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MULTIVARIATE FACTOR ANALYSIS OF HEAVY MINERALS CONCENTRATE FROM ATHABASCA OIL SANDS TAILINGS BY XPS

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National Research
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Presentation Overview :

- 1) Motivation & Research Objectives
- 2) Multivariate Factor Analysis
- 3) Large-Area Spectroscopy
- 4) Surface Component Imaging

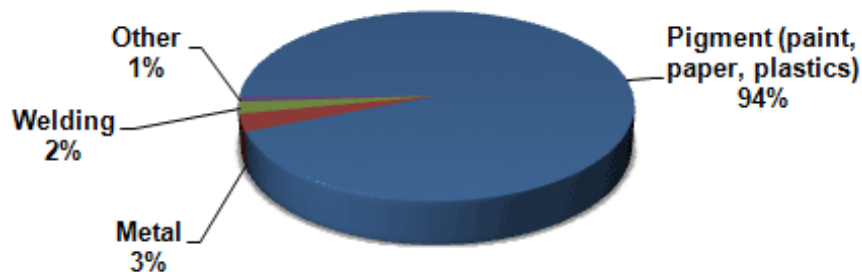


Motivation & Research Objectives

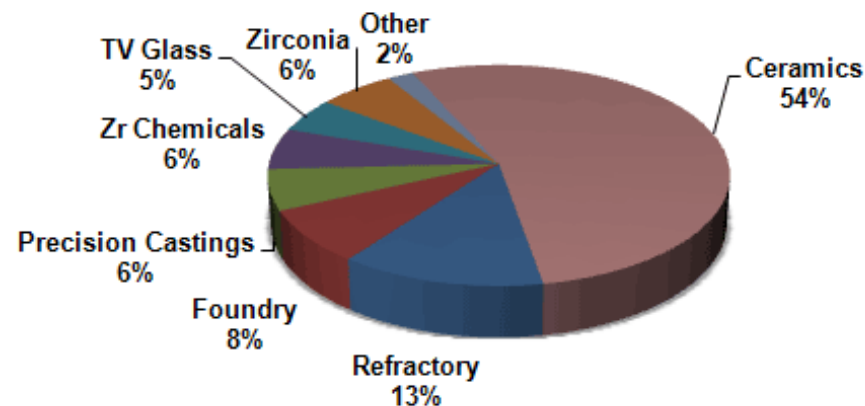
Commercial Oil Sands Processing

- hot water extraction → bitumen froth floatation / tailings solids
- heavy mineral solids concentrate in froth

Global Consumption of Titanium



Global Consumption of Zircon

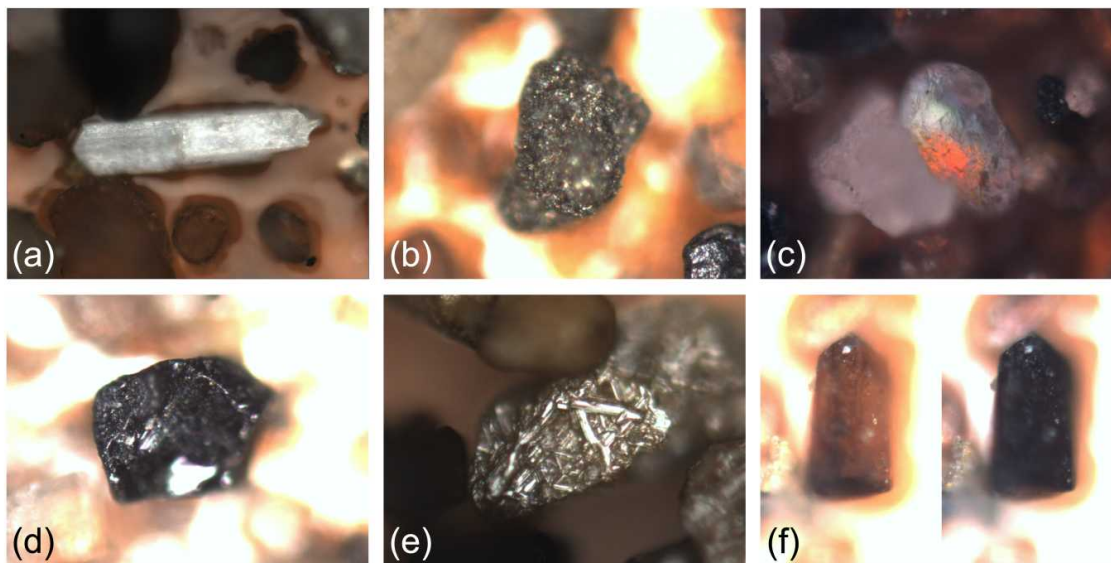


<http://www.titaniumcorporation.com>

Motivation & Research Objectives

Electrostatic and magnetic separation of HMC

- f) zircon (ZrSiO_4); e) rutile (TiO_2); d) ilmenite (FeTiO_3)
- c) quartz (SiO_2); b) pyrite (FeS_2); a) gypsum ($\text{CaSO}_4 \cdot 2\text{H}_2\text{O}$)

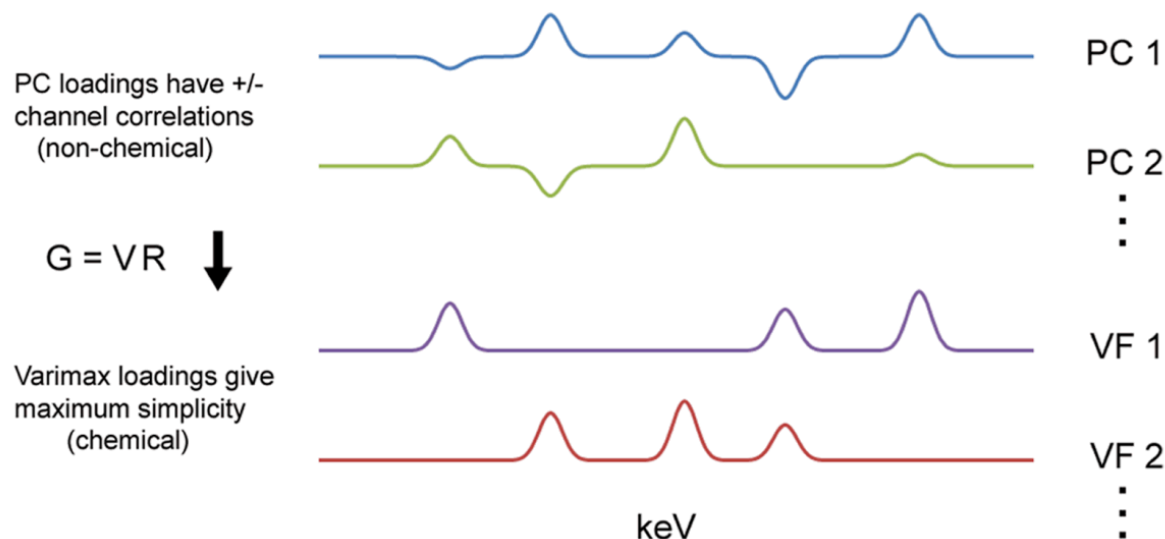


XPS study ←
1) mineral associations
2) surface condition

Multivariate Factor Analysis

Varimax rotation (R)

- improves factor interpretability
- component or spectral maximum simplicity*



* few minerals / spot, or
few elements / spectrum

Varimax criterion

$$\max_j \sum \sigma_j^2 (V_{i,j}^2)$$

spectral basis

$$G = VR$$

or

component basis

$$H = UR$$

Multivariate Factor Analysis

Varimax con't

- preserves orthonormality of rotated basis
- relaxed orthogonality in complementary domain

spectral basis

$$(VR)^T VR = I$$

$$(U\Sigma R)^T U\Sigma R \neq D$$

component basis

$$(UR)^T UR = I$$

$$(V\Sigma R)^T V\Sigma R \neq D$$

like factor
modeling



- * trade simplicity in one domain for contrast in other
- * choose constraints based on physical characteristics

Keenan, M. R. *Surf. Interface Anal.* **2009**, 41, 79.

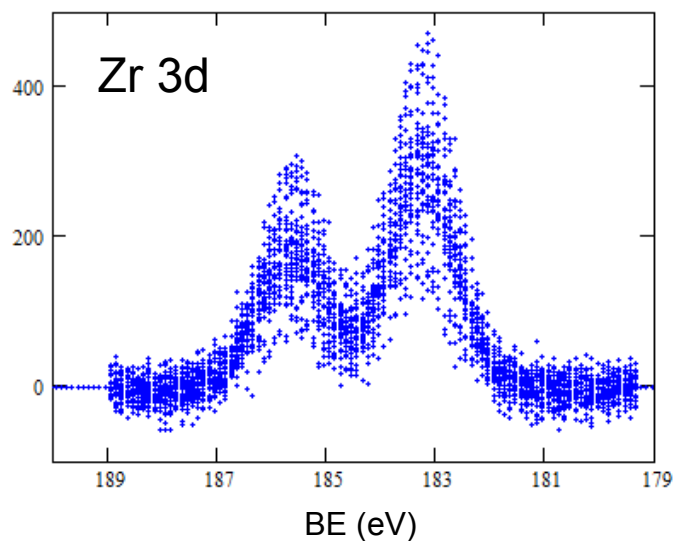
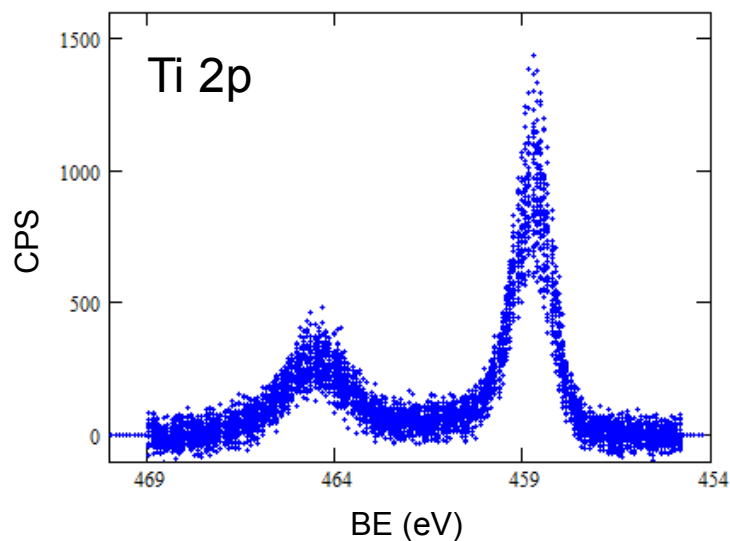
Smentkowski, V. S.; Ostrowski, S. G.; Keenan, M. R. *Surf. Interface Anal.* **2009**, 41, 88.



Large-Area Spectroscopy

Measurement - 300 x 700 μm spot area (5-10 particles per spot)

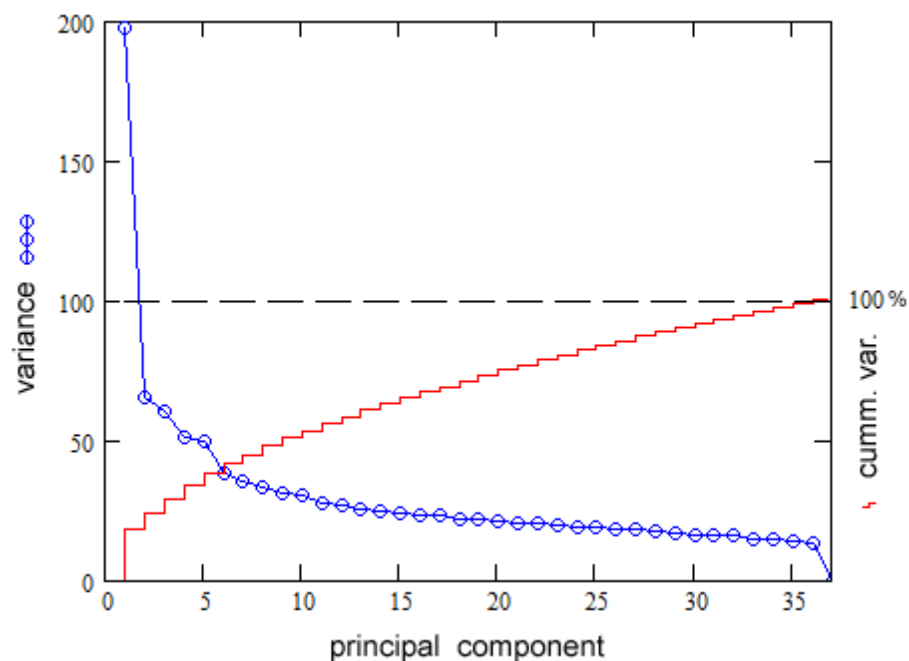
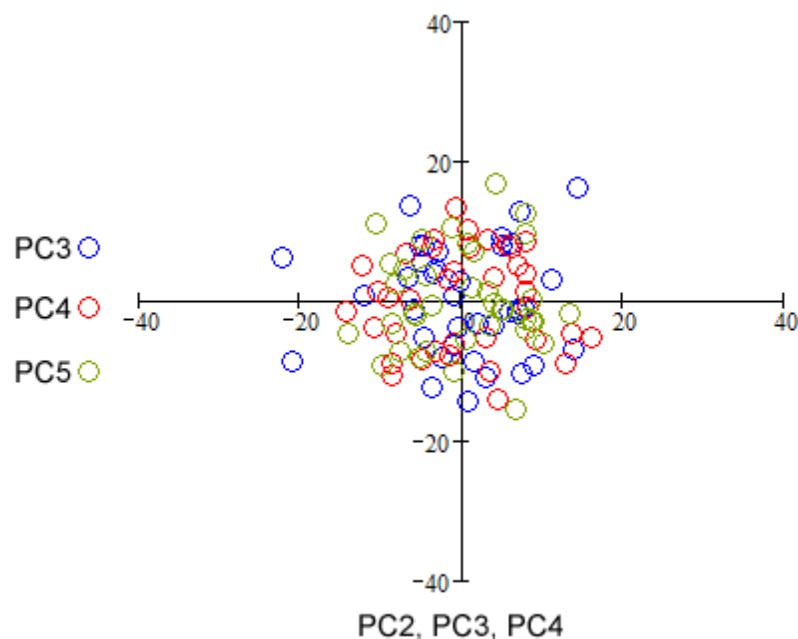
Pre-processing i) background subtraction / concatenate regions
ii) standardization (mean-center / unit variance)



raw data
37 spots

Large-Area Spectroscopy

PCA score plot and variance (eigenvalues)



- no component classification
- 6 factors retained for spectral rotation

Large-Area Spectroscopy

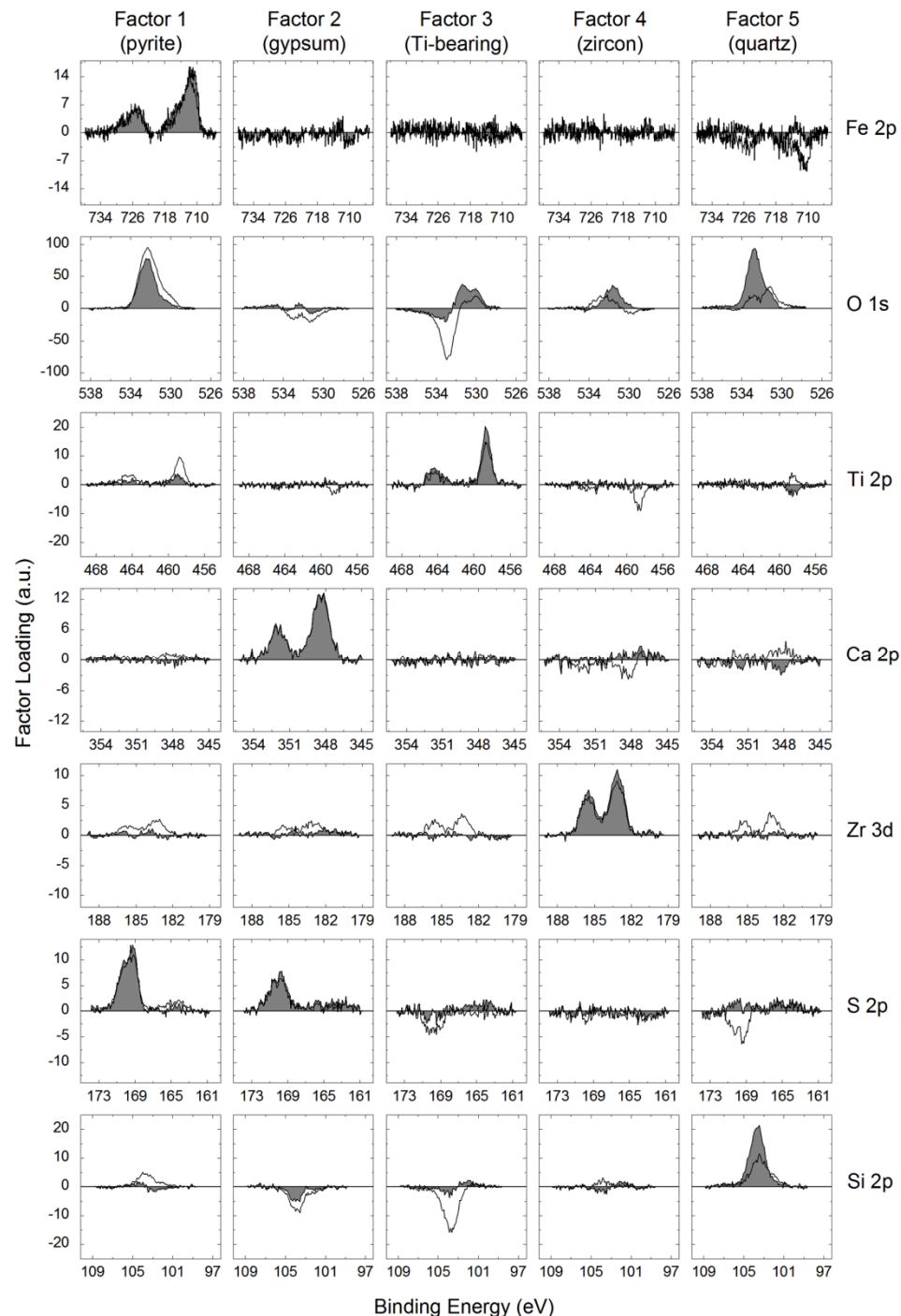
Loadings Spectra (σV and σVR)

- orthonormal V and VR
- Varimax rotation (filled)
- PCA (solid line)

Interpretation

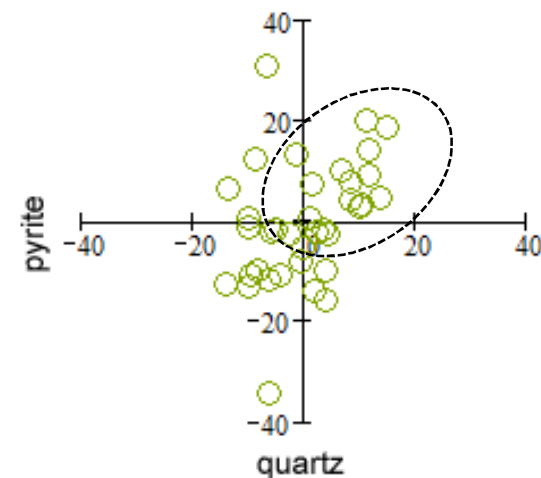
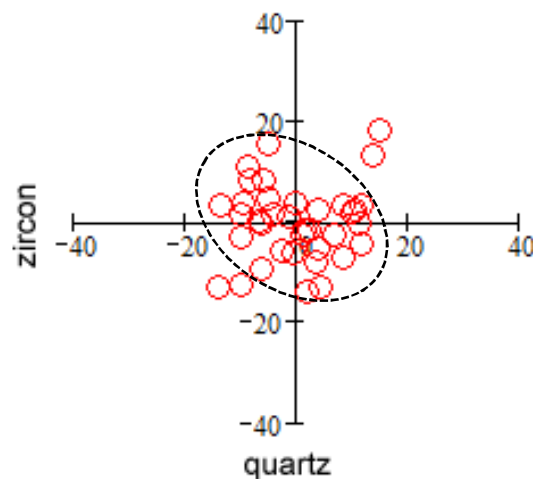
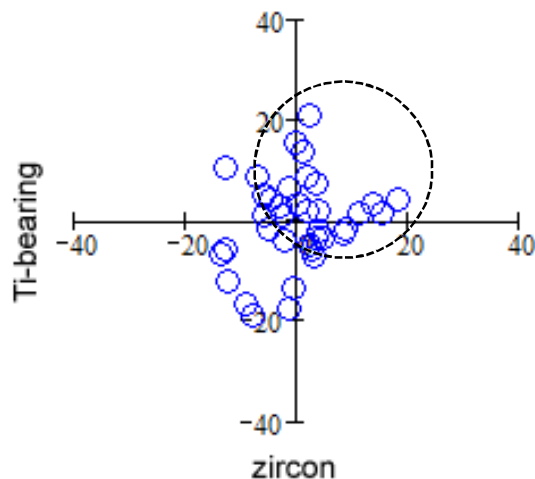
- simplifies factor correlations
→ better chemical representation
- Ti-bearing: can't distinguish TiO_2 from *altered* ilmenite

$\downarrow$ *weathering*
 spectral overlap
 $\text{FeTiO}_3 \rightarrow \text{TiO}_2$



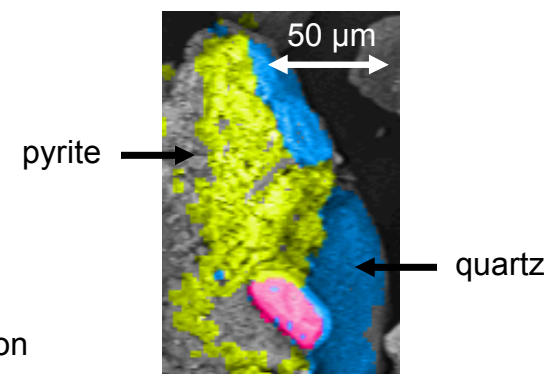
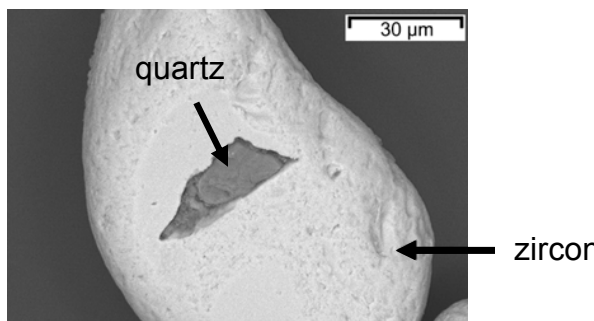
Large-Area Spectroscopy

Rotated Factor Scores



- some inclusion in smaller particles

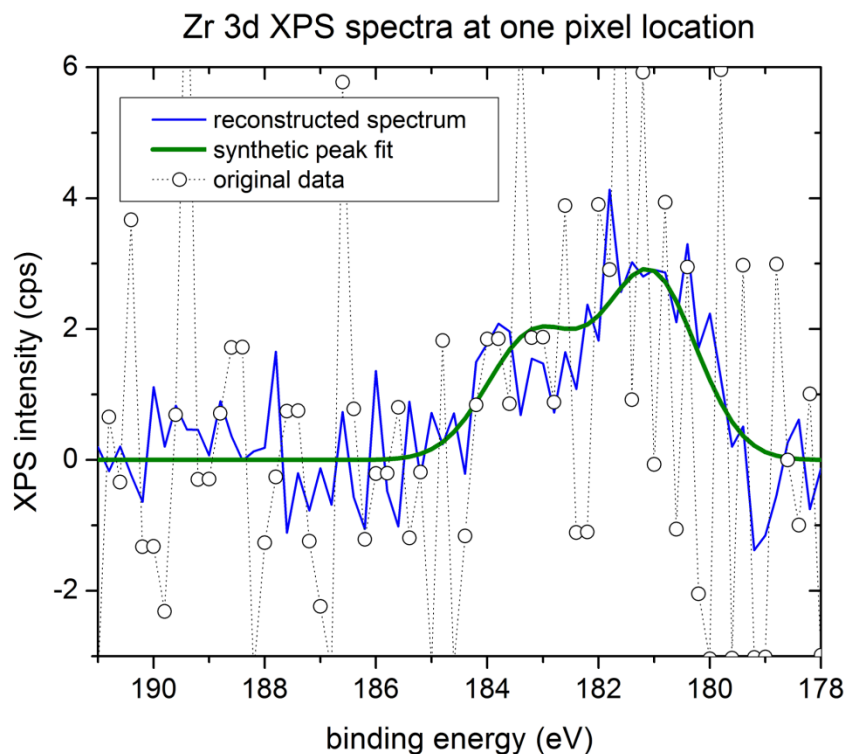
- large liberated particles
- electrostatic separation !



Surface Component Imaging

Data Cube

- 256 x 256 pixels (3 x 3 μm / pixel) ~ 20 μm features
- 567 BE channels in 0.2 eV steps



PCA data reconstruction

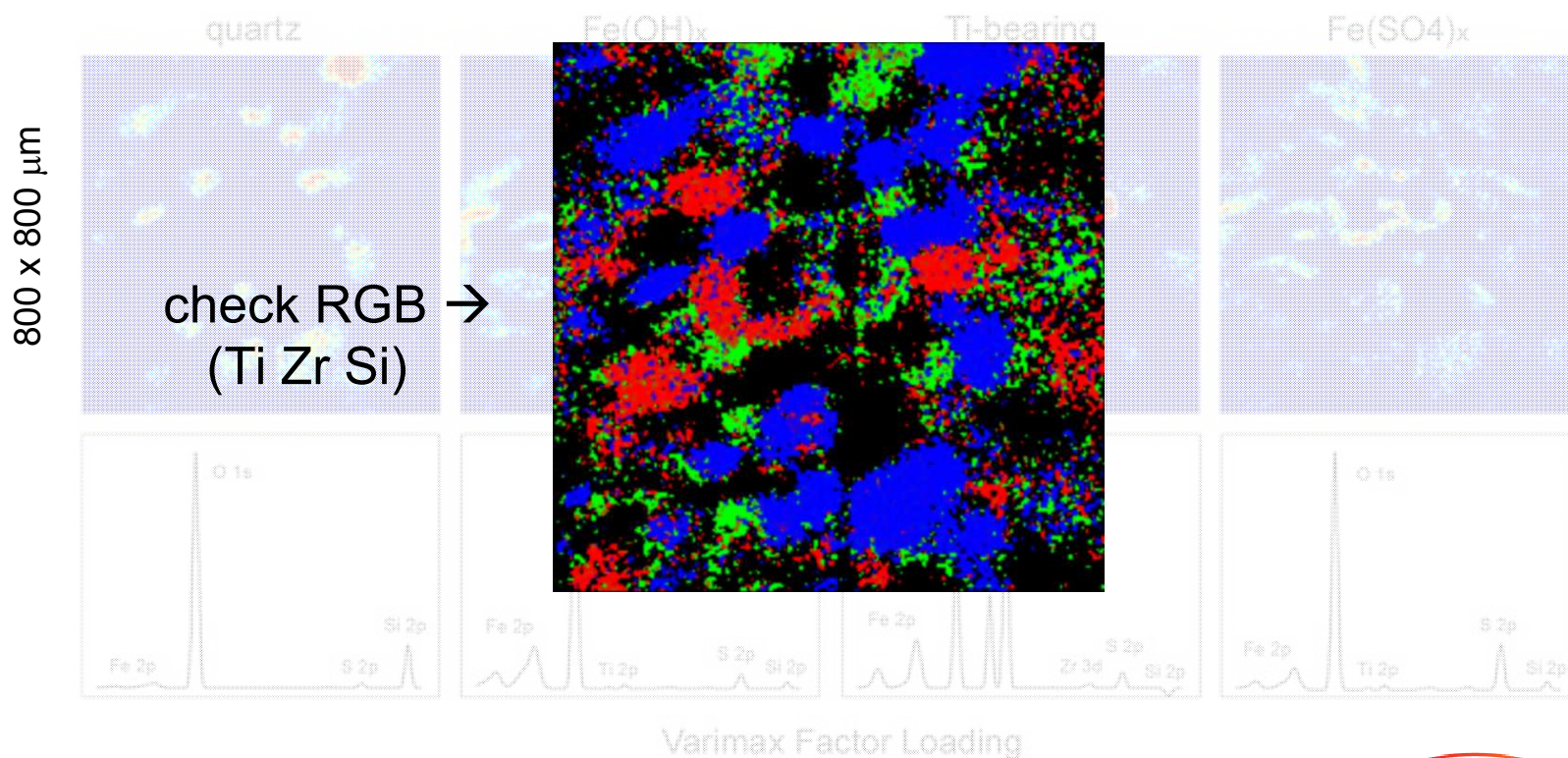
- noise reduction / peak fitting
- spectral integration
- elemental RGB images



Surface Component Imaging

Varimax Rotation ($V\Sigma R$) on synthetic fit spectra

- orthonormal score images (UR), but w/o spatial simplicity
- surface components $\rightarrow$ pyrite weathering



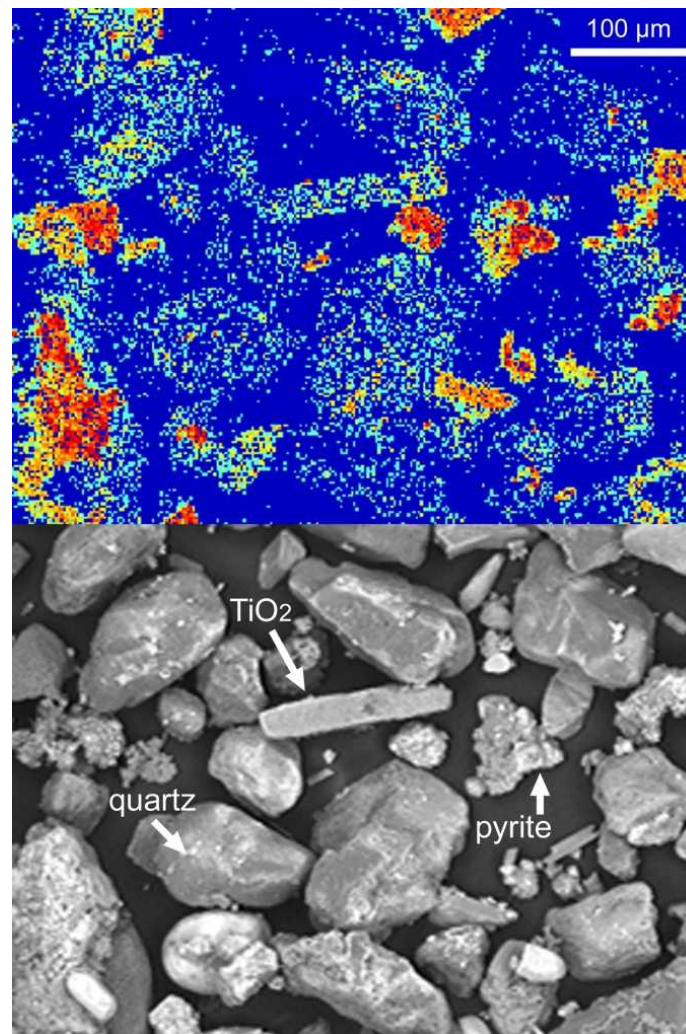
Surface Component Imaging

check SEM-EDX

- sulphur channel $K\alpha$ 2.3 keV
- off-peak background subtraction
- compare to backscattering image



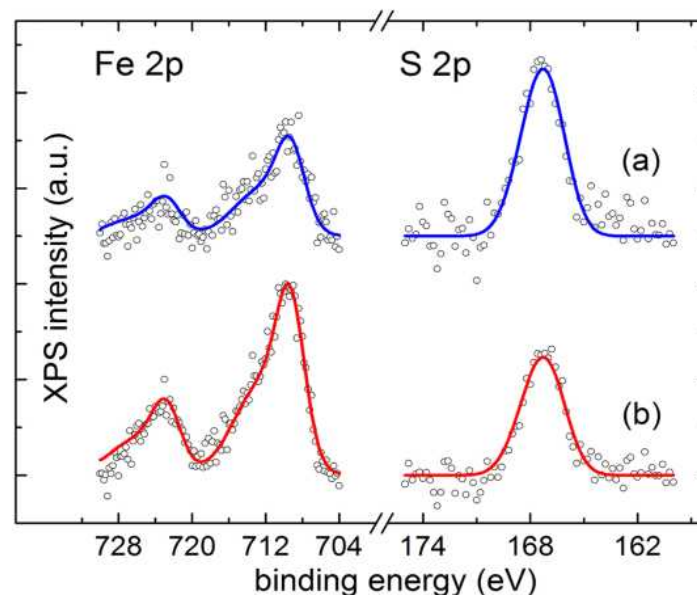
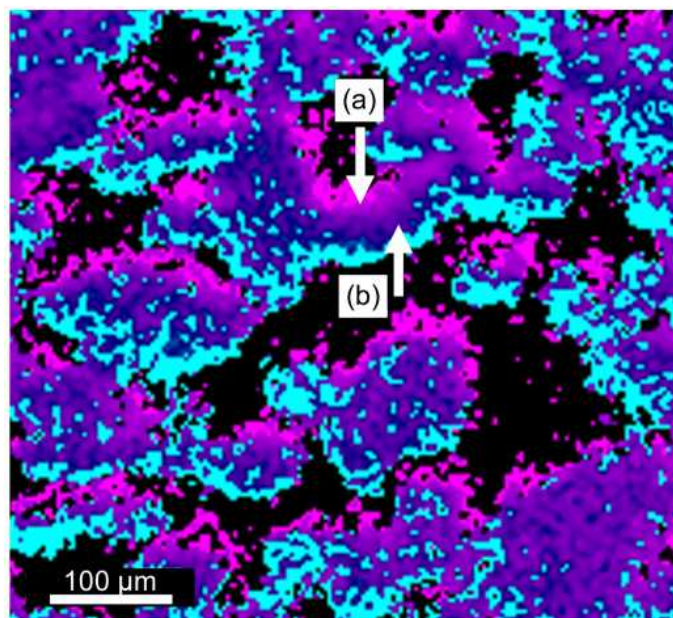
solid pyrite and surficial component



Surface Component Imaging

check PCA reconstructed image

- Fe (cyan) and S (magenta)
- relative proportion maps to new vector in 3-colour space
- shadow effect suggests bi-layering



Summary:

- LAS Varimax rotation VR → factor loadings like mineral chemistry
- LAS factor scores indicate mineral associations
 - i) particle liberation for Ti and Zr heavy minerals
 - ii) quartz / zircon inclusions
 - iii) pyrite / quartz physical association
- imaging Varimax rotation ($V\Sigma R$) → uncorrelated score images (UR)
- surface components resolved consistent with pyrite weathering (iron hydroxides / iron sulphates)





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