Multivariate factor analysis of heavy minerals concentrate from Athabasca Oil Sands tailings by XPS

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

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TITANIUM CORPORATION

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Presentation Overview :

1) Motivation & Research Objectives

2) Multivariate Factor Analysis

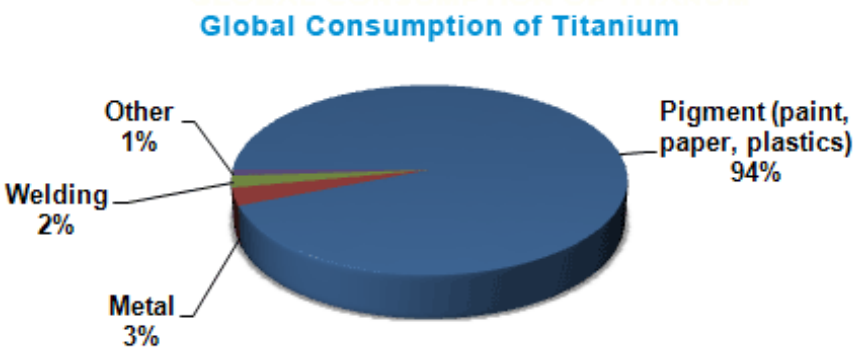
3) Large-Area Spectroscopy

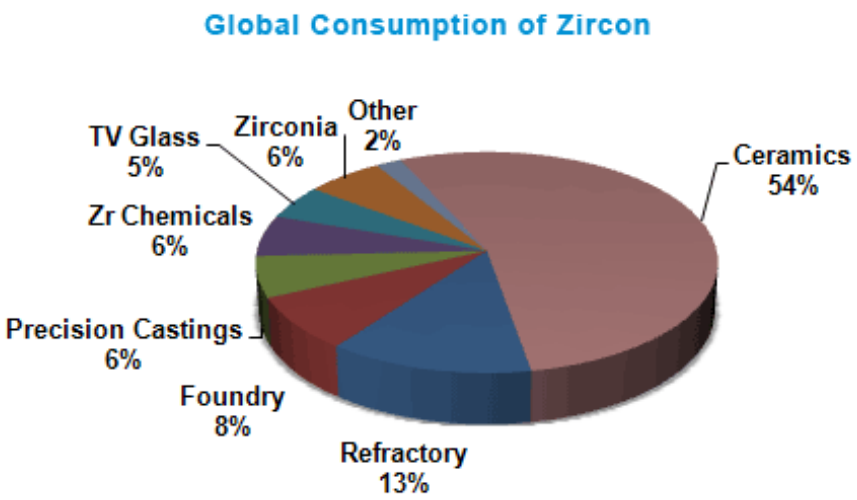
4) Surface Component Imaging

Motivation & Research Objectives

Commercial Oil Sands Processing

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



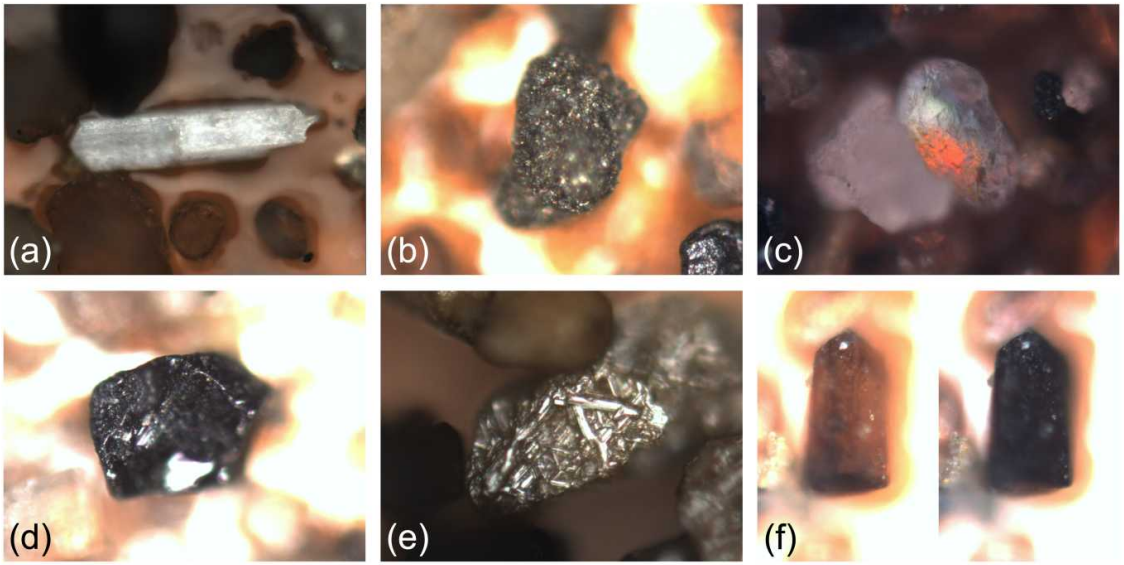


http://www.titaniumcorporation.com

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 ($CaSO_4 \cdot 2H_2O$)



XPS study ↵

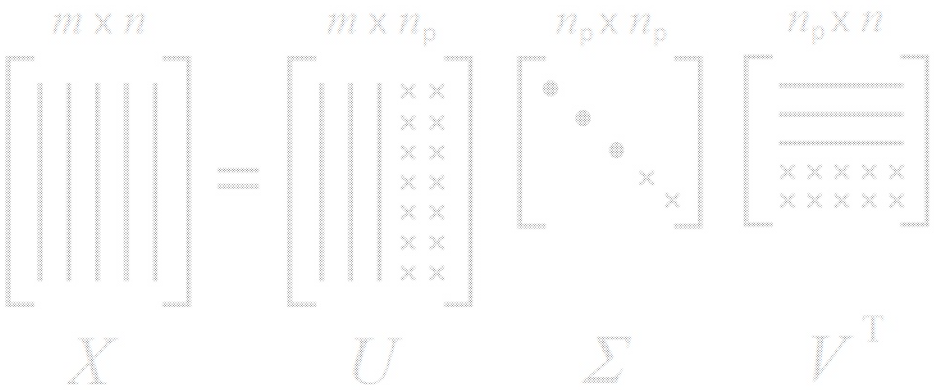
1) mineral associations
2) surface condition

Multivariate Factor Analysis

Principal Components Analysis (PCA) $X = S V^{T}$

- → variable reduction
- → scores (S) & loadings (V)
- → orthogonal factors (uncorrelated)
- → within factor variable correlations

Spectral Analysis



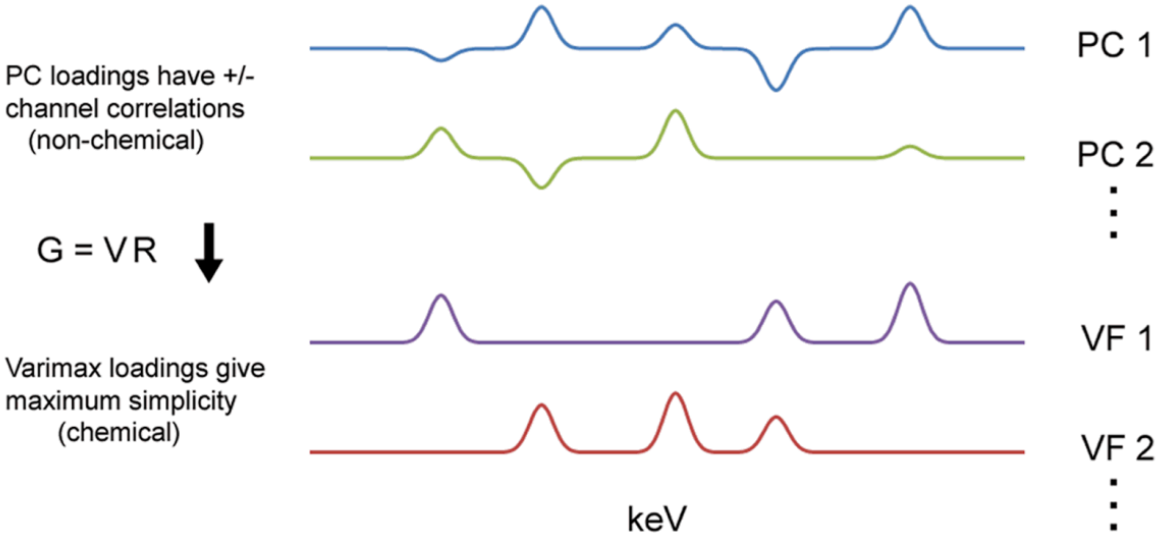
- PCA factorization by SVD
- component & spectral bases
- ordered by significance
- noise reduction

Multivariate Factor Analysis

Varimax rotation (R)

→ improves factor interpretability

→ component or spectral maximum simplicity*



Varimax criterion

$$\max \sum_j \sigma_j^2 (V_{i,j}^2)$$

spectral basis

$$G = VR$$

or

component basis

$$H = UR$$

* few minerals / spot, or
few elements / spectrum

Multivariate Factor Analysis

Varimax con't

→ preserves orthonormality of rotated basis

→ relaxed orthogonality in complementary domain

spectral basis	component basis
$(VR)^{\mathrm{T}} VR = I$	$(UR)^{\mathrm{T}} UR = I$
$(U\Sigma R)^{\mathrm{T}} U\Sigma R \neq D$	$(V\Sigma R)^{\mathrm{T}} V\Sigma R \neq D$

like factor modeling

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

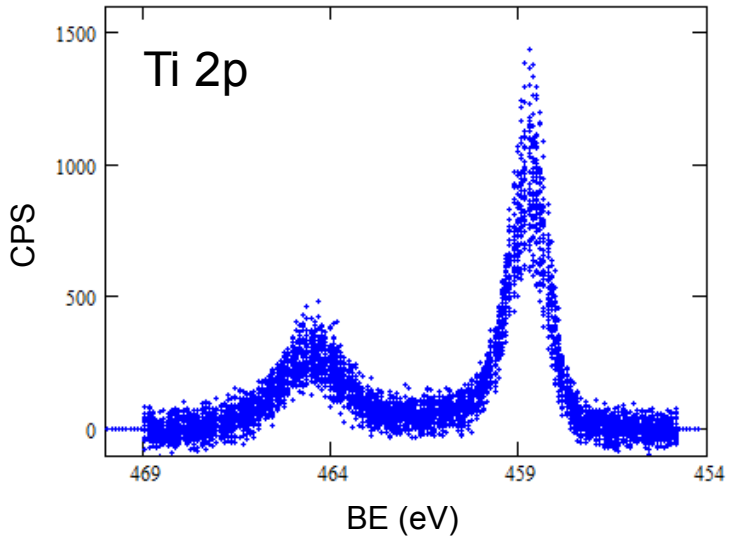
Keenan, M. R. *Surf. Interface Anal.* **2009**, *41*, 79.

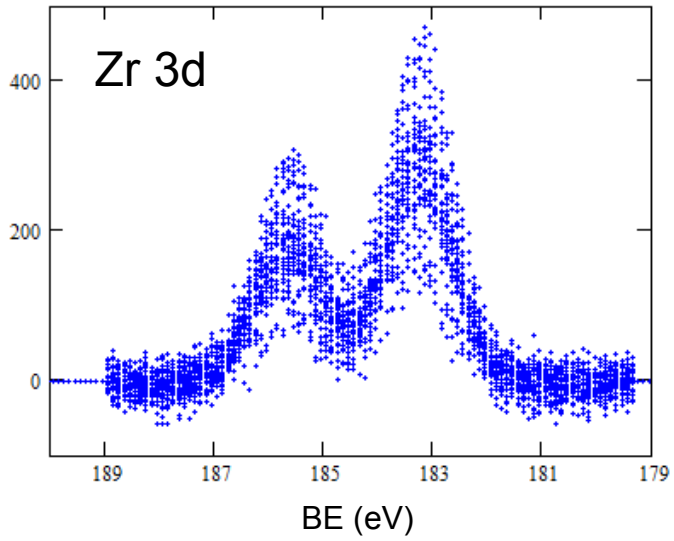
Smentkowski, V. S.; Ostrowski, S. G.; Keenan, M. R. *Surf. Interface Anal.* **2009**, *41*, 88.

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)

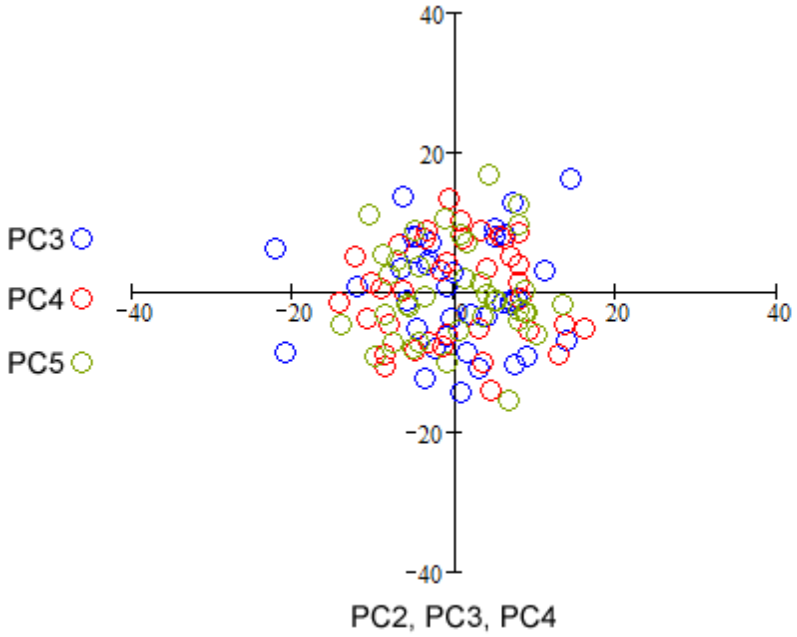


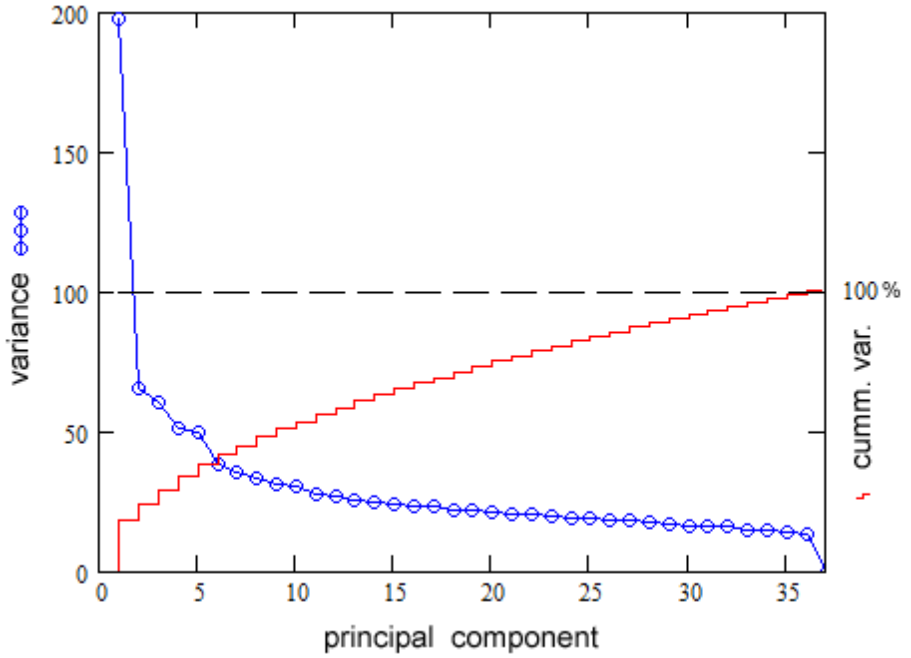


raw data
37 spots

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)

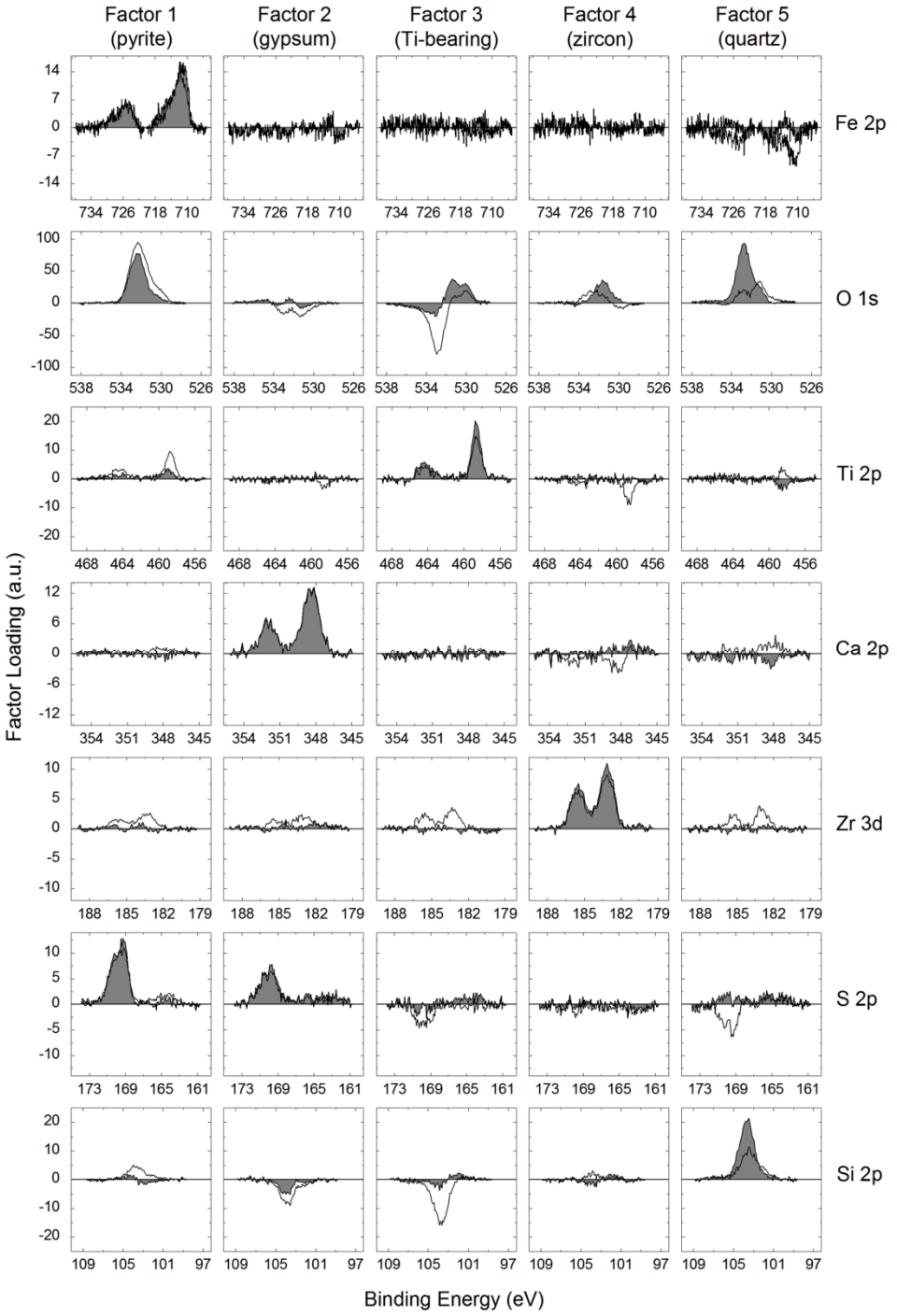
Interpretation

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

↓ *weathering*

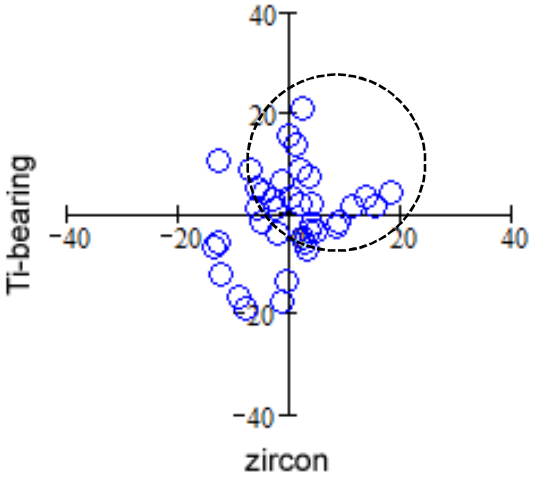
spectral overlap

$FeTiO_3$ → TiO_2

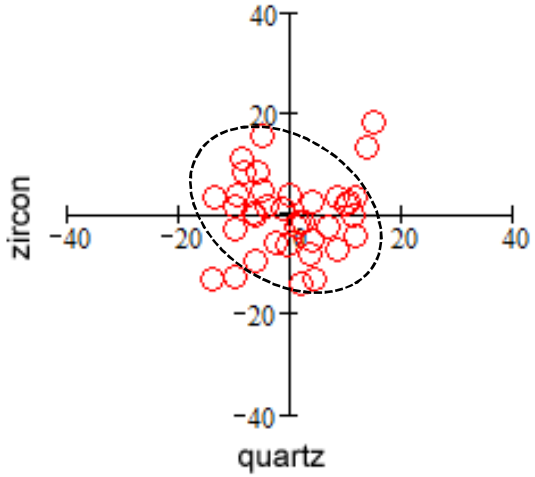


Large-Area Spectroscopy

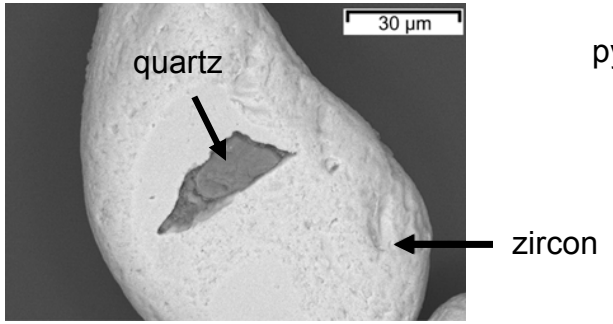
Rotated Factor Scores

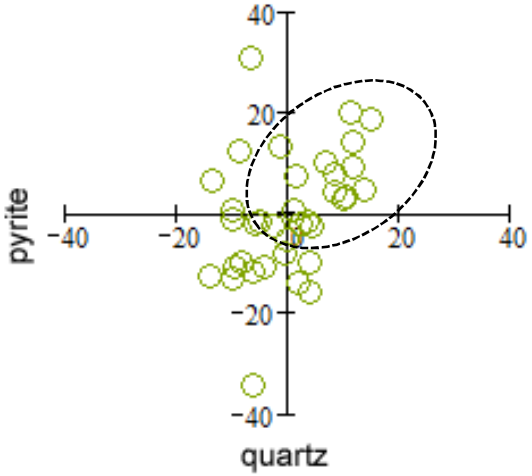


- large liberated particles
- electrostatic separation !

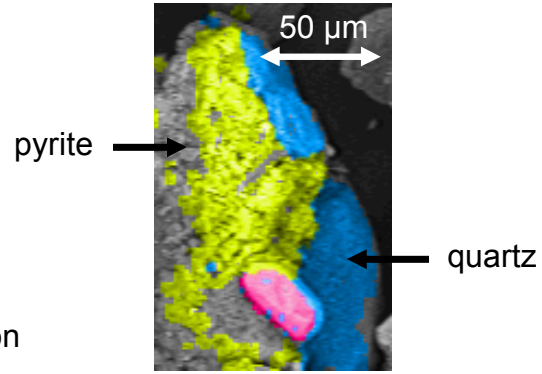


- some inclusion in smaller particles





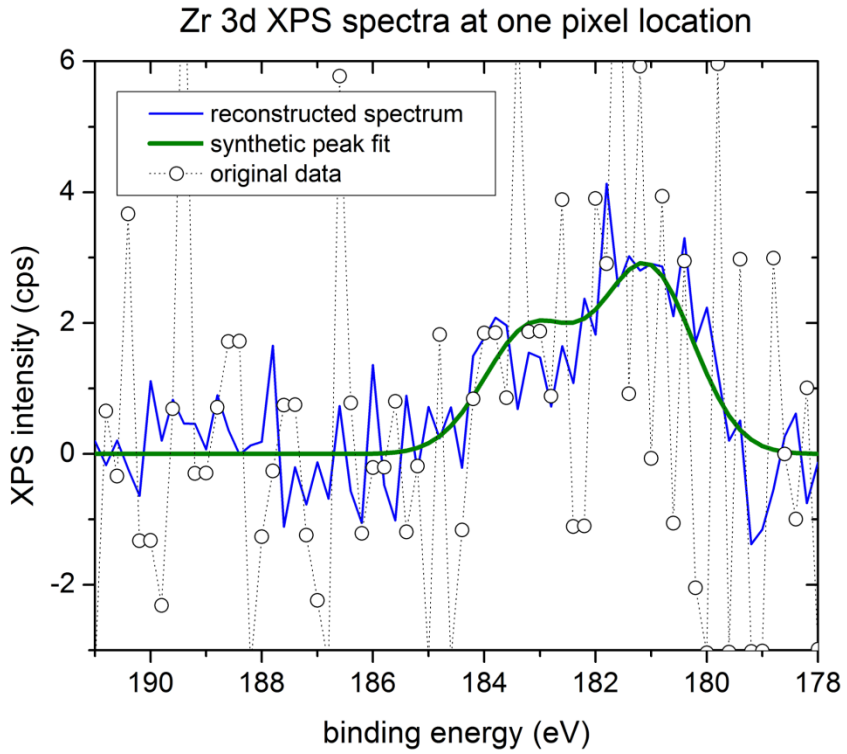
- physical association
- pyrite floatation



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



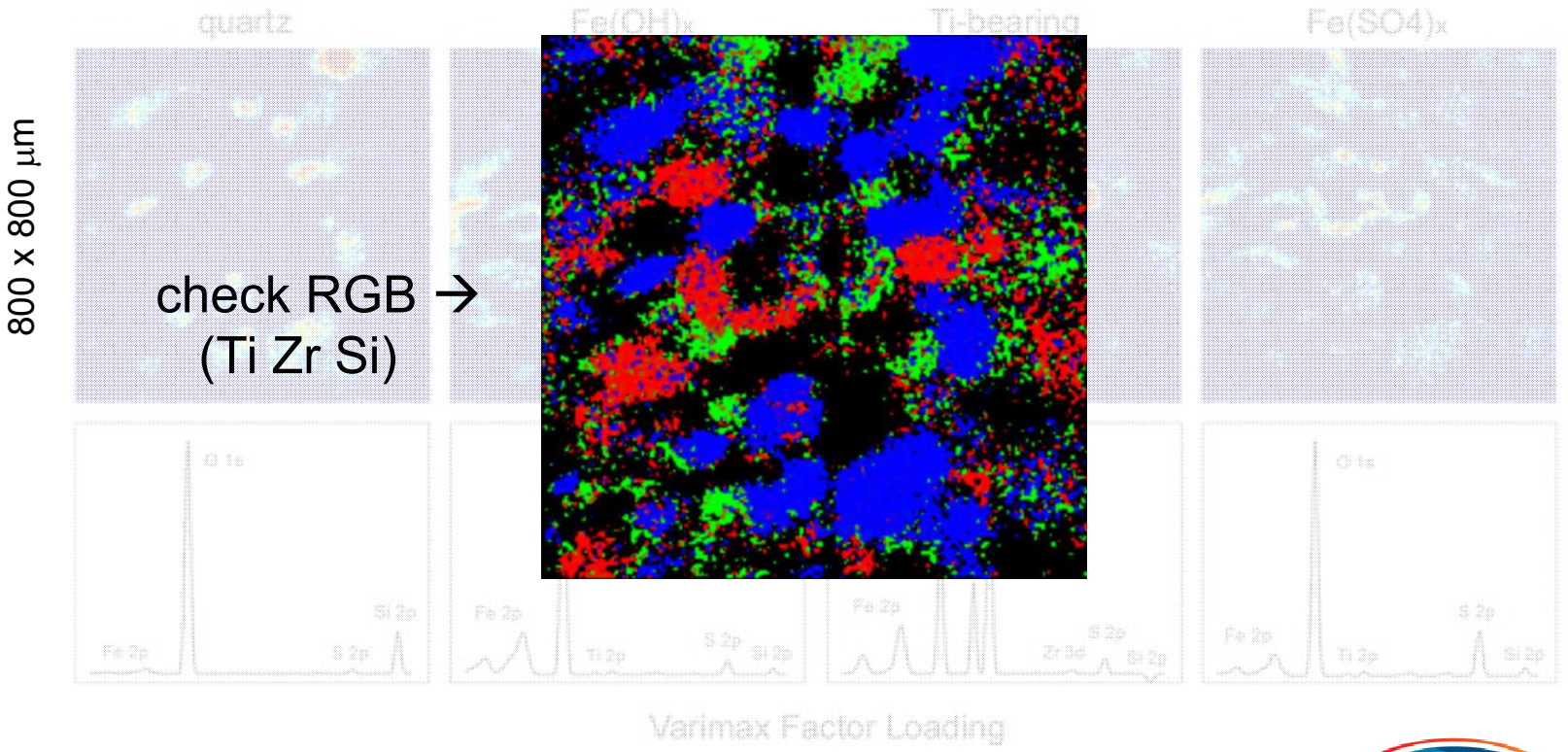
PCA data reconstruction

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

Surface Component Imaging

Varimax Rotation (VΣR) on synthetic fit spectra

- orthonormal score images (UR), but w/o spatial simplicty
- surface components → pyrite weathering



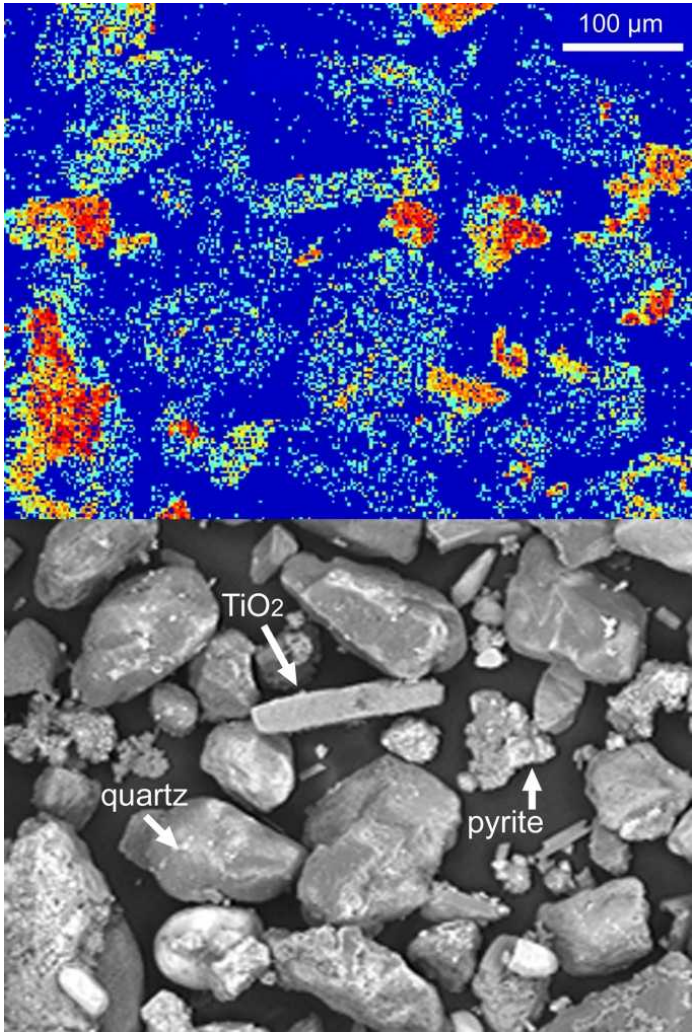
Surface Component Imaging

check SEM-EDX

- sulphur channel Kα 2.3 keV
- off-peak background subtraction
- compare to backscattering image

↓

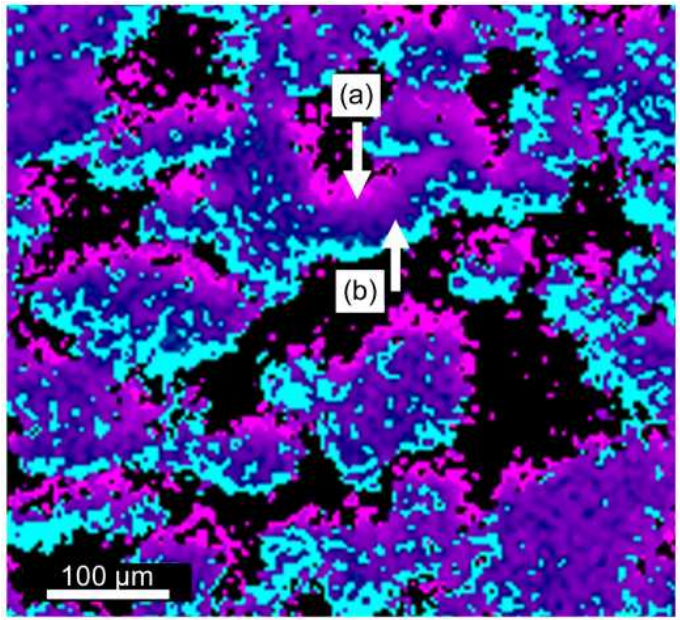
solid pyrite and surficial component

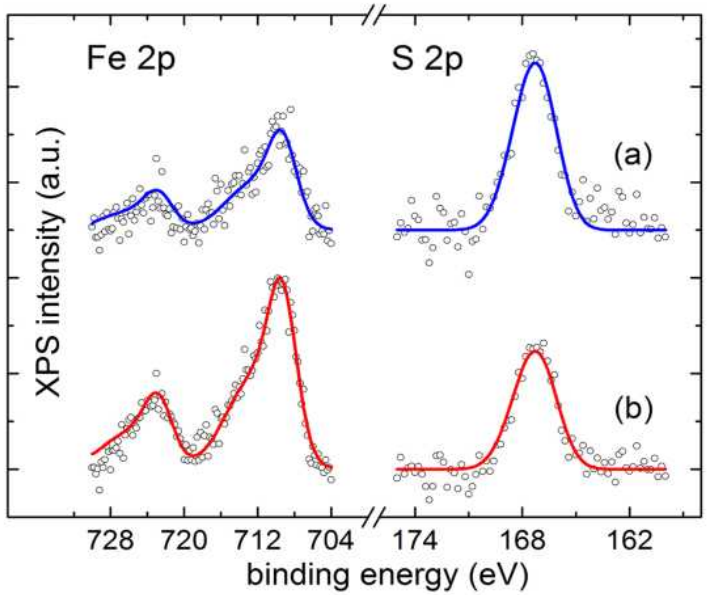


Surface Component Imaging

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 liberatation for Ti and Zr heavy minerals
  - ii) quartz / zircon inclusions
  - iii) pyrite / quartz physical association
- imaging Varimax rotation (VΣR) → uncorrelated score images (UR)
- surface components resolved consistent with pyrite weathering (iron hydroxides / iron sulphates)

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