Site-specific electron diffraction resolved via nuclear recoil

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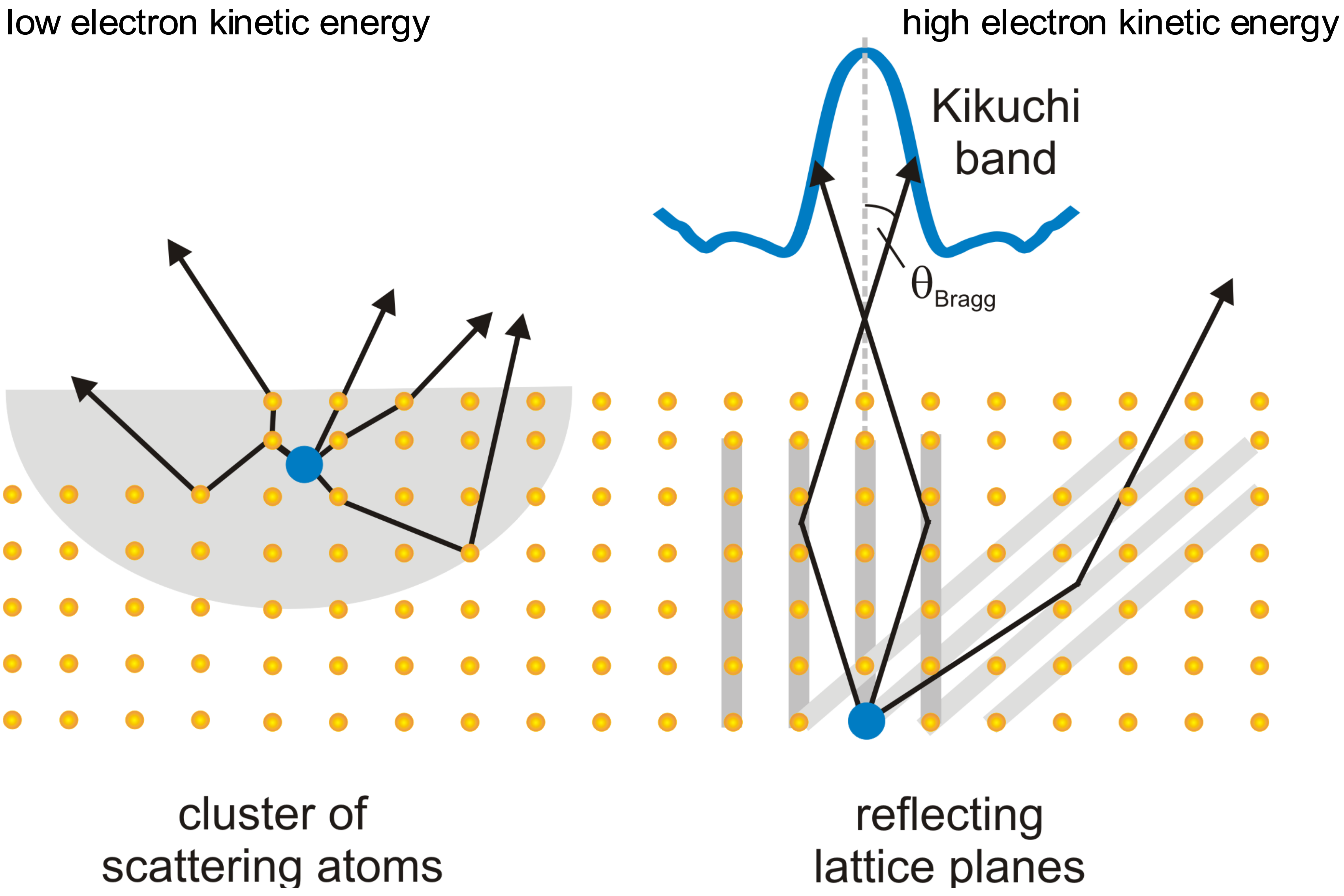
Canberra, Australia

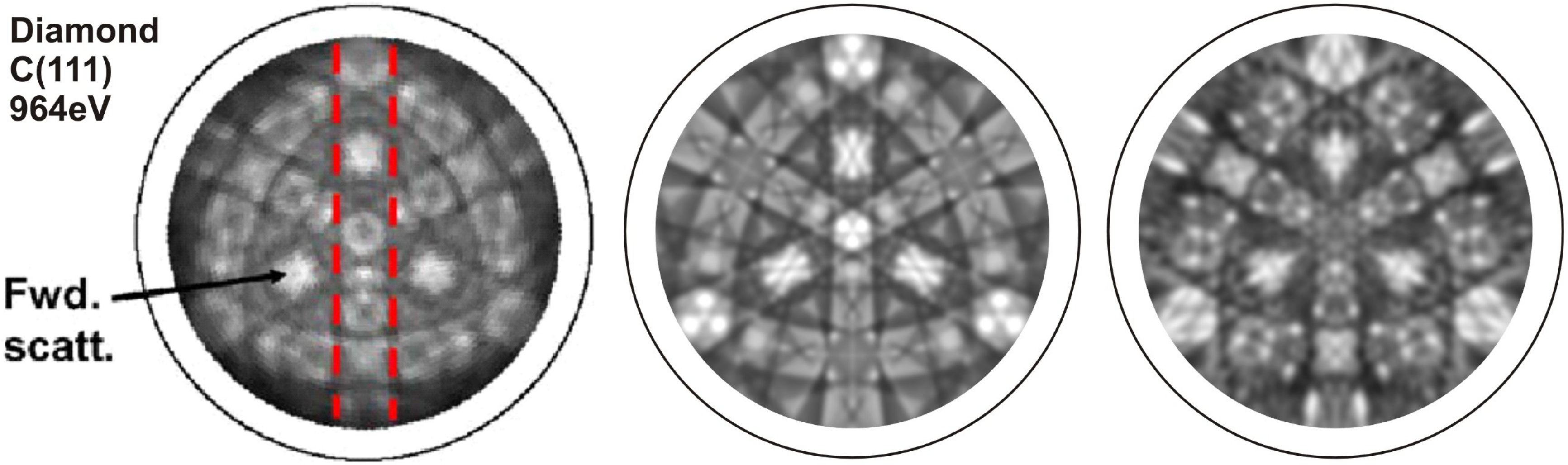
MAX-PLANCK-GESELLSCHAFT

NATURAM PRIMUM COGNOSCERE RERUM

Diffraction of electrons from localized sources



X-ray Photoelectron Diffraction: Diamond



(a) experiment

(b) dynamical simulation

(c) multiple scattering simulation (EDAC)

~10min

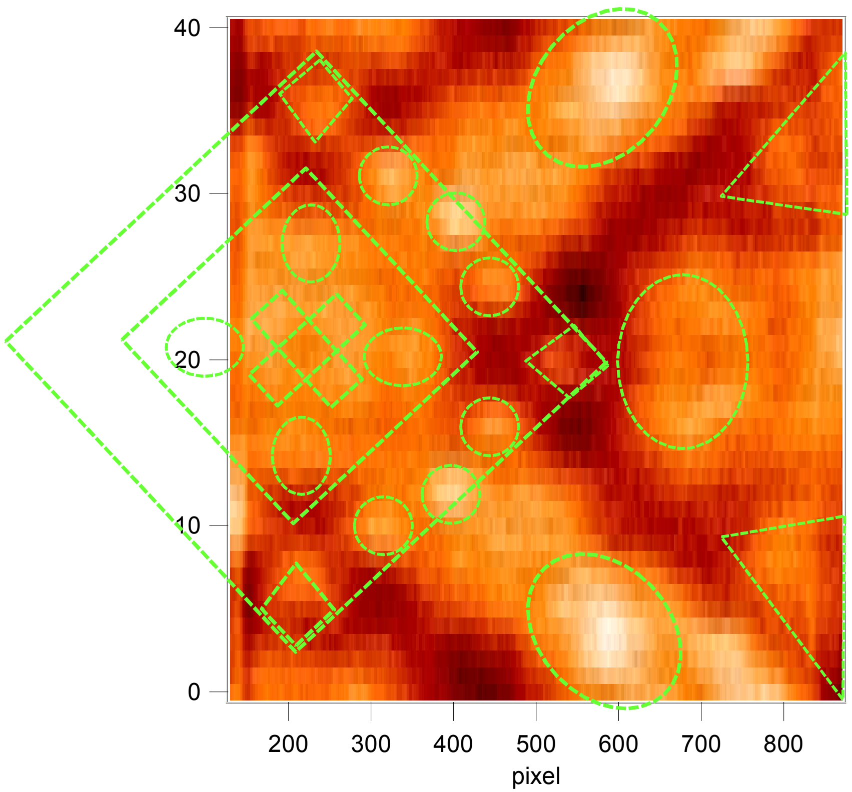
~12d

A. Winkelmann, C.S. Fadley, F. J. Garcia de Abajo
New Journal of Physics **10** (2008) 113002

X-ray Photoelectron Diffraction: $LaSrMnO_3$

Experiment

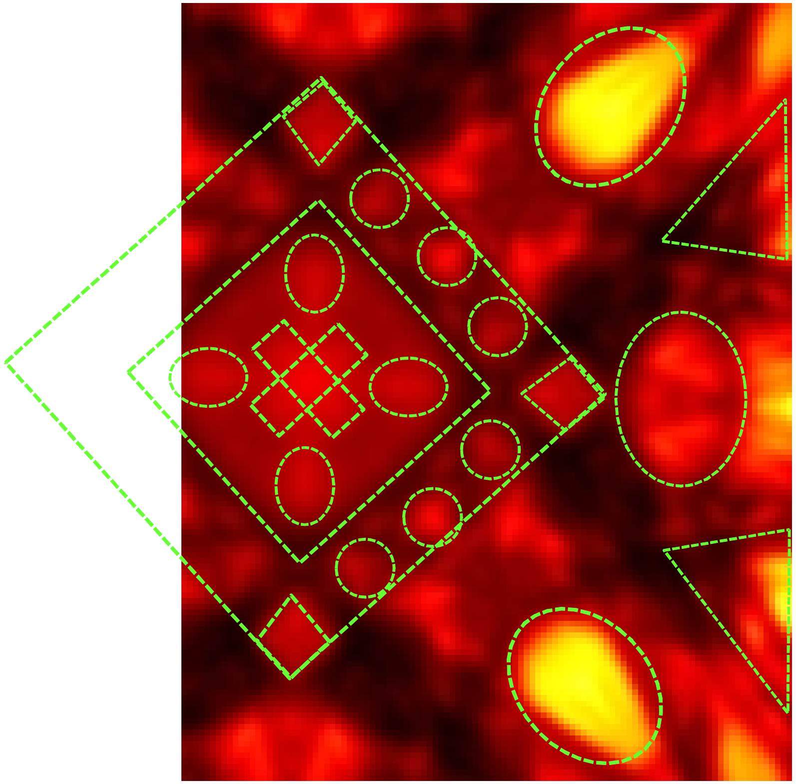
STO/LSMO Multilayer
Mn 3p emission
E=793eV
hv = 833.2 eV



Experiment: Fadley Group

XPD Theory

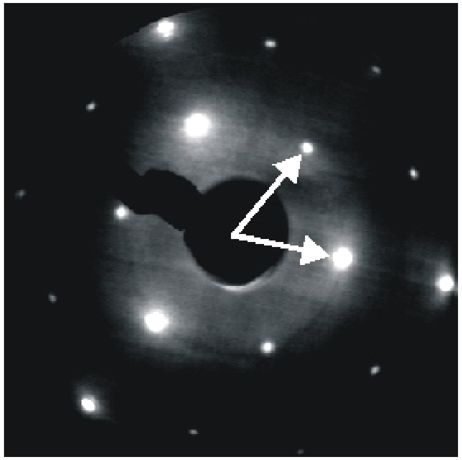
LSMO 5nm „bulk“
Kikuchi Mn emission
E=793eV
hv = 833.2 eV



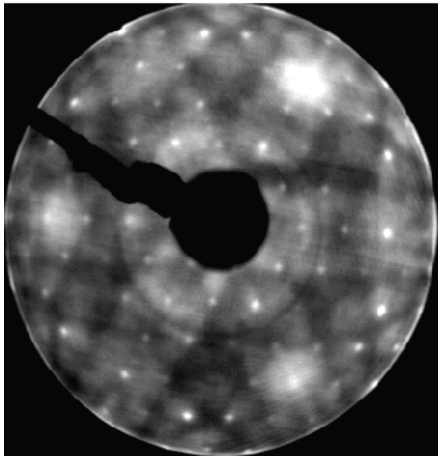
Theory: A. Winkelmann

Diffraction of backscattered and back-reflected electrons

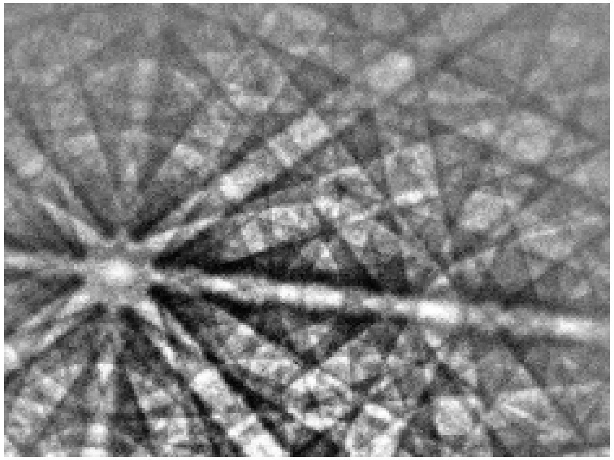
6H SiC 170eV



6H SiC 1kV



Mo bcc 25kV

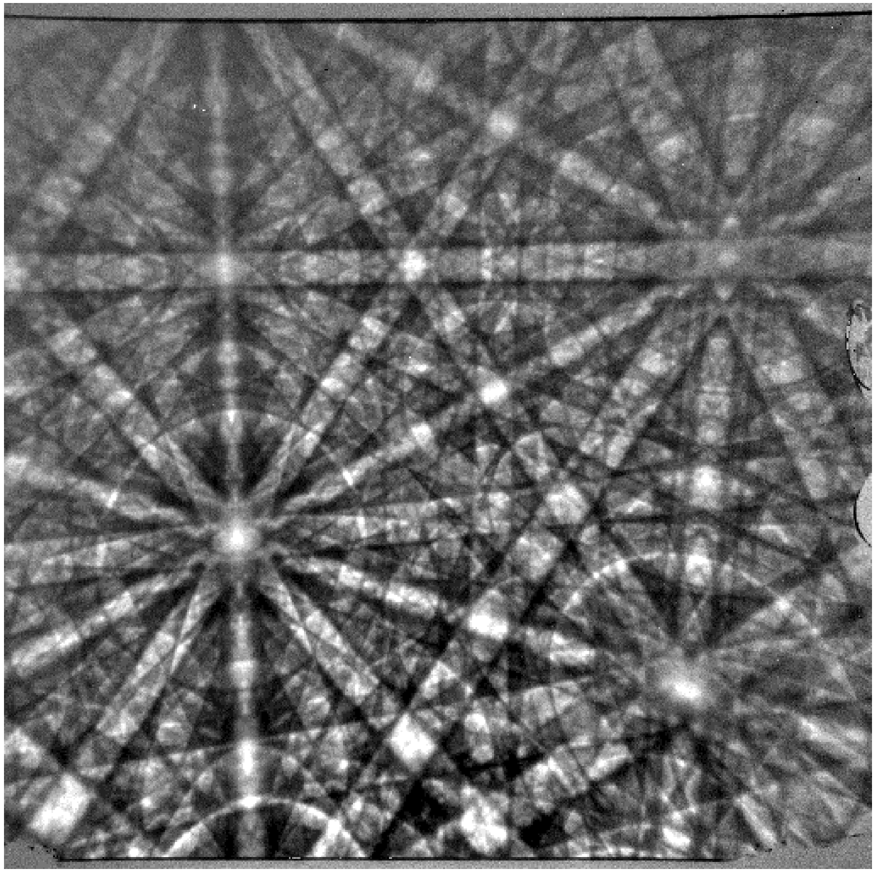


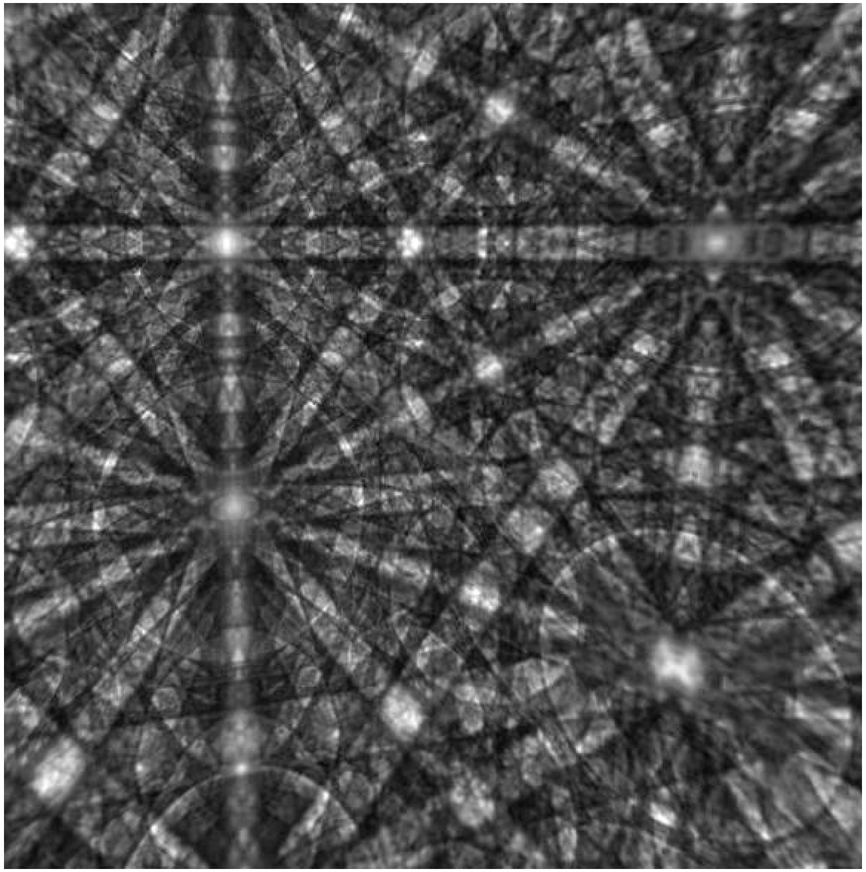
low energy

high energy

LEED

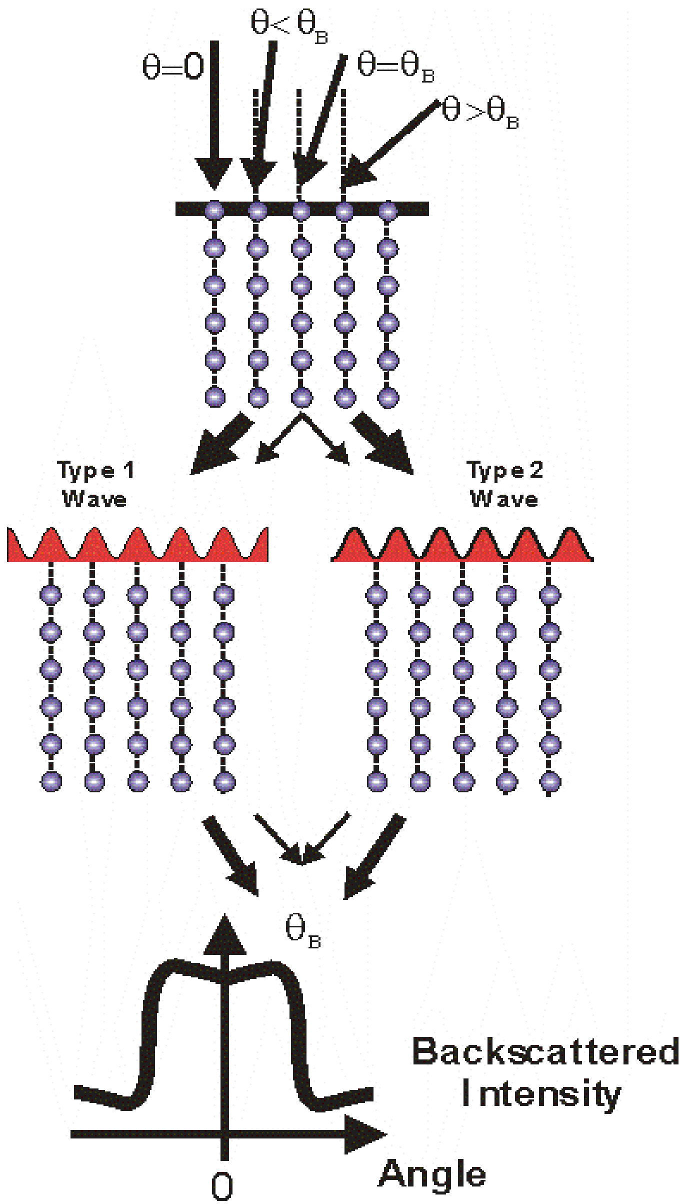
diffraction in the
scanning electron microscope



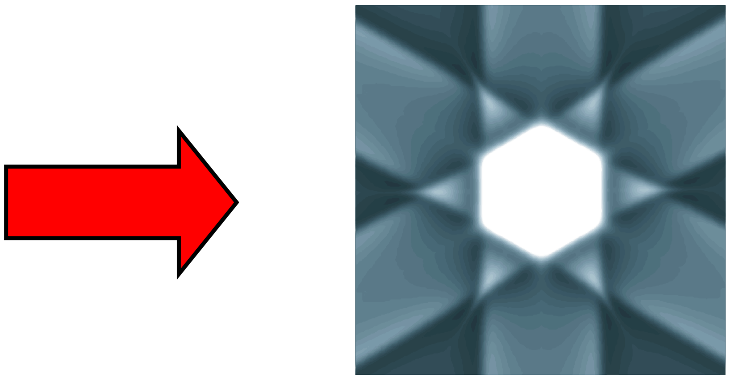


experiment RuO_2 20kV dynamical simulation

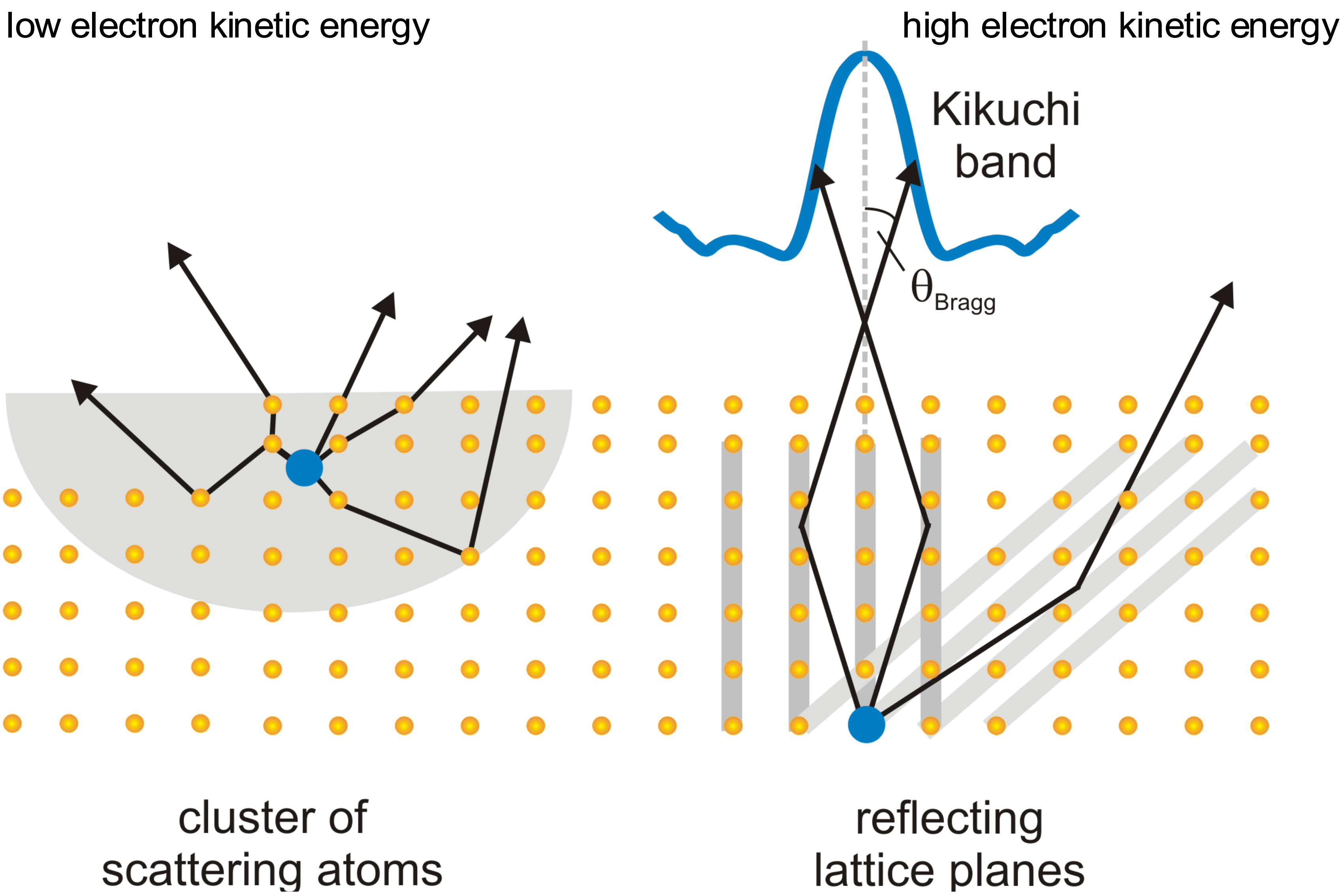
Bloch wave model of Electron Diffraction



- excitation of two types of Bloch waves near a Bragg reflection
- changing backscattering probability away from Bragg reflection
- formation of Kikuchi-band
- sources / detectors localized at atomic positions



Mechanisms for independent electron emitters in crystals?



momentum conservation

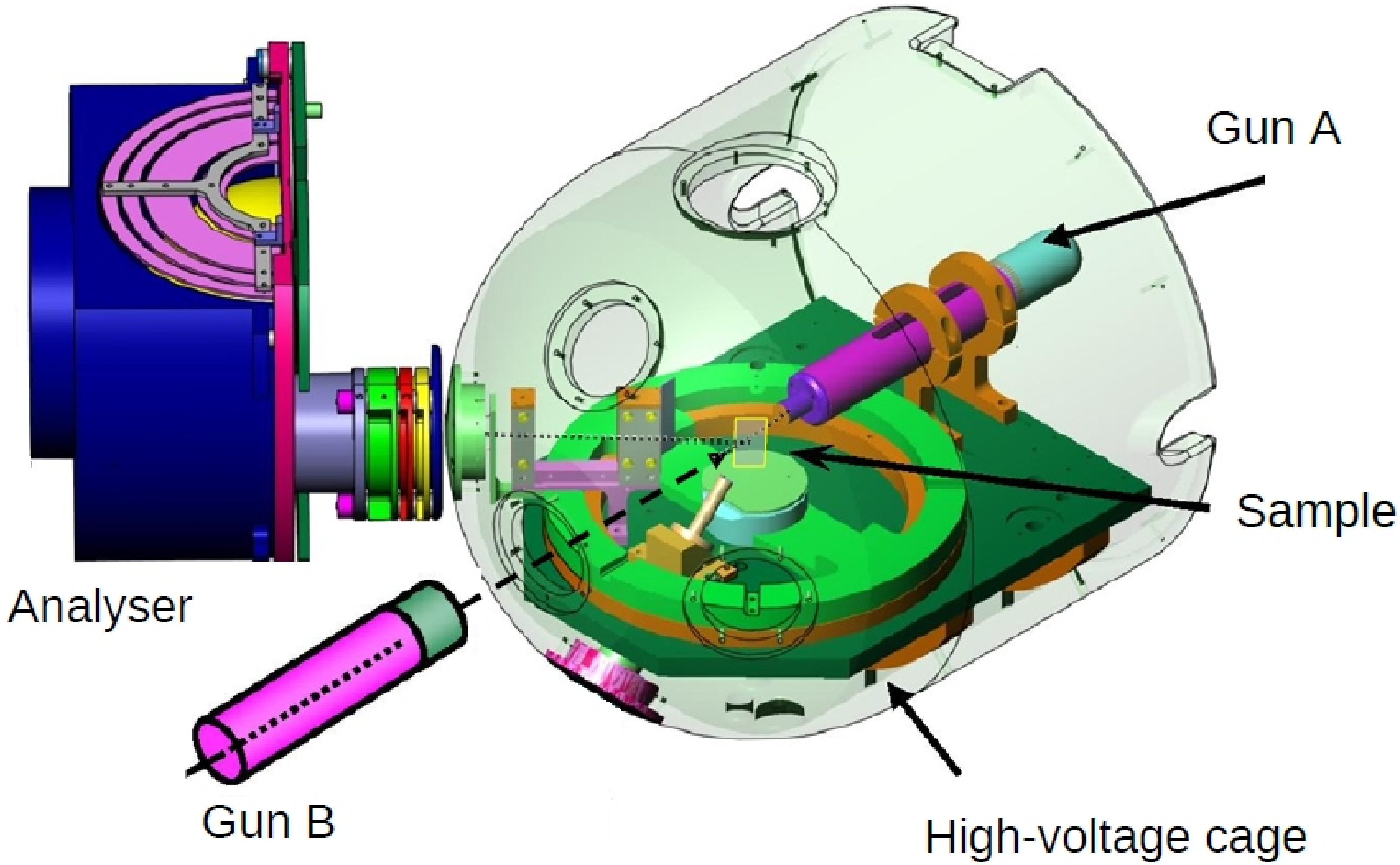
Recoil effects: Photoemission, Electron Scattering, Neutron Scattering

M. Vos, M. R. Went, Y. Kayanuma, S. Tanaka, Y. Takata, and J. Mayers

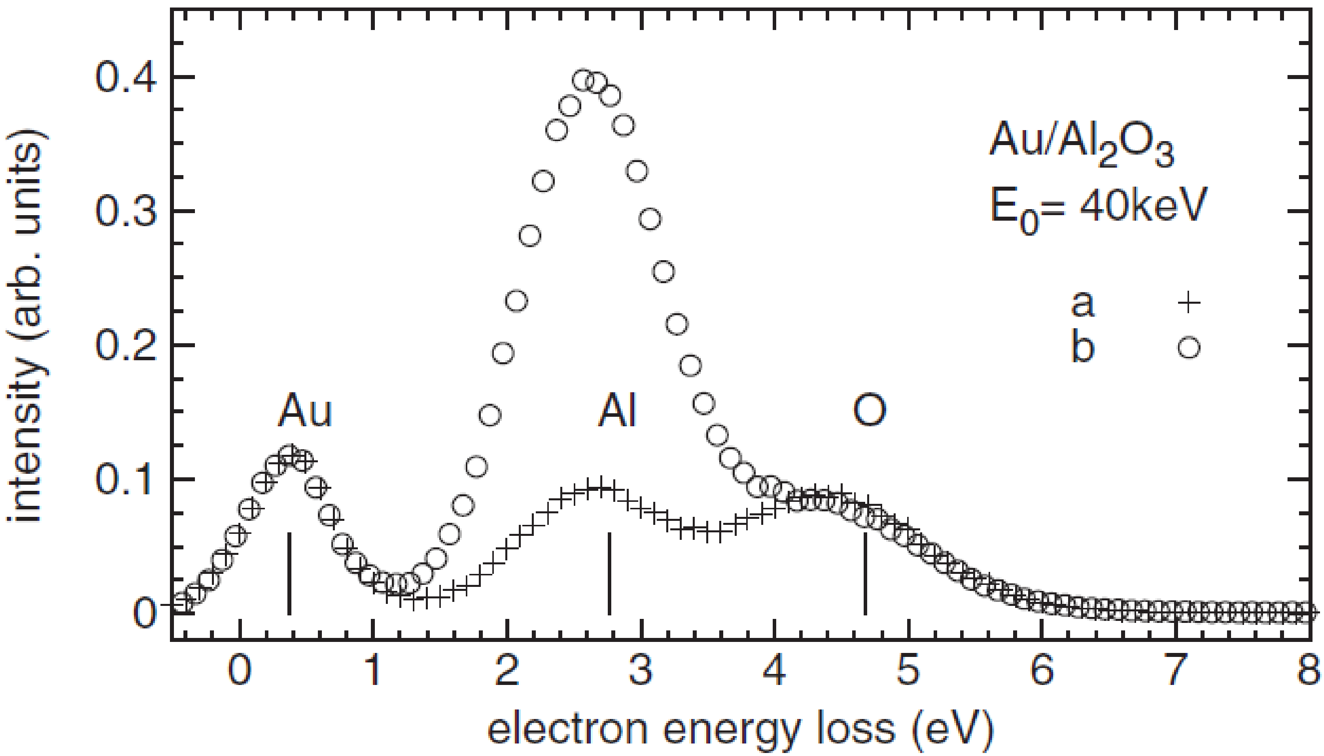
Phys.Rev. B 78, 024301 (2008)

Energy dependent measurements of Kikuchi band profiles

High energy Electrostatic electron energy analyzer, Australian National University, Canberra
$\Delta E < 0.5eV$ @10..40kV



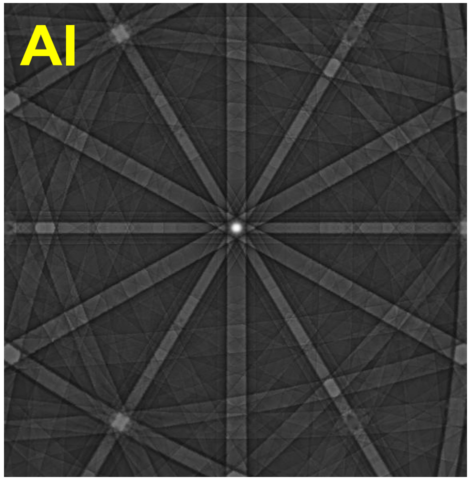
Electron Rutherford Backscattering Spectroscopy

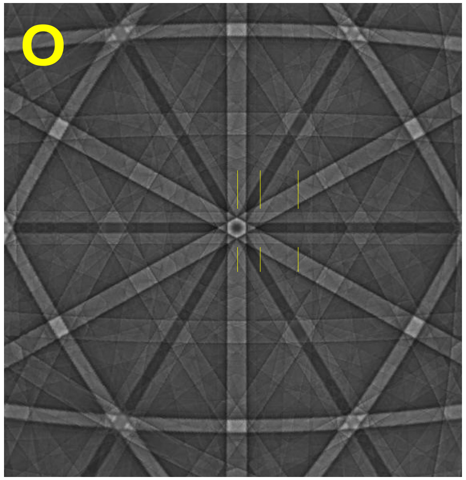


element-selective
recoil energy
of elastically scattered
electrons: Au atoms on Al_2O_3

M. Vos, K. Aizel, A. Winkelmann
Surface Science **604** (2010) 893–897

Element-resolved Kikuchi bands in Sapphire

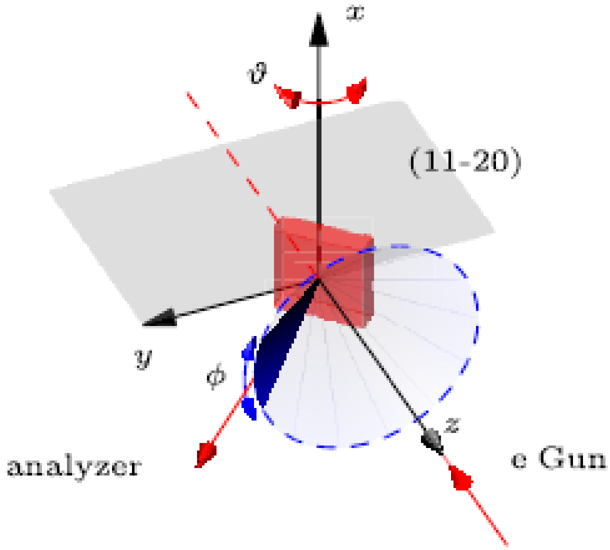




Simulation

Al_2O_3

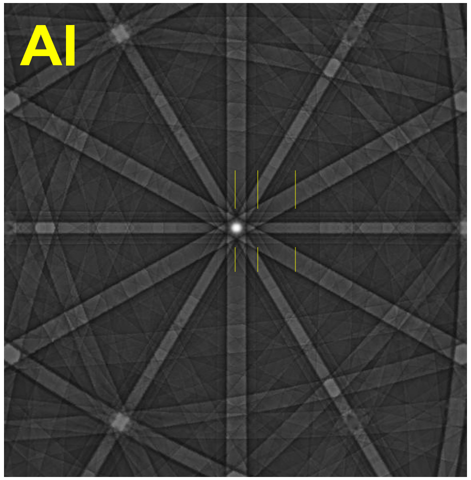
35kV

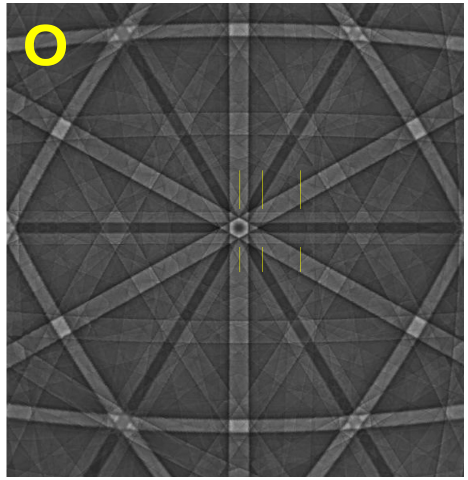


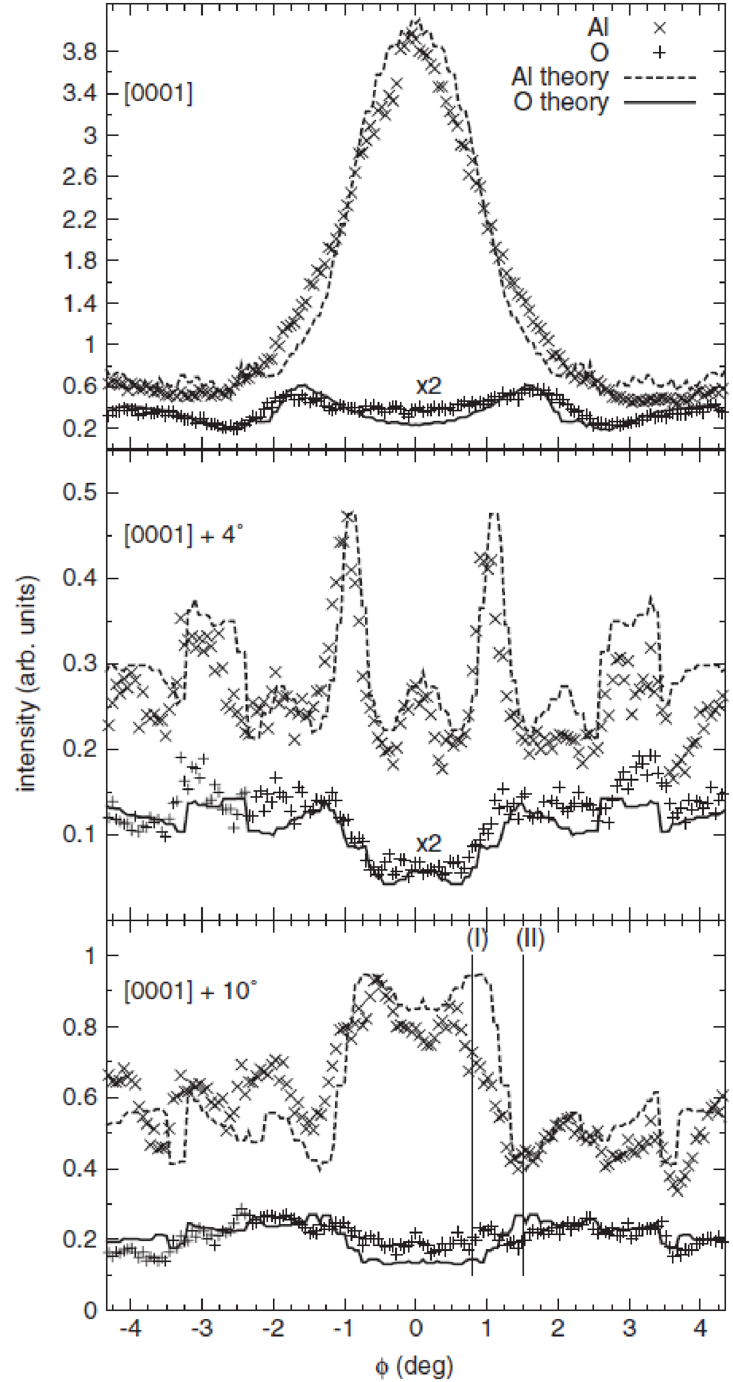
A. Winkelmann, M. Vos

Physical Review Letters **106** (2011) 085503

Element-resolved Kikuchi bands in Sapphire



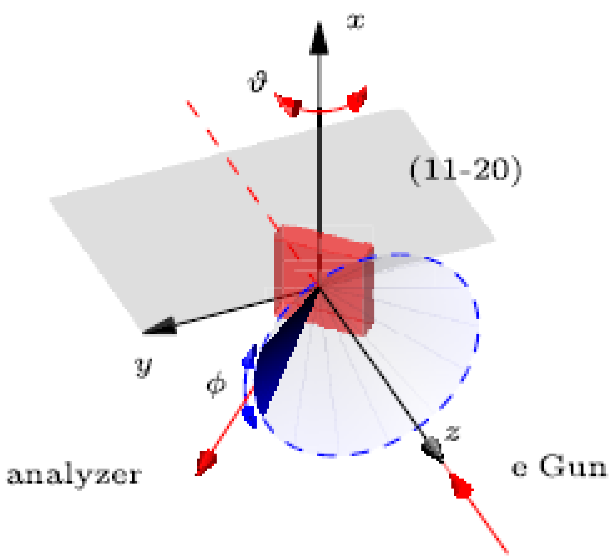




Simulation

Al_2O_3

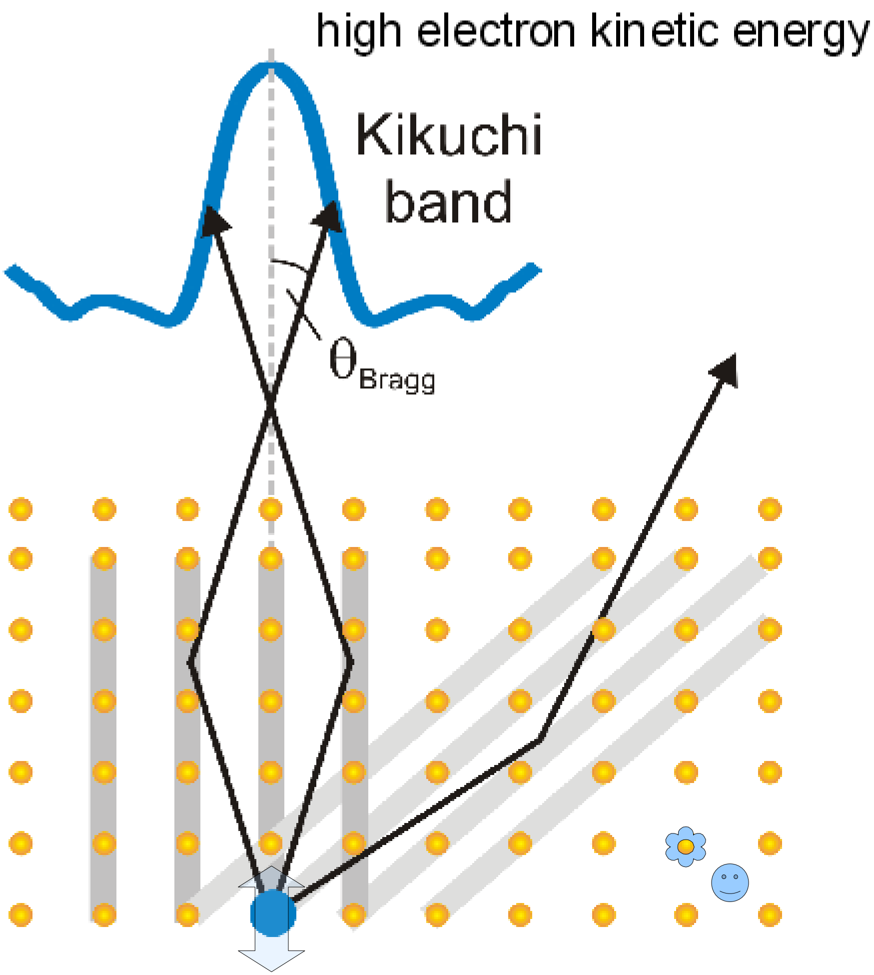
35kV

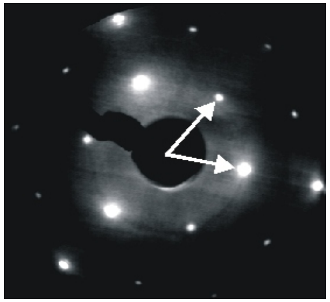


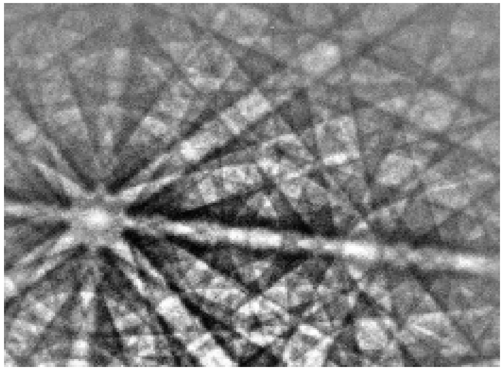
A. Winkelmann, M. Vos
Physical Review Letters **106** (2011) 085503

Summary

simulation of high energy electron diffraction
from internal sources by 3D Bloch wave approach





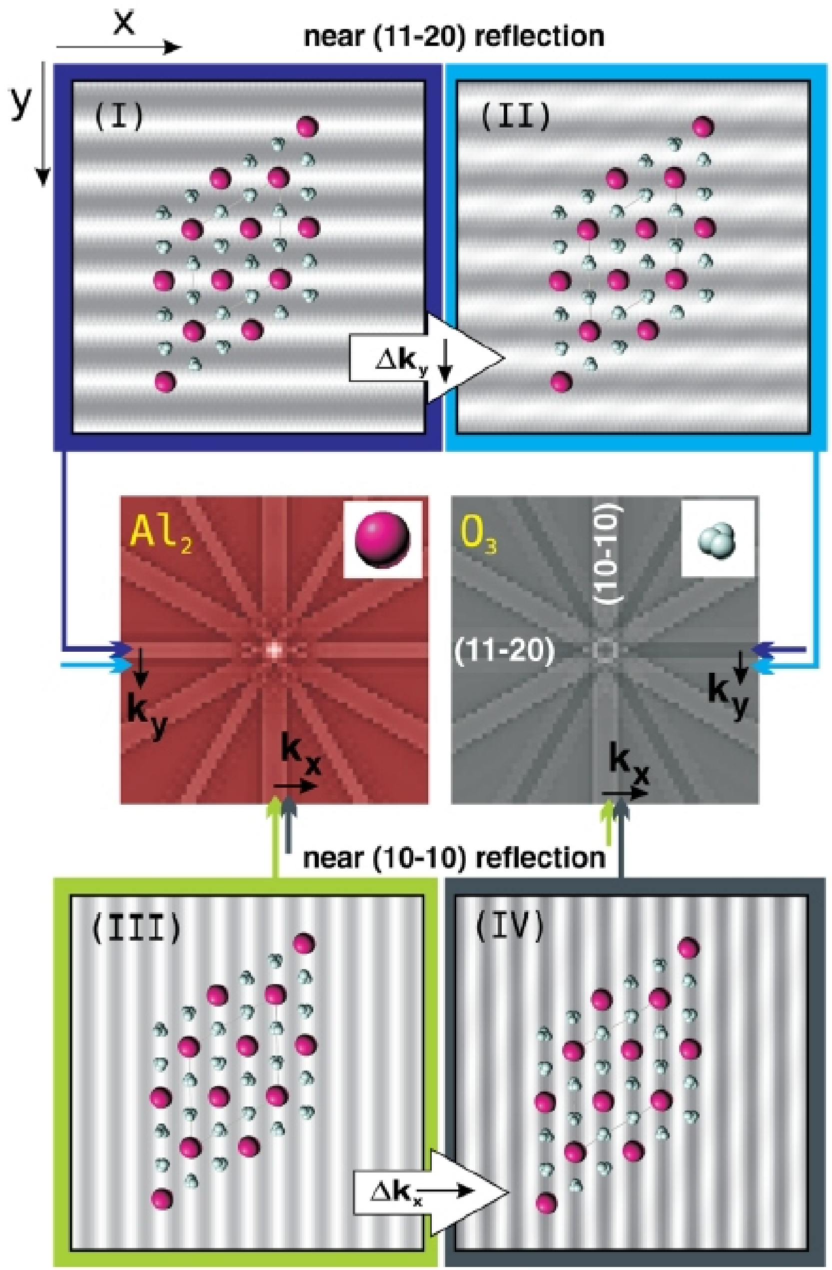


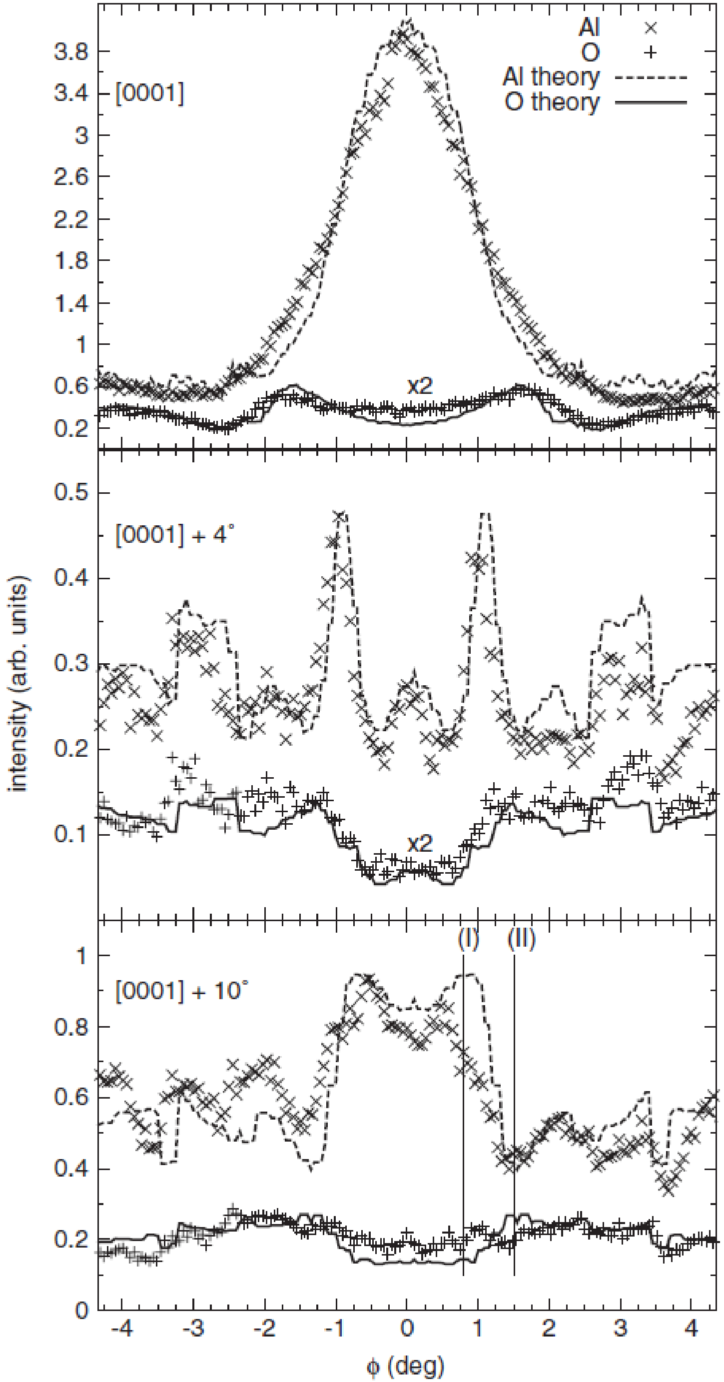
nuclear recoil can cause incoherence and change from low energy spot diffraction patterns to high-energy Kikuchi patterns

crystallographic information by diffraction

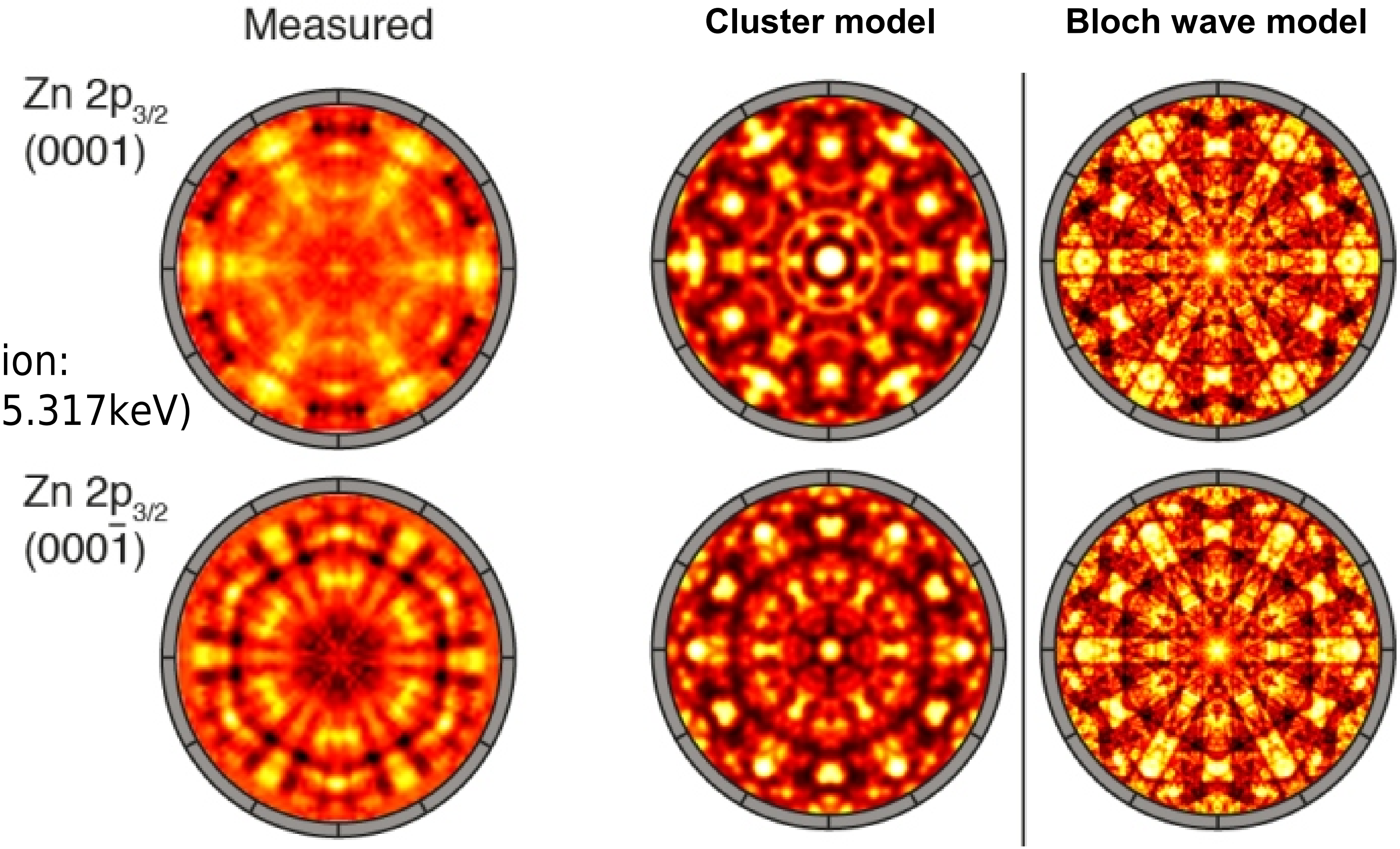
of high energy electrons with specific recoil losses

Element-resolved Kikuchi bands in Sapphire





X-ray Photoelectron Diffraction: ZnO Polarity



excitation:
Cr Kα (5.317keV)

E_{kin}=4.387keV

J. Williams, I. Pis, A. Winkelmann, M. Kobata,Y. Adachi, K. Kobayashi, and N. Ohashi (submitted)

Bloch wave model of electron diffraction

Wave function is sum of Bloch waves

$$\Psi(\vec{r}) = \sum_j c_j \exp(i\vec{k}^{(j)}\vec{r}) \sum_g^{(N)} C_g^{(j)} \exp(i\vec{g}\vec{r})$$

Fourier expansion of crystal potential

$$V(\vec{r}) = \sum_g^{(N)} V_g \exp(i\vec{g}\vec{r})$$

Schrödinger Equation

$$\frac{-\hbar^2}{2m}\nabla^2\Psi(\vec{r}) - |e|V(\vec{r})\Psi(\vec{r}) = \frac{\hbar^2 K_0^2}{2m}\Psi(\vec{r})$$

Eigenvalue problem (Matrix) + boundary conditions

Wave function of diffracted electrons $c_j, C_g^{(j)}, \vec{k}^{(j)}$

CBED
J.M. Zuo, K. Gjonnes, J.C.H. Spence, J.Electr.Micr.Techn. 12, 29 (1989)

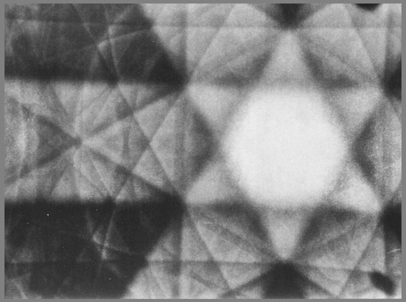
Backscattering proportional to probability density of electrons near atomic cores

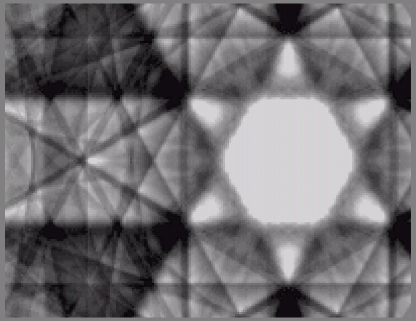
$$I_{ECP} \propto \sum_n Z_n^2 \sum_{i,j} B_{ij}(t) \sum_{g,h} C_g^i C_h^{j*} \exp(-M) \exp[i(\vec{h} - \vec{g})\vec{r}_n]$$

Theory: Rossouw C J, Miller P R, Josefsson T W and Allen L J
Phil. Mag. A 70, 985 (1994)

ECP/EBSD
Simulation program

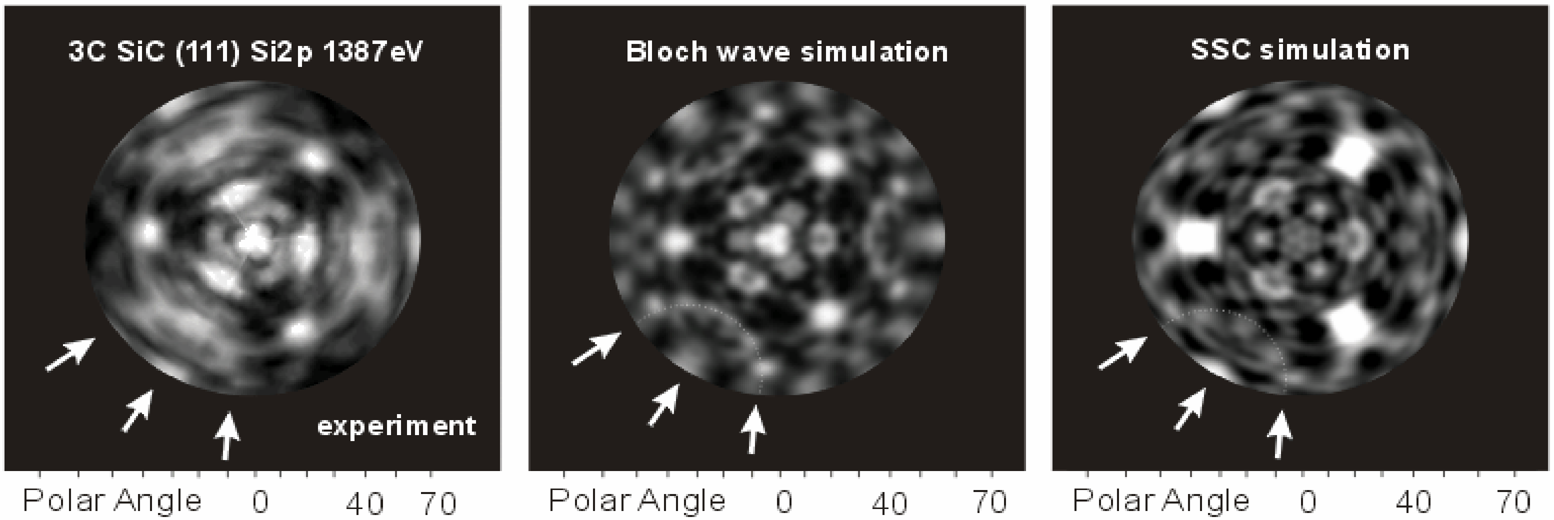
Experiment 6HSiC 15kV

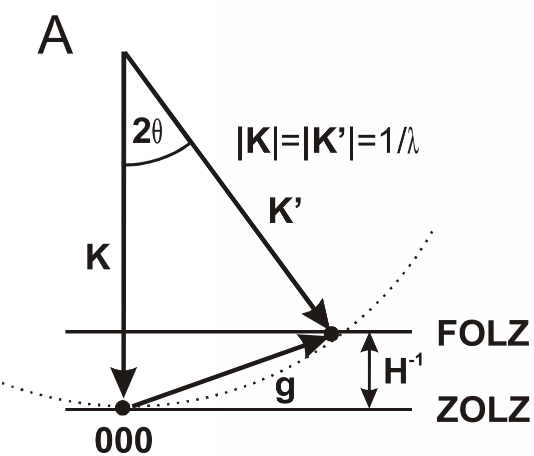


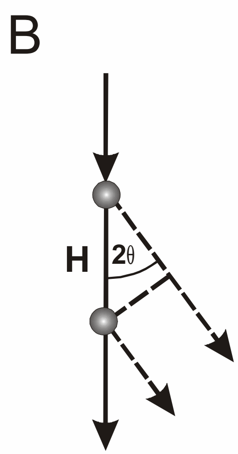


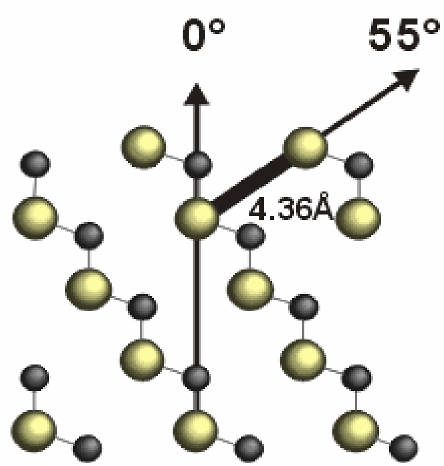
Simulation

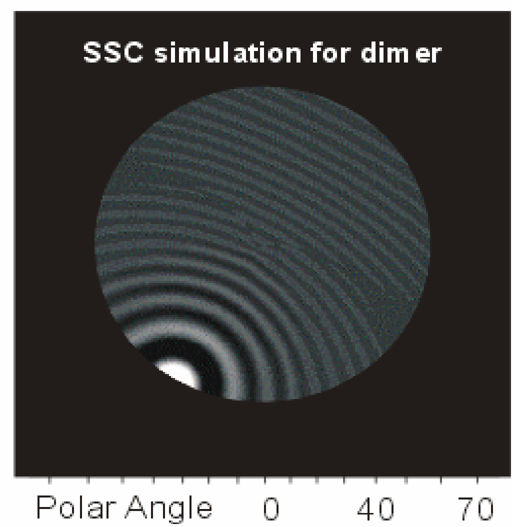
3C SiC(111) Si2p ring-like structures







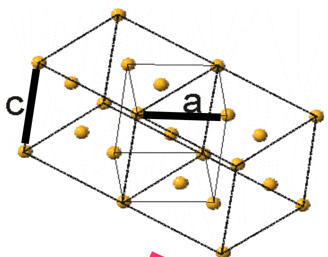




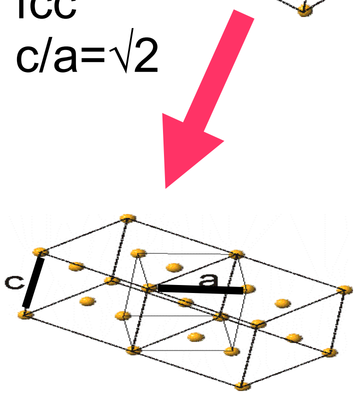
A. Winkelmann et al., Phys. Rev. B 69, 245417 (2004)

Ultrathin magnetic films: Tetragonally distorted FeCo alloys on Pd(001)

Definition
of c/a ratio



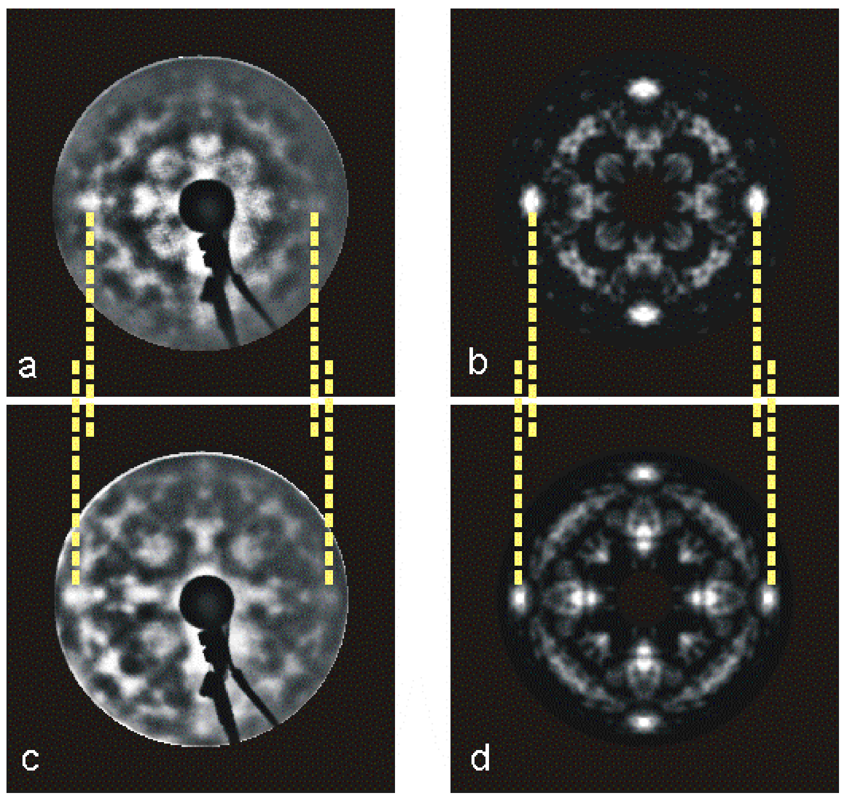
fcc
c/a=√2



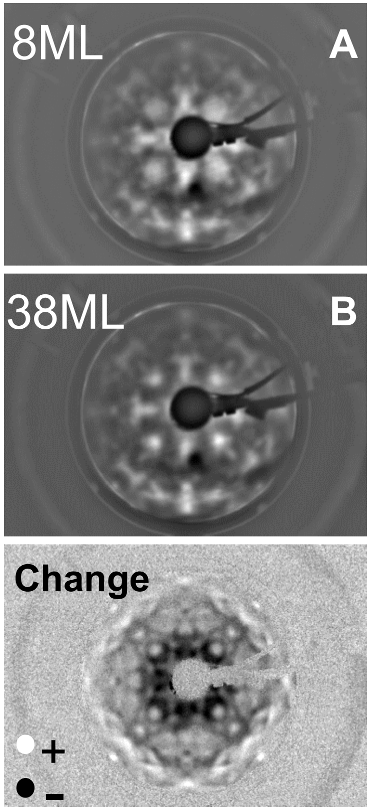
bcc
c/a=1

Pd(001)

experiment | cluster simulation



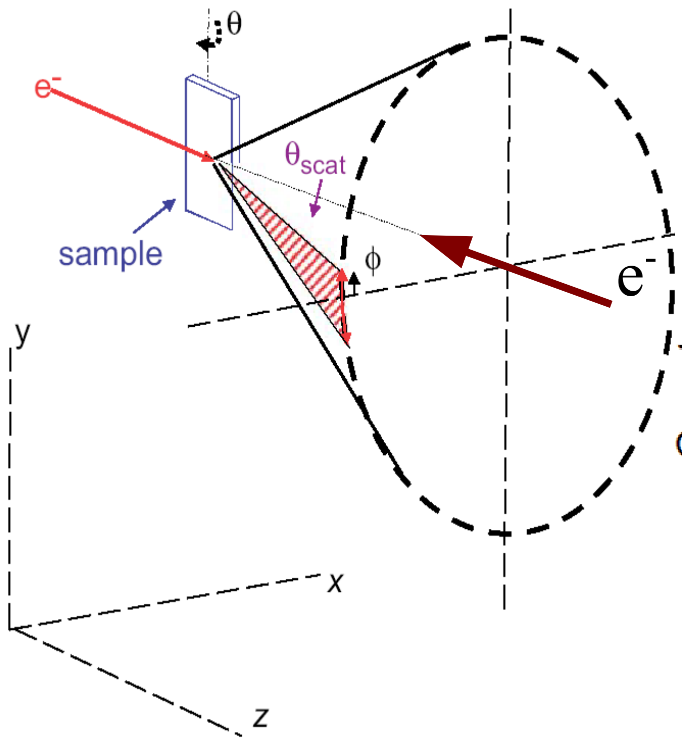
15 ML $Fe_{0.4}Co_{0.6}$/Pd(001)
c/a=1.13



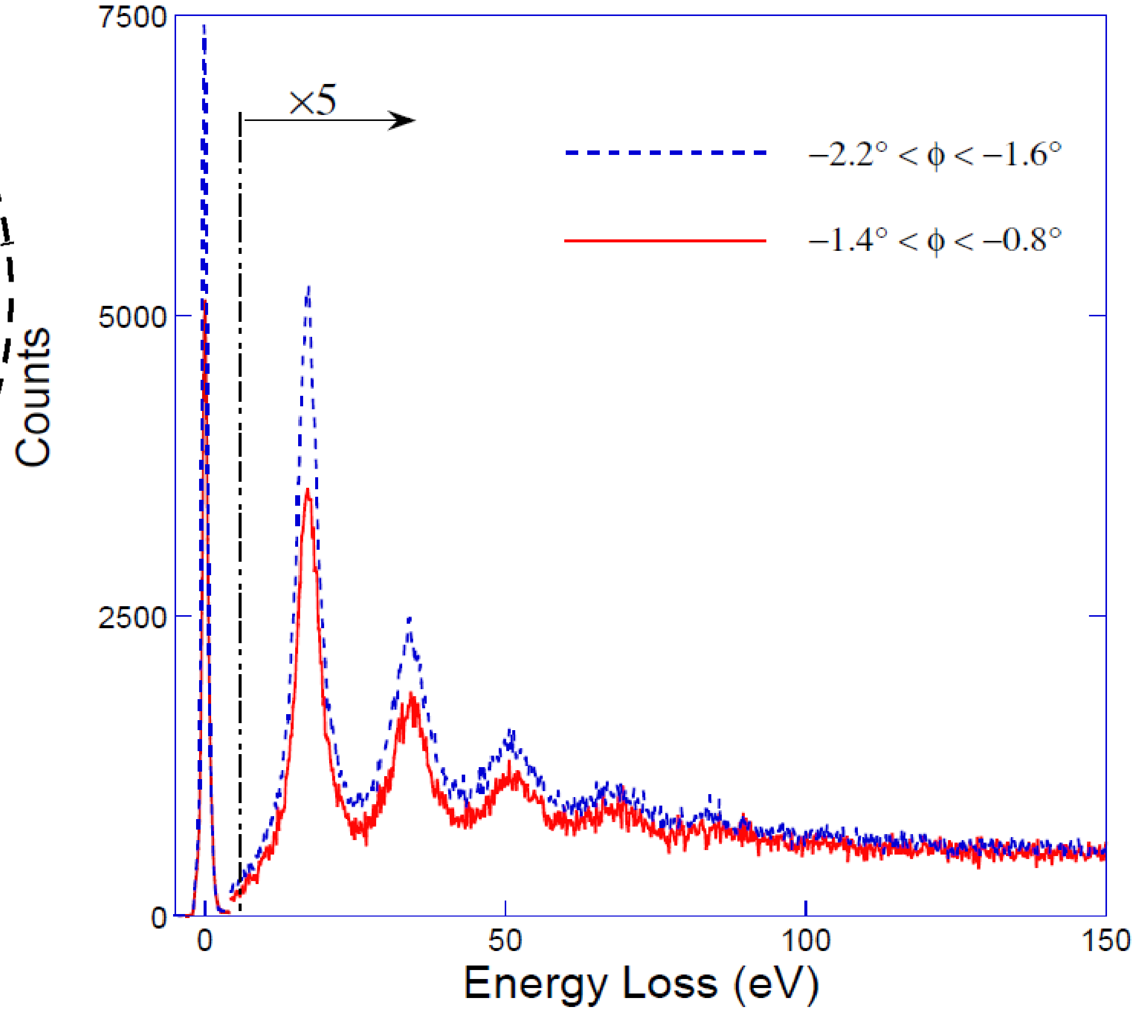
decreasing c/a ratio
with thickness

A. Winkelmann *et al.*,
Phys. Rev. Lett. 96, 257205 (2006)

Inelastic Scattering : Energy dependence of Kikuchi band profiles



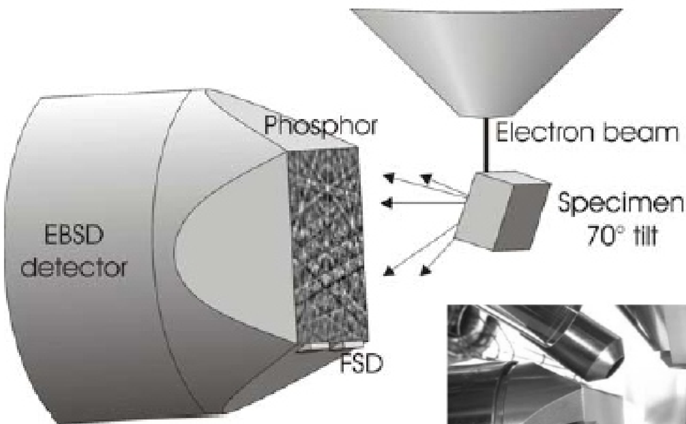
Si(001) angle-resolved energy loss spectra of backscattered electrons E_0=30kV

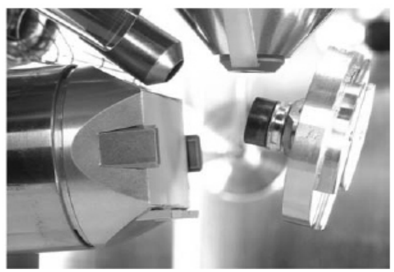


A. Winkelmann, K.Aizel, M. Vos,
New Journal of Physics **12** (2010) 053001

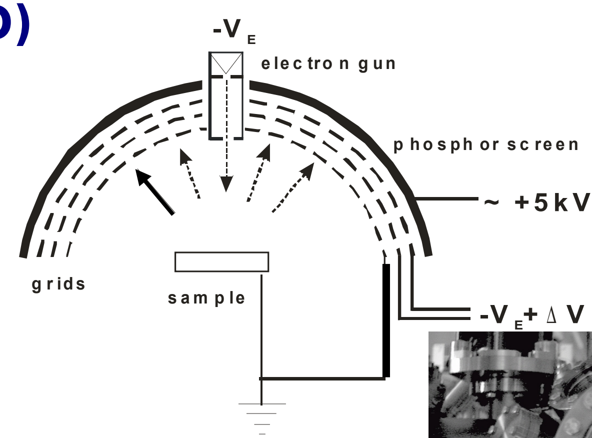
Diffraction of backscattered and back-reflected electrons

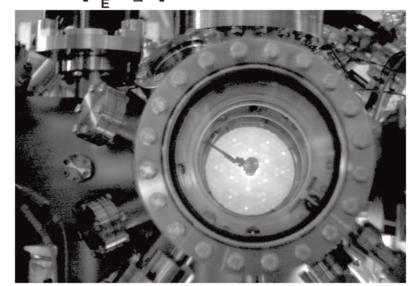
Scanning electron microscopy: Electron Backscatter Diffraction (EBSD)



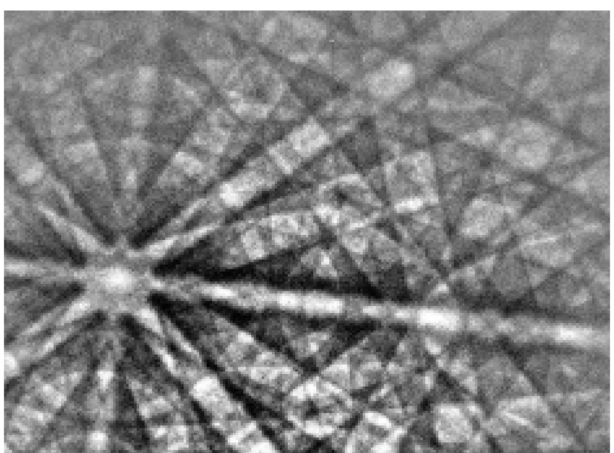


Low Energy Electron Diffraction (LEED)

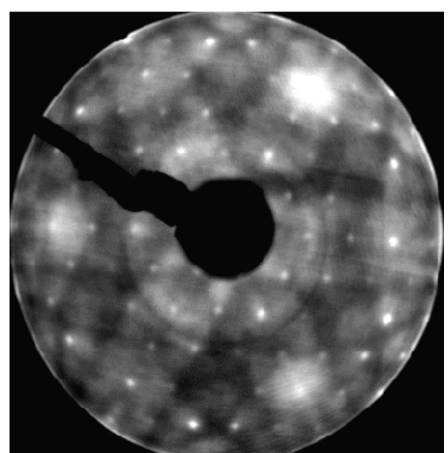




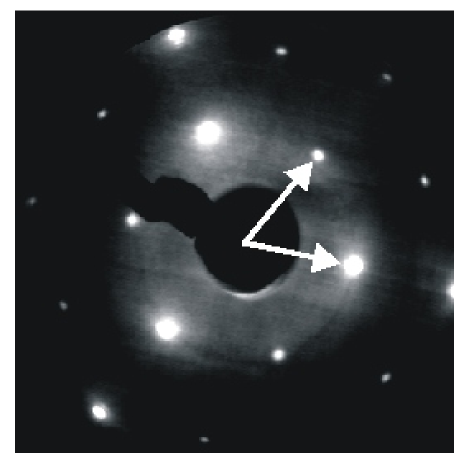
Mo bcc 25kV



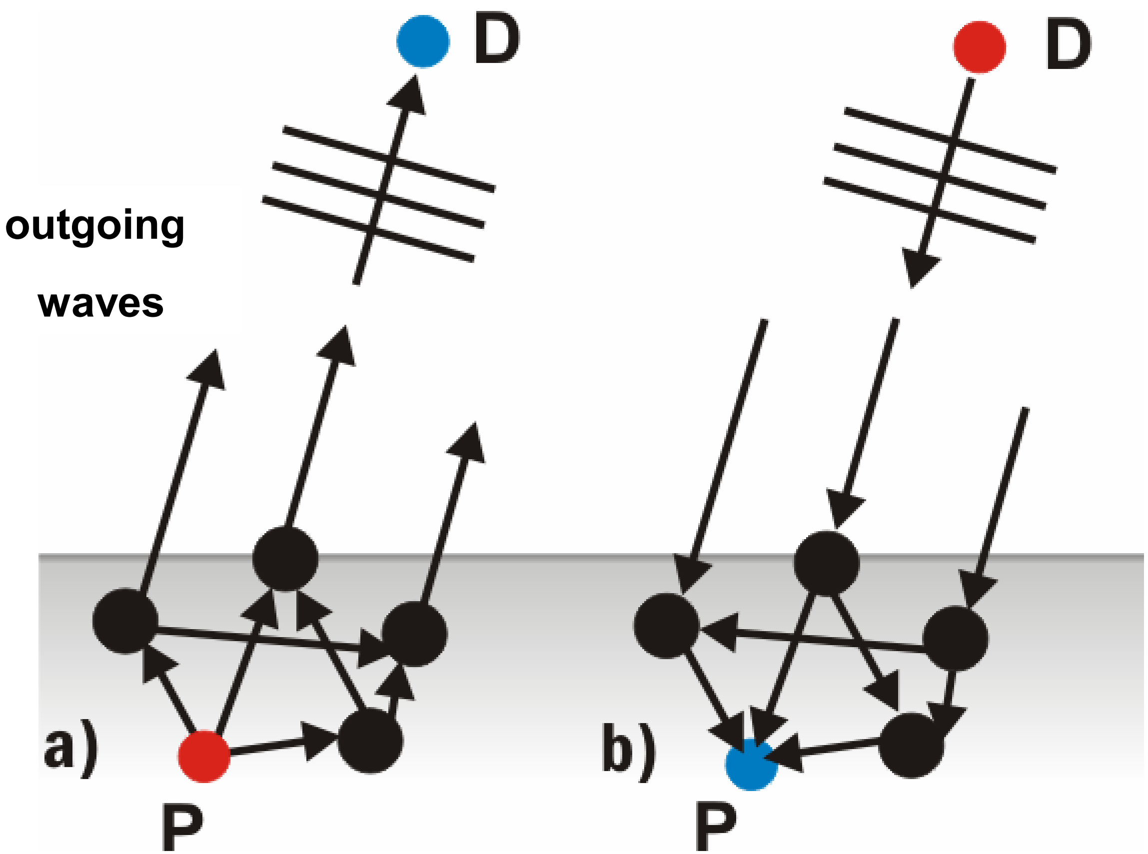
6H SiC 1kV

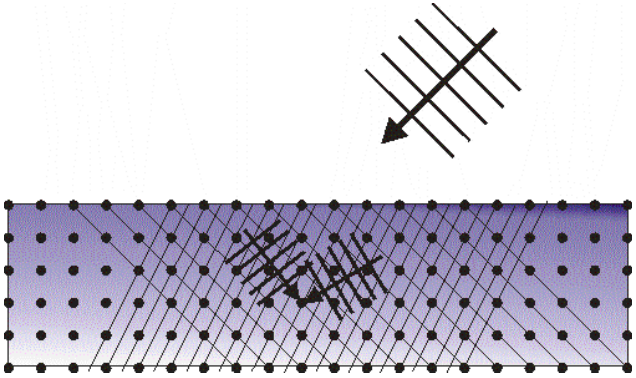


6H SiC 170eV



Using the reciprocity principle





diffraction of incoming plane waves

(e.g. TEM)

Simple model of backscatter diffraction

A. Winkelmann "Dynamical Simulation of Electron Backscatter Diffraction Patterns"
in "Electron Backscatter Diffraction in Materials Science" 2nd ed., 2009
www.springer.com/materials/book/978-0-387-88135-5