united nations
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international centre for theoretical physics

ICTP 40th Anniversary

SCHOOL ON SYNCHROTRON RADIATION AND APPLICATIONS
In memory of J.C. Fuggle & L. Fonda

19 April - 21 May 2004

Miramare - Trieste, Italy

1561/39

Spectral and image analysis

L. Gregoratti

Spectral and image analysis

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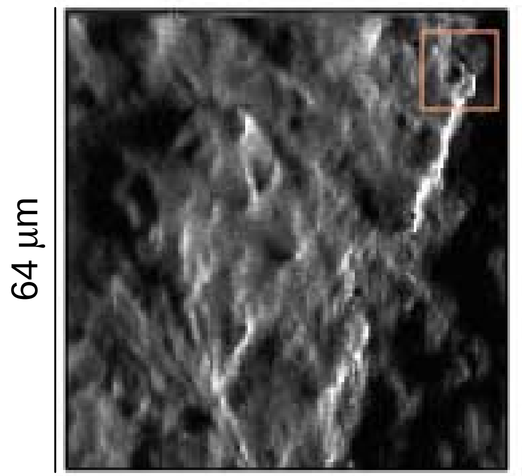
Contrast mechanisms in a photoemission image

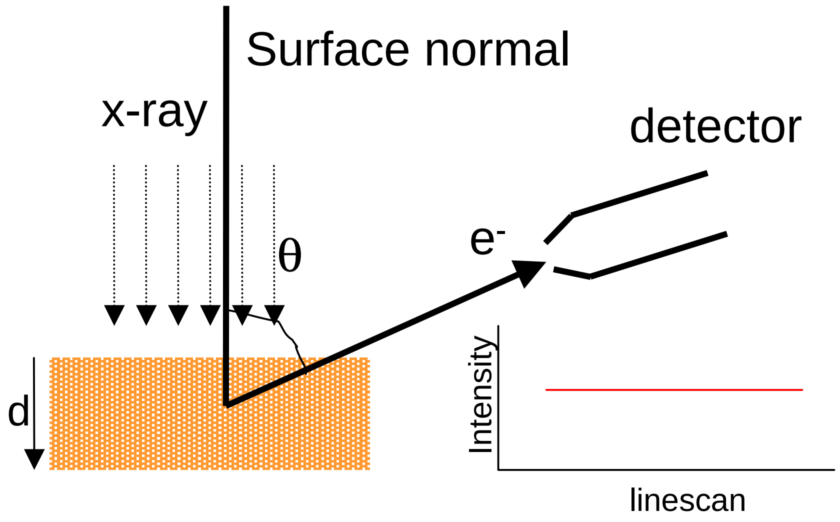
- Topography

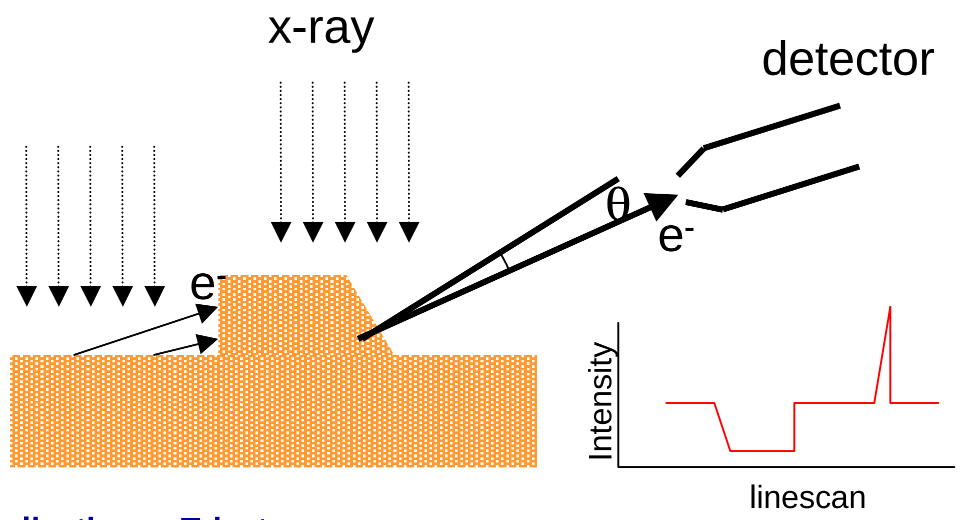
$$I = I_0\, e^{-\frac{d}{\lambda \cos\theta}}$$

λ = inhelastic mean free path

Blob of C nanotubes







- **Chemical inhomogeneity**

Ni islands on Si

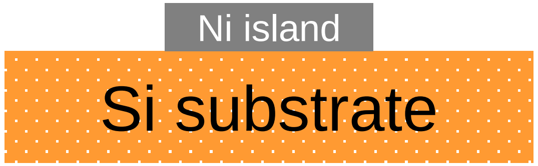


Image on Ni

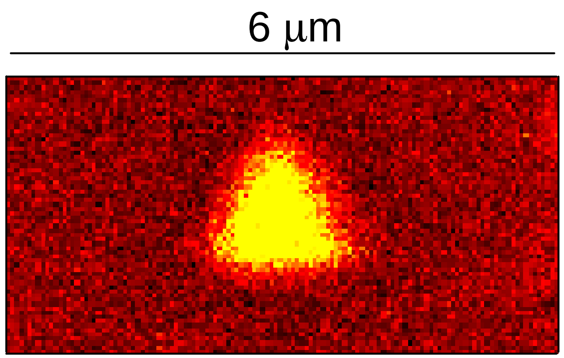
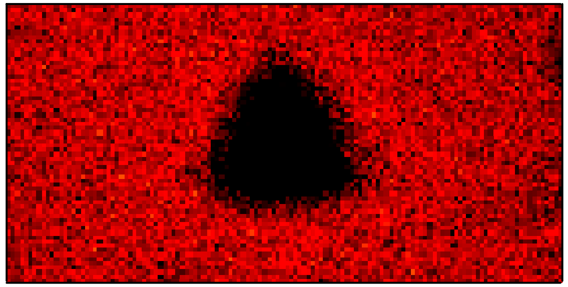


Image on Si



Au patch on Rh(110)

Image on Rh

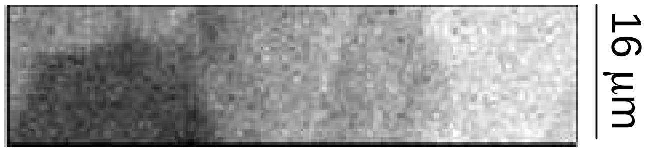
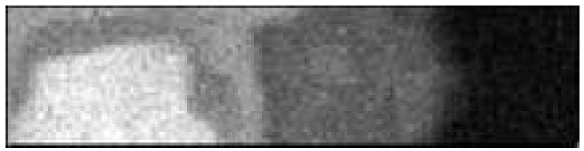
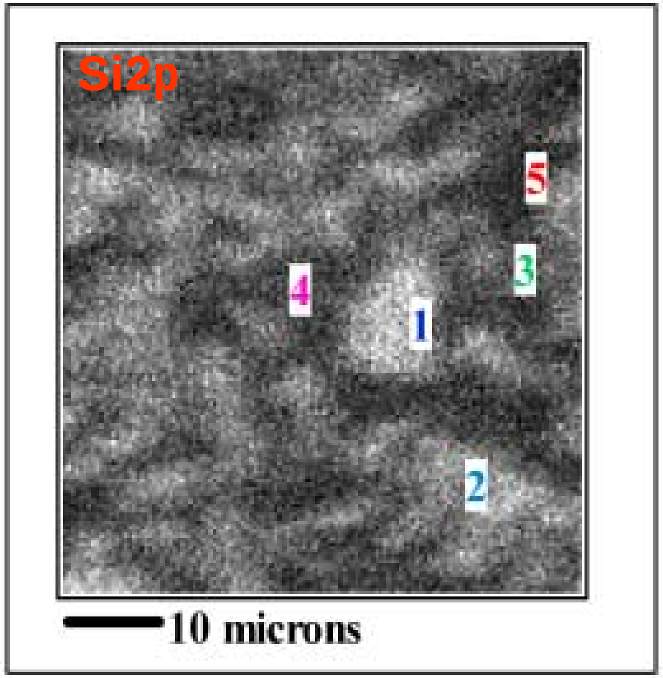


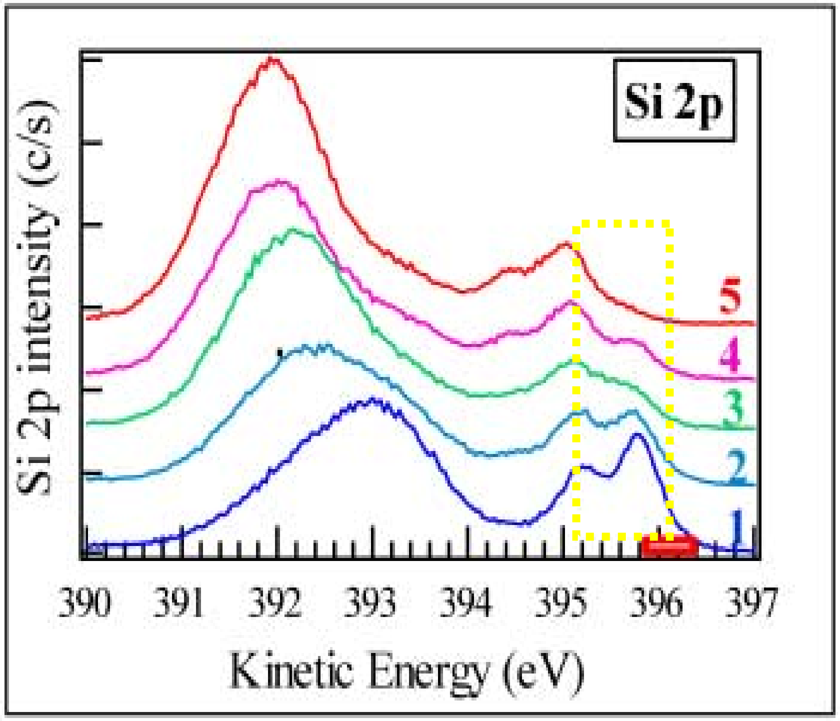
Image on Au



- Other sources of contrast

charging





Getting the chemical information out of the artefacts

Artefacts

1. Topography
2. Beam induced effects:
   - C deposition (residual gases)
   - O_2 reduction
   - Charging
3. Background level

General formulas:

$$I = \frac{I_{peak} - I_{bkg}}{I_{peak} + I_{bkg}}$$

$$I = \frac{I_{peak} - I_{bkg}}{I_{bkg}}$$

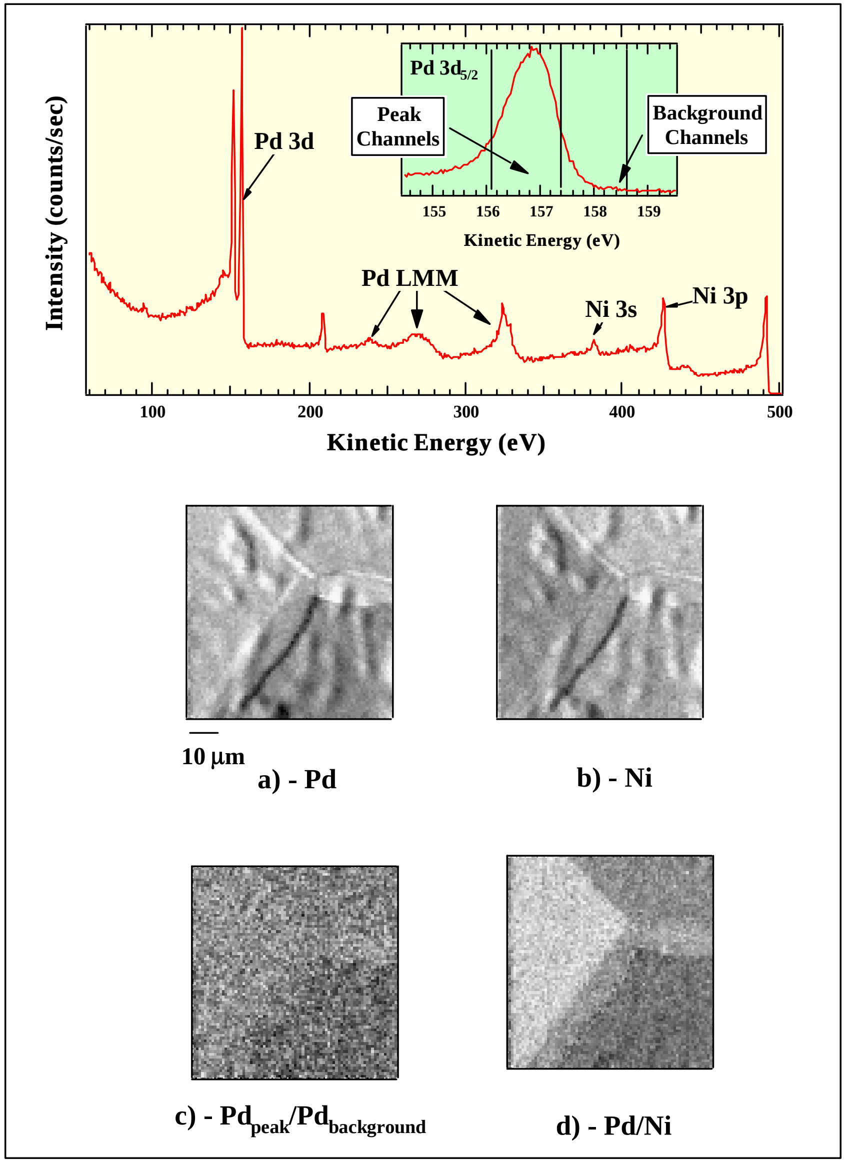
$$I = \frac{I_{peak}}{I_{bkg}}$$

sometimes only:

$$\frac{I_{peak1}}{I_{peak2}}$$

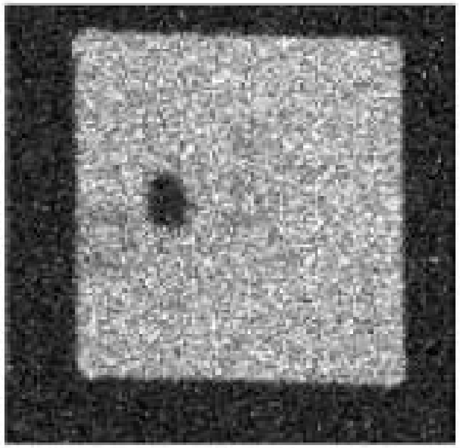
Which I_{bkg} ?

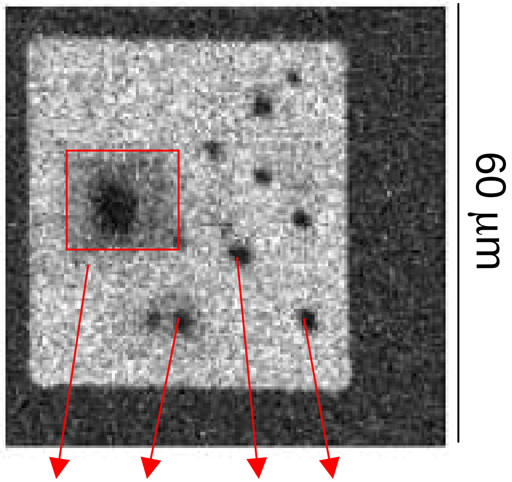
- $I_{bkg\ left}$
- $I_{bkg\ right}$
- $I_{bkg\ (left+right)}$
- *secondaries*



C growth

SiO_x sample
Si2p maps

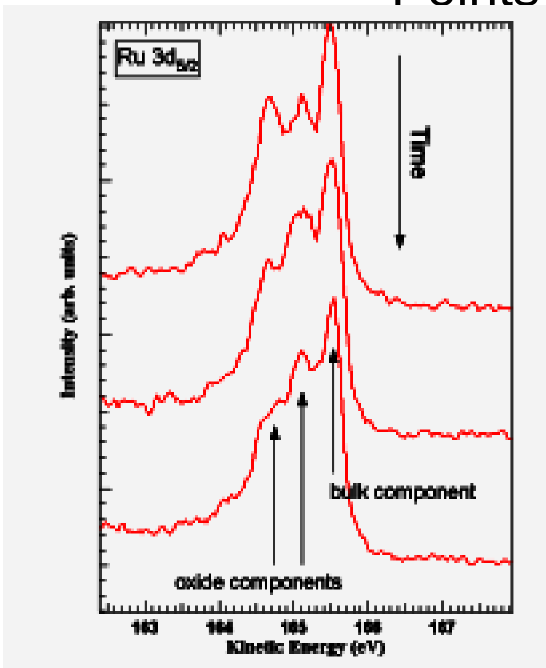




Points irradiated (>10 min)

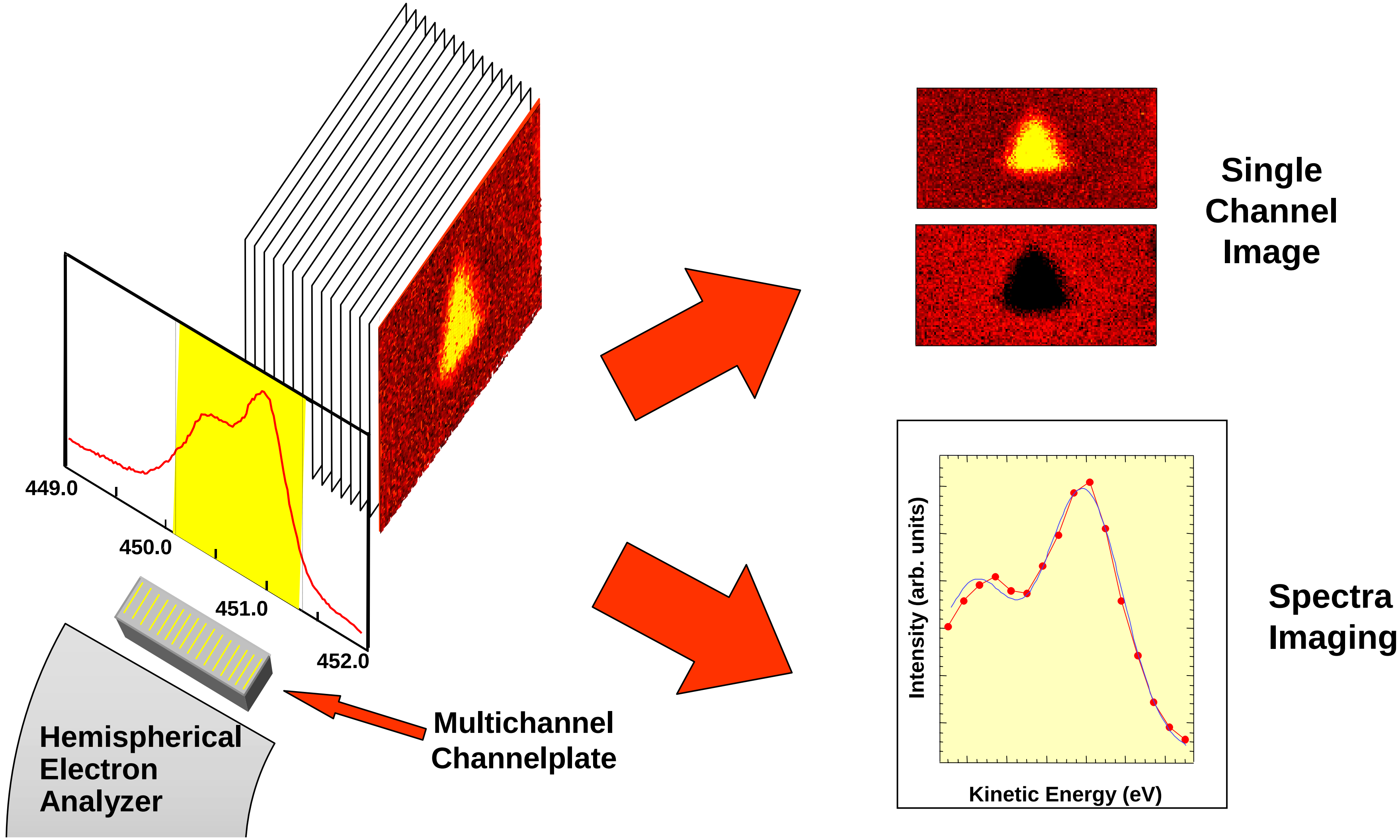
O_2 reduction

RuO_x sample



Each spectrum every 1 min

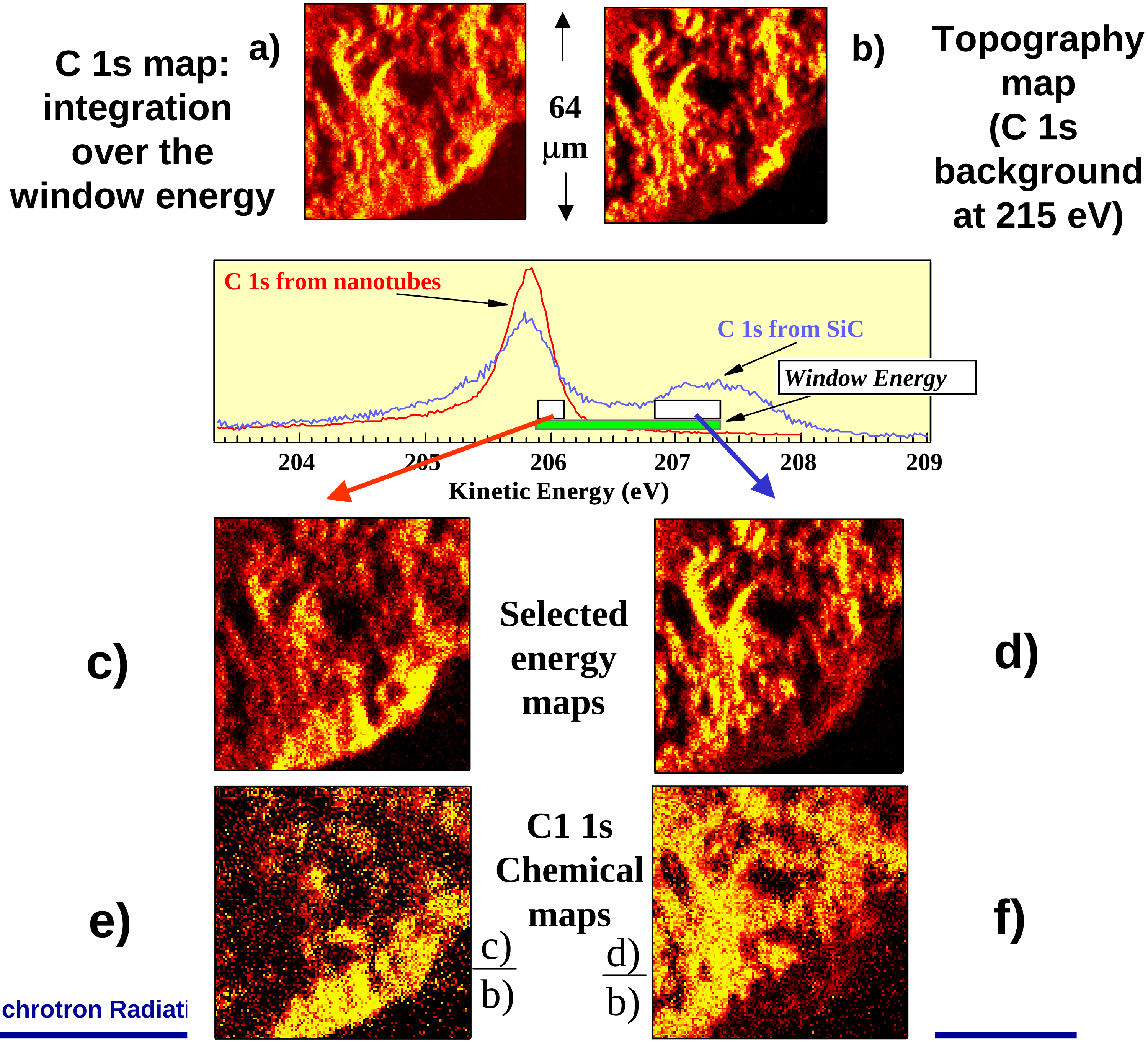
Multichannel detection



Single Channel Analysis

Carbon nanotubes on SiC

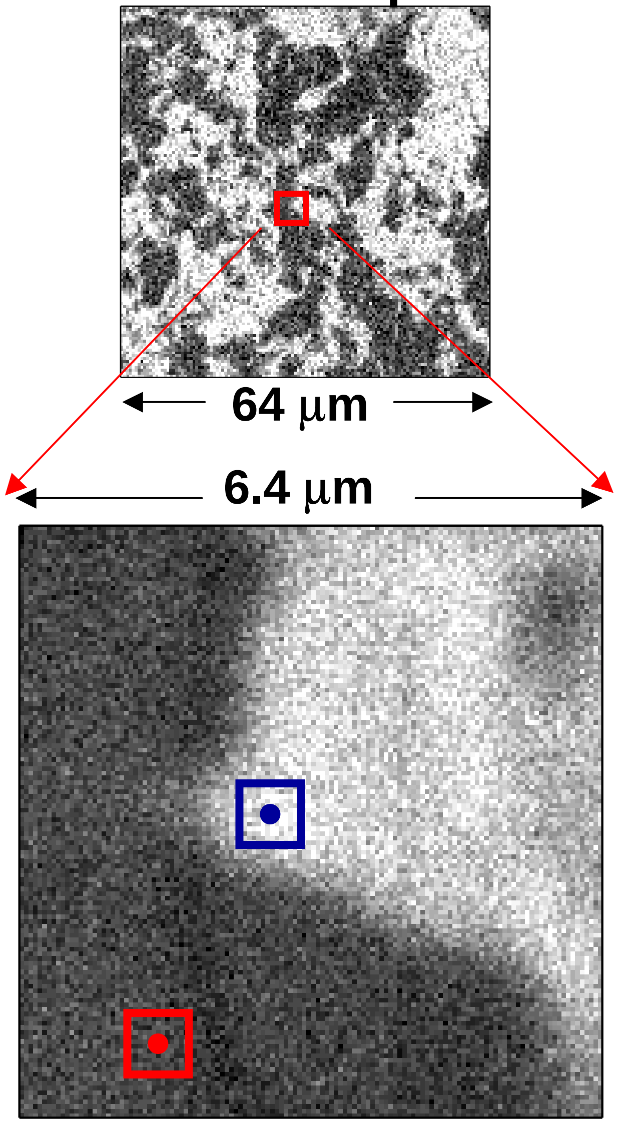
R. Larciprete – Enea - Italy



Spectra Imaging

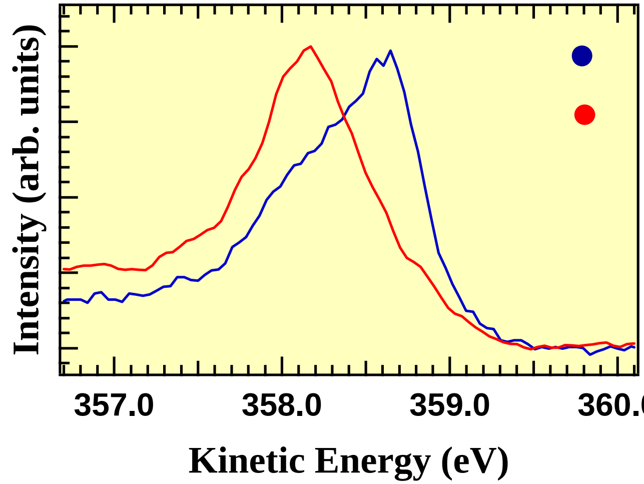
Ru(0001) oxidation
H. Conrad – FHI - Germany

Ru 3d maps

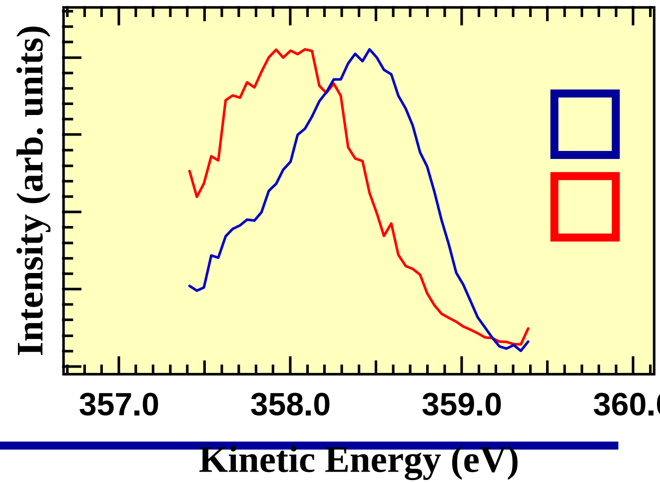


Ru $3d_{5/2}$ spectra

Conventional Scanning Spectroscopy (48 points - 70 sec)

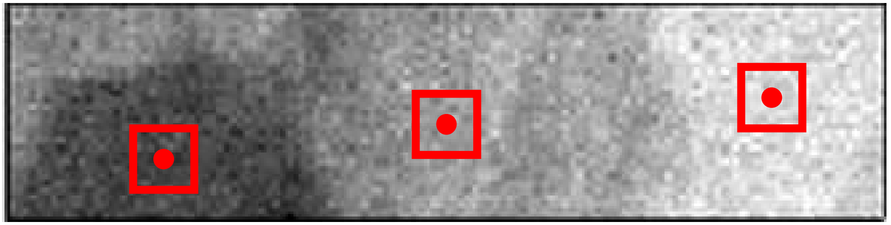


Inherent Dispersion Energy Spectroscopy (48 points - 10 sec)



Spectra Imaging

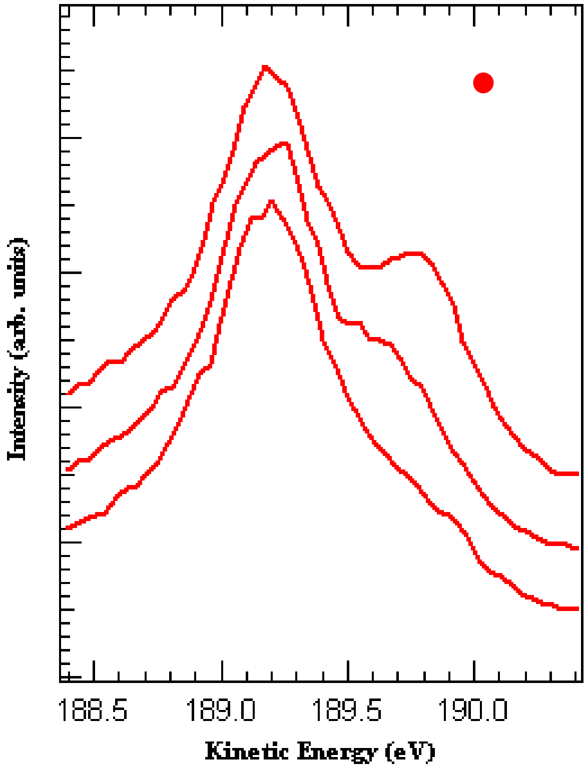
Rh 3d map

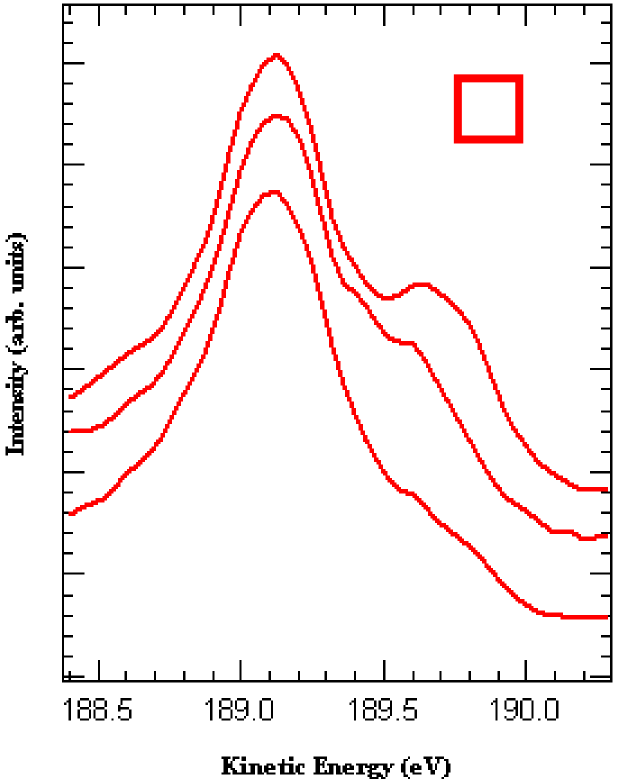


Conventional Scanning Spectroscopy

Inherent Dispersion Energy Spectroscopy

Rh 3d$_{3/2}$ spectra





Spectra analysis

Natural linewidth or core hole lifetime (Lorentzian)

Good for insulators and semiconductors

$$L(E) = \frac{1}{\left(1 + 4\left(\frac{E - E_L}{\Gamma_L}\right)^2\right)}$$

E_L = centroid
Γ_L = FWHM

Instrumental resolution and phonon broadening (Gaussian)

$$G(E) = \exp\left[-4\ln 2\left(\frac{E - E_G}{\Gamma_G}\right)^2\right]$$

E_G = centroid
Γ_G = FWHM

Convolution of the Gaussian and the Lorentzian (Voigt)

$$I(E_G) = \int_{-4\sigma}^{+4\sigma} \exp\left[-4\ln(2)\left(\frac{E - E_G}{\Gamma_G}\right)^2\right] \times \frac{1}{\left(1 + 4\left(\frac{E - E_L}{\Gamma_L}\right)^2\right)} \mathrm{d}E$$

Natural linewidth or core hole lifetime (Doniach-Sunjic)

Good for metals

$$DS(E) = \frac{Gamma(1-\alpha)\cos\left[\frac{\pi\alpha}{2} + (1-\alpha)\arctan\left(2\left(\frac{E-E_L}{\Gamma_L}\right)\right)\right]}{\left((E-E_L)^2 + 4\Gamma_L^2\right)^{\frac{1-\alpha}{2}}}$$

E_L = centroid

Γ_L = FWHM

α = asymmetry

Lineshape for metals

$$I(E_G) = \int_{-4\sigma}^{+4\sigma} \exp\left[-4\ln(2)\left(\frac{E-E_G}{\Gamma_G}\right)^2\right] \times DS(E)\mathrm{d}E$$

Fitting procedure

Background removal

Background functions:

- Tougaard

$$F(E) = j(E) - \lambda \int_{E}^{\infty} dE' K(E' - E) j(E')$$

F(E)=primary excitation spectrum
j(E)=flux of emitted electrons
K(E,T)=probability for an electron of loosing energy
λ=mean free path for inelastic scattering

- Shirley

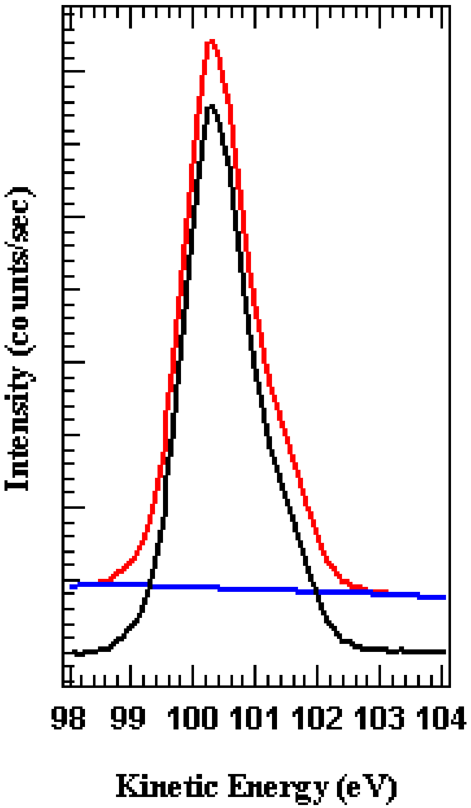
$$b_i = k \sum_{j=i+1}^{N} p_j$$

b_i=background of the point i
p_j=signal of the point j
N=highest kinetic energy
k=constant

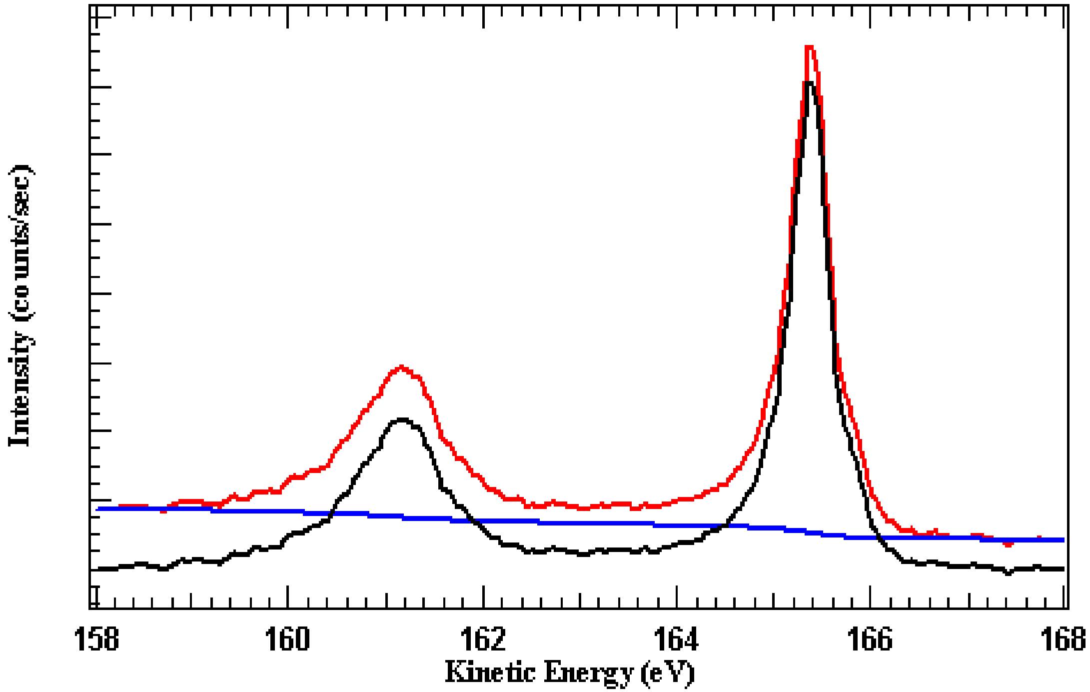
- Linear

- Cubic

Linear background: N1s



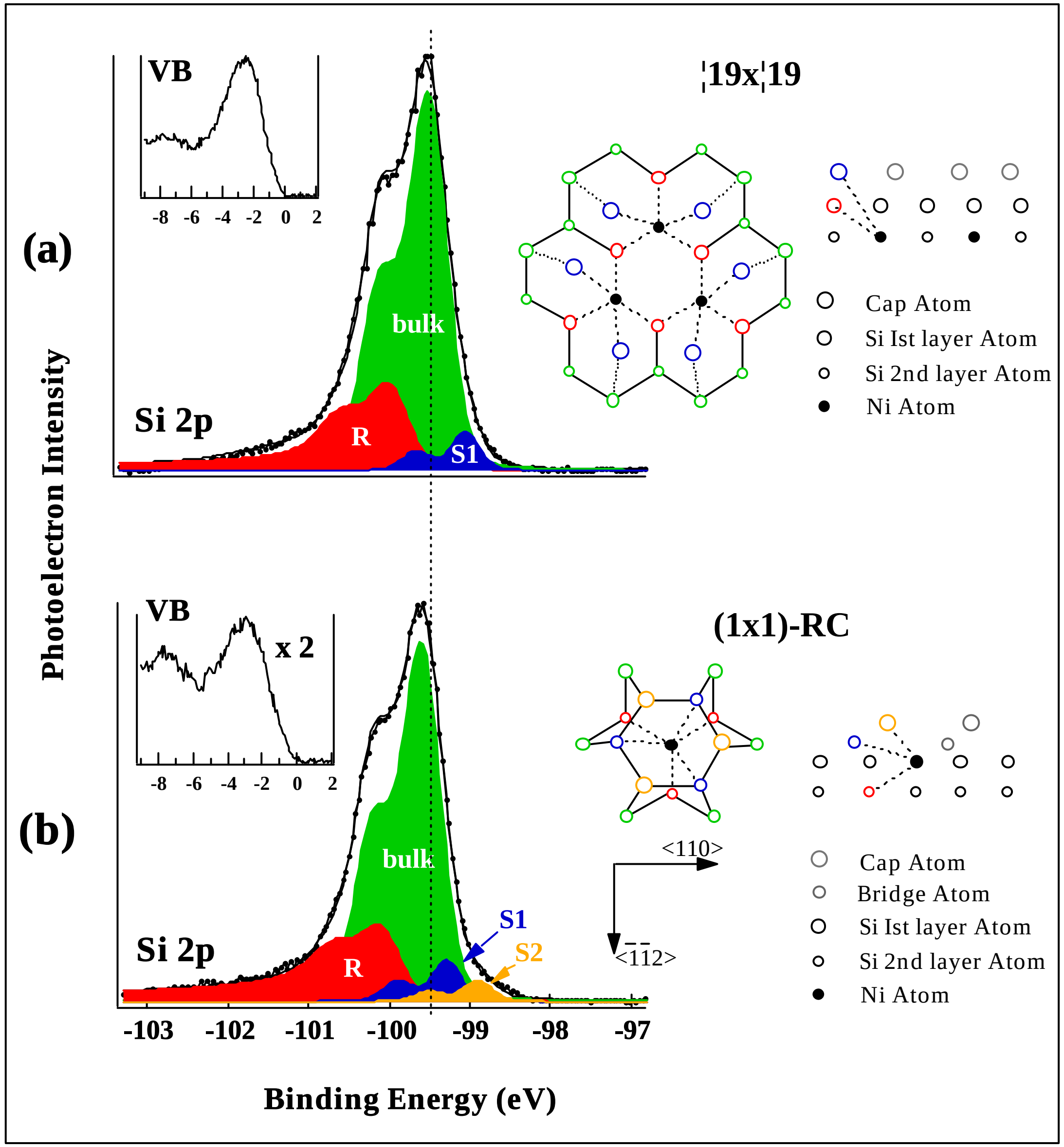
Shirley background: Rh3d



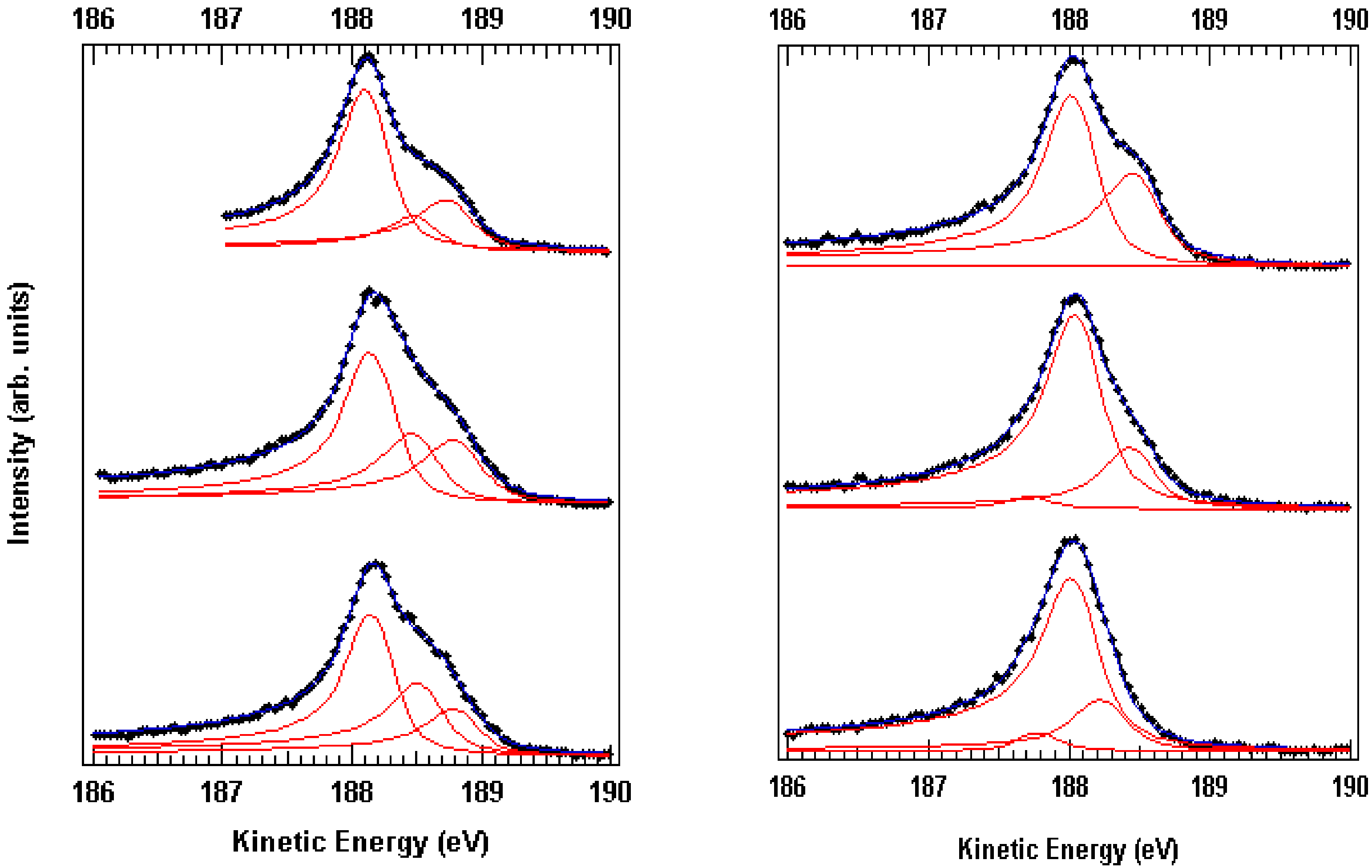
Fitting

Ni/Si(111)
2D recostructions

Si2p
spectra



Rh $3d_{3/2}$ fitting procedure (same experiment)



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Stefan Hufner, “Photoelectron spectroscopy, principles and applications”, Springer