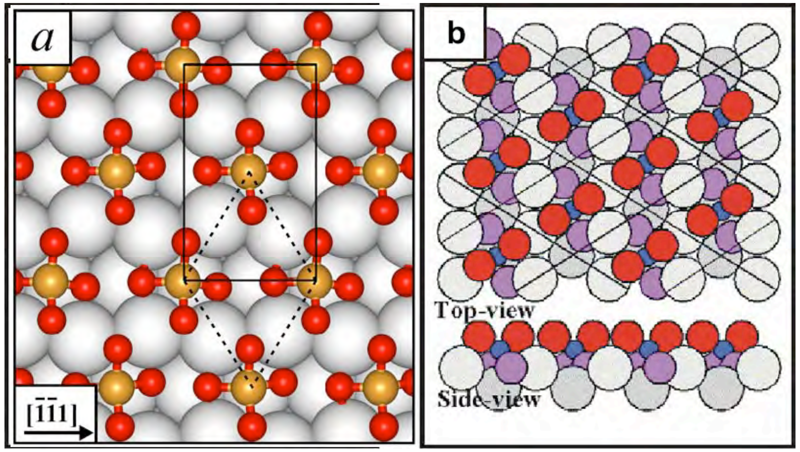
- J. Seifert, H. Winter
  Structure of monolayer silica film on Mo(112) investigated by rainbow scattering under axial surface channeling
  *Surface Science Letters **603** (2009)* L109

- J. Seifert, M. Busch, A. Schüller, D. Blauth, S. Wethekam, H. Winter
  Structure of ultrathin silica films on Mo(112) studies via classical and quantum mechanical rainbow scattering of fast atoms
  Surface and interface analysis (2010) submitted

- J. Seifert, A. Schüller, H. Winter, R. Wlodarczyk, M. Sierka, J. Sauer
  Fast atom diffraction during scattering from a monolayer silica film on Mo(112)
  Physical Review B (2010) to be submitted

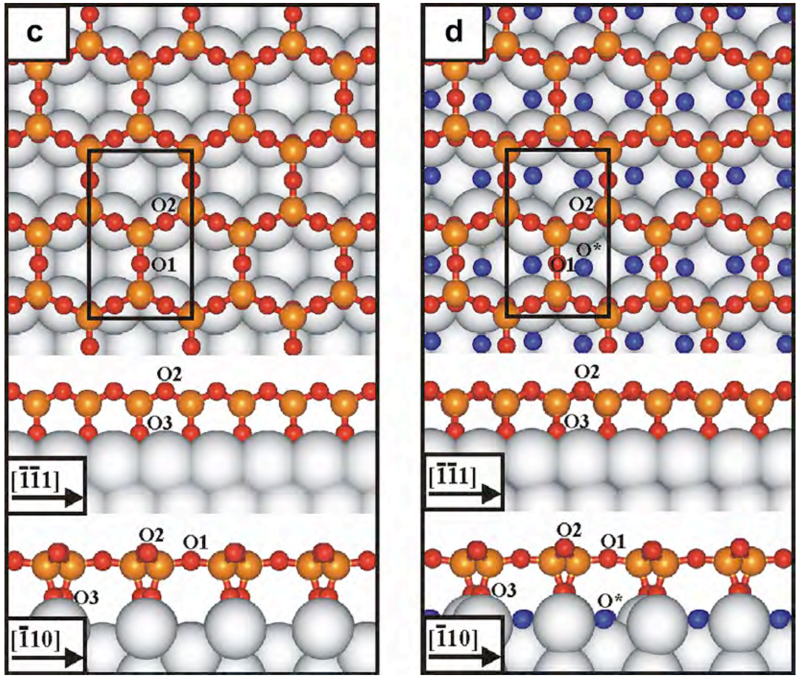
structure of Mo(112)/SiO_2: „cluster vs. 2D-network“

Goodman et al.
„[SiO_4] cluster model“



M. Chen, A.K. Santra and D.W. Goodman, Phys. Rev. B 69 (2004) 155404
M. Chen and D.W. Goodman, Surf. Sci. 600 (2006) L255

Sierka et al.
„2D-network model“



T.K. Todorova et al., Phys. Rev. B 73 (2006) 165414
J. Weissenrieder et al., Phys. Rev. Lett. 95 (2005) 076103
M. Sierka et al., Chem. Phys. Lett. 424 (2006) 115

Structure of Mo(112)/SiO_2: „cluster vs. 2D network“

Available online at www.sciencedirect.com
ScienceDirect
Surface Science 601 (2007) 588–590
SURFACE SCIENCE
www.elsevier.com/locate/susc

Discussion

Comment on "The structure of monolayer SiO_2 on Mo(112): A 2-D [Si–O–Si] network or isolated [SiO_4] units?"

Livia Giordano [a], Davide Ricci [a], Gianfranco Pacchioni [a,*], Piero Ugliengo [b]

[a] Dipartimento di Scienza dei Materiali, Università di Milano-Bicocca, Via R. Cozzi, 53, 20125, Milano, Italy
[b] Dipartimento di Chimica IFM, Università di Torino and NIS, Nanostructured Interfaces and Surfaces Centre of Excellence Via P. Giuria 7, I-10125 Torino, Italy

Received 11 October 2006; accepted for publication 14 November 2006
Available online 4 December 2006

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Surface Science 601 (2007) 591–593
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Mingshu Chen, D. Wayne Goodman *

Department of Chemistry, Texas A&M University, College Station, TX 77843, United States

Received 11 November 2006; accepted for publication 14 November 2006
Available online 5 December 2006

IOP PUBLISHING JOURNAL OF PHYSICS: CONDENSED MATTER
J. Phys.: Condens. Matter 20 (2008) 264013 (11pp) doi:10.1088/0953-8984/20/26/264013

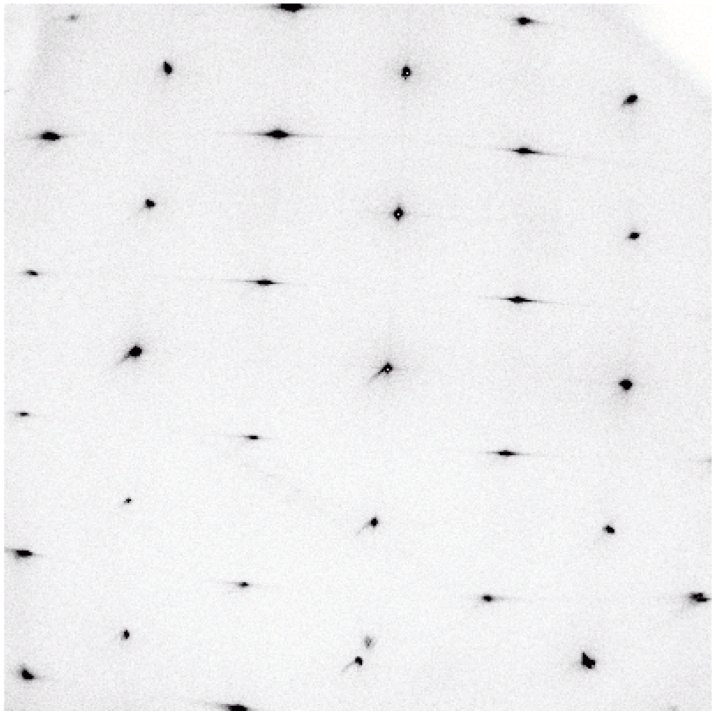
Ultrathin, ordered oxide films on metal surfaces

M S Chen[1,2] and D W Goodman[1]

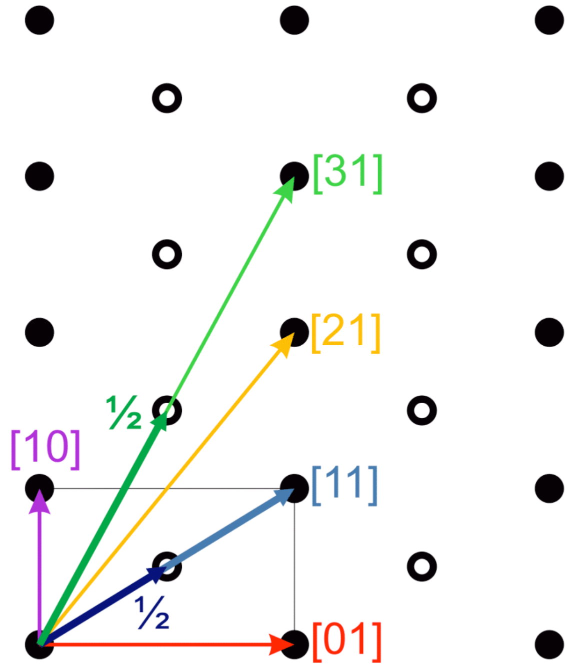
are entirely inconsistent with the 2D network model. Therefore the detailed structure of monolayer SiO_2/Mo(112) is still an issue yet to be resolved.

SiO on Mo(112) – well defined ML-film

a)



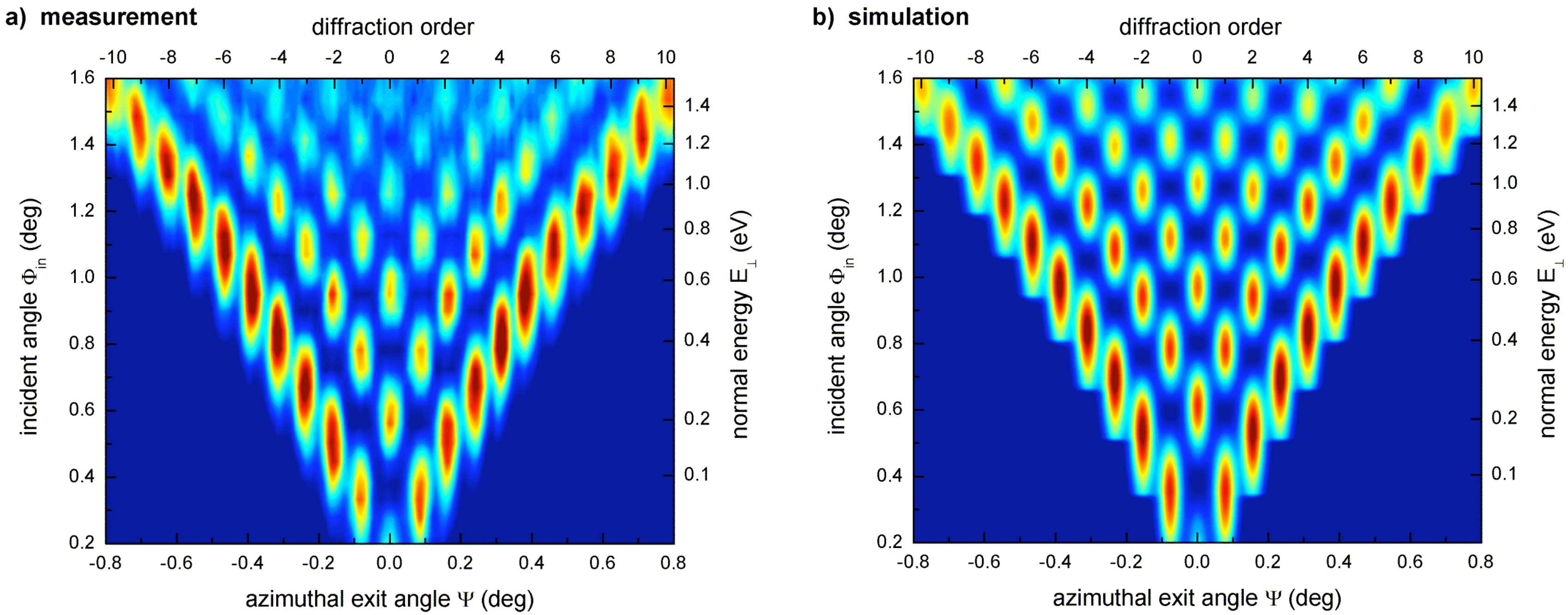
b)



LEED shows c(2x2)

Mo(112)/SiO_2: „diffraction charts“

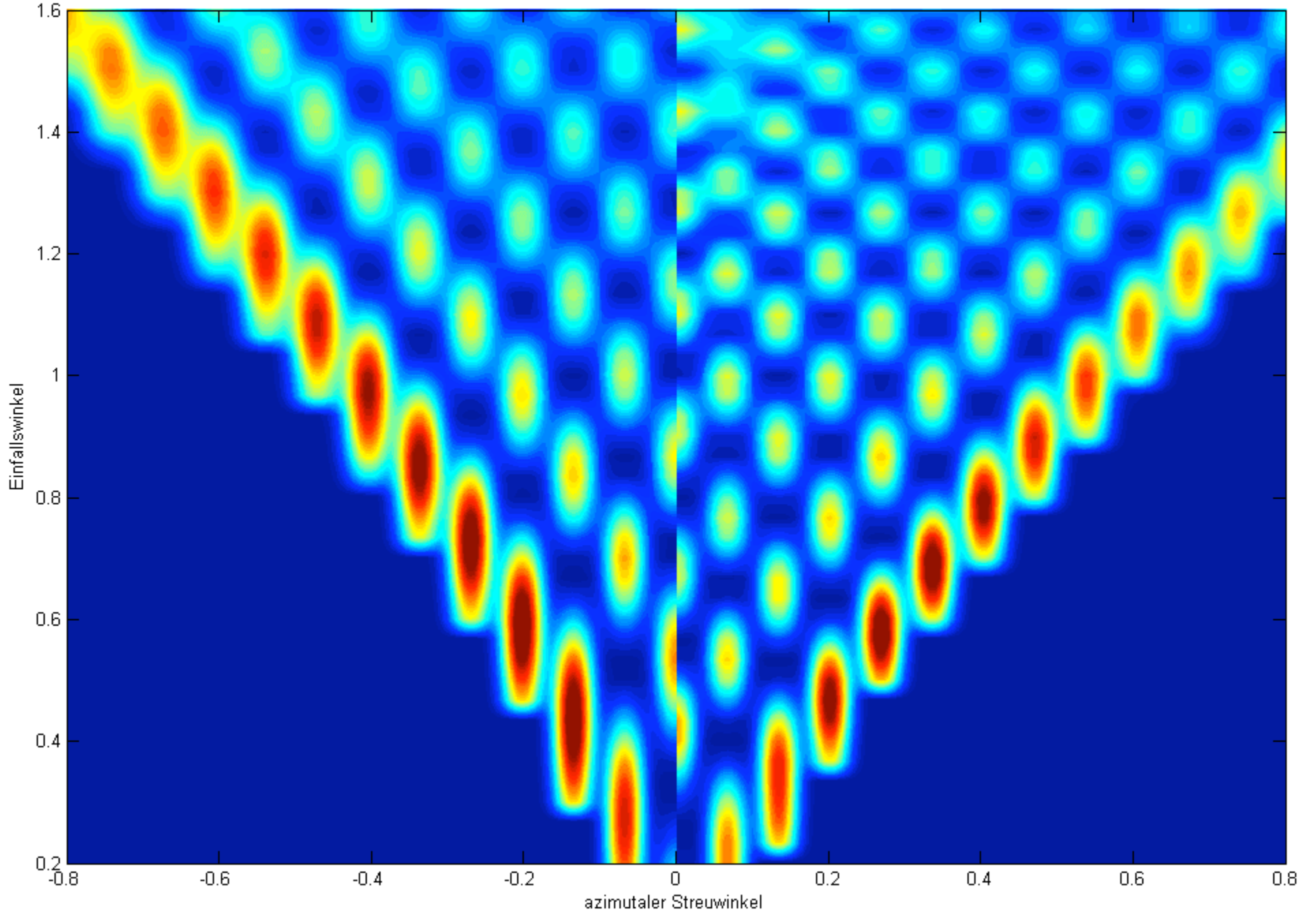
experiment | 2D-network model



DFT-calculations: Sierka et al. (2009)

Mo(112)/SiO_2: „diffraction charts“

2D-network model | cluster model



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[b] Dipartimento di Chimica IFM, Università di Torino and NIS, Nanostructured Interfaces and Surfaces Centre of Excellence, Via P. Giuria 7, I-10125 Torino, Italy

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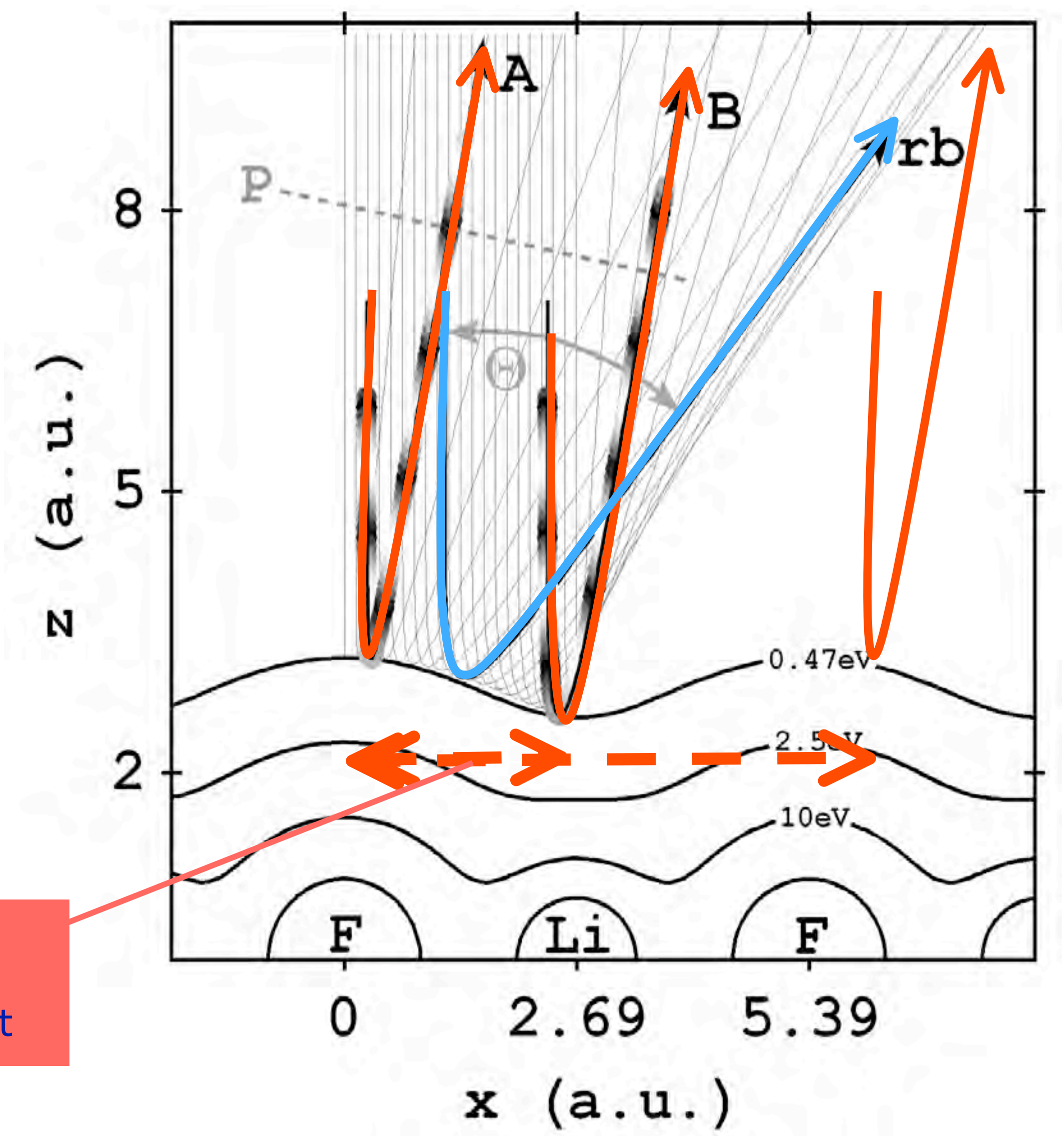
Ultrathin, ordered oxide films on metal surfaces

M S Chen[1,2] and D W Goodman[1]

→ are entirely inconsistent with the 2D network model. Therefore the detailed structure of monolayer SiO_2/Mo(112) is still an issue yet to be resolved.

rainbow scattering and diffraction (corrugation)



can be much smaller than lattice constant

„supernumerary rainbows“

Multiple supernumerary bows. *The supernumeraries are the closely spaced greenish purple arcs on the inner (blue) side of the primary bow. Captured by Mark Nankman at Oltjärn in Sweden after two heavy showers on a late afternoon in August '99.*

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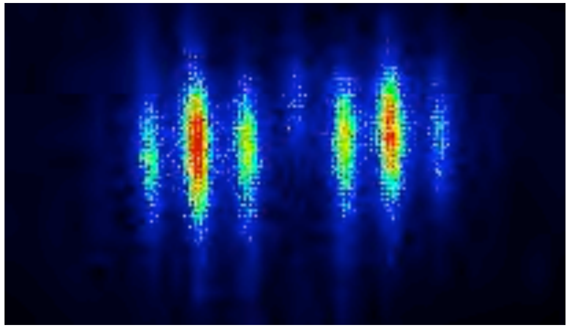
insulators

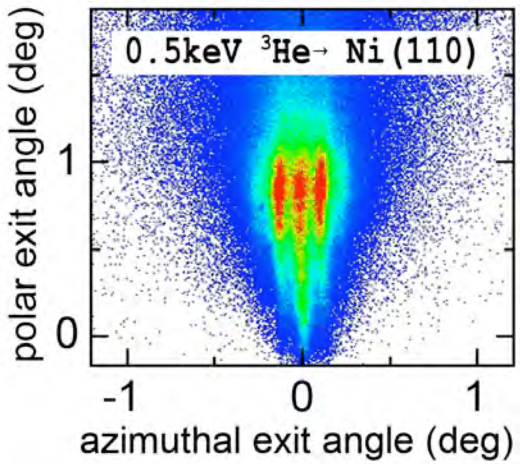
LiF(100)
NaCl(100) → Rousseau

MgO(100)



metals

Ni(110)

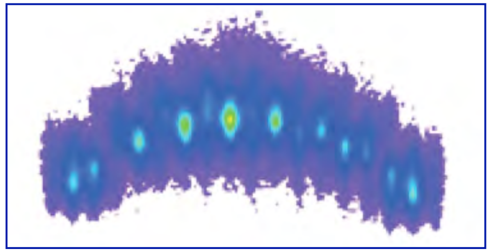


semi conductors

→ Rousseau, Khemliche, Roncin

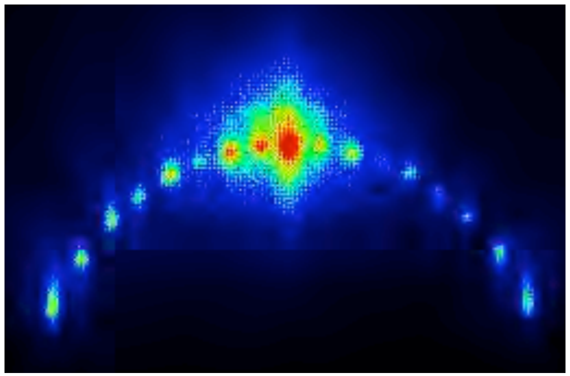
GaAs(001)

ZnSe(001)



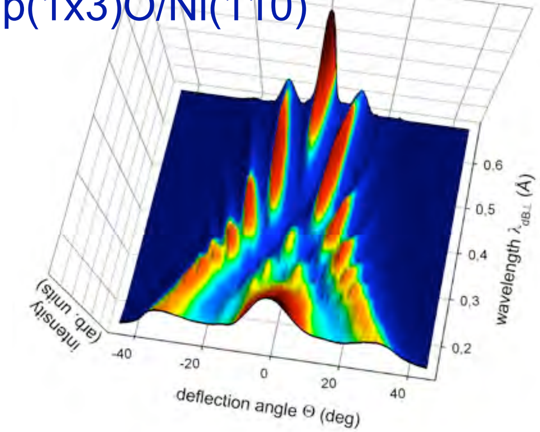
superstructures

c(2x2)O/Fe(110)
c(12x16)S/Fe(110)
c(1x3)S/Fe(110)



reconstruction

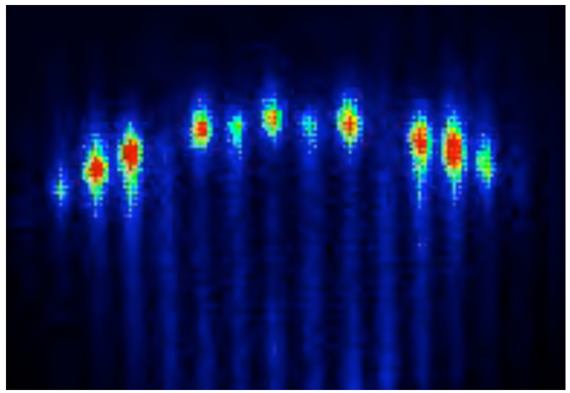
p(1x2)O/Ni(110)
p(1x2)O/Mo(112) → J. Seifert
p(1x3)O/Ni(110)



thin films

→ J. Seifert

SiO/Mo(112)



Sfb 546 "Übergangsmetalloxid-Aggregate"

Stellung innerhalb des Sfb546

Teilprojekt B1 **Teilprojekt C5**

structure of Mo(112) / O and Mo(112) / SiO

Teilprojekt C1

titania films on metal substrates

coadsorption V –Ti (complementary methods)

Teilprojekt C4

bulk vanadia crystals

Teilprojekt C8

TiO_2 surfaces (complementary methods)

low energy ion scattering