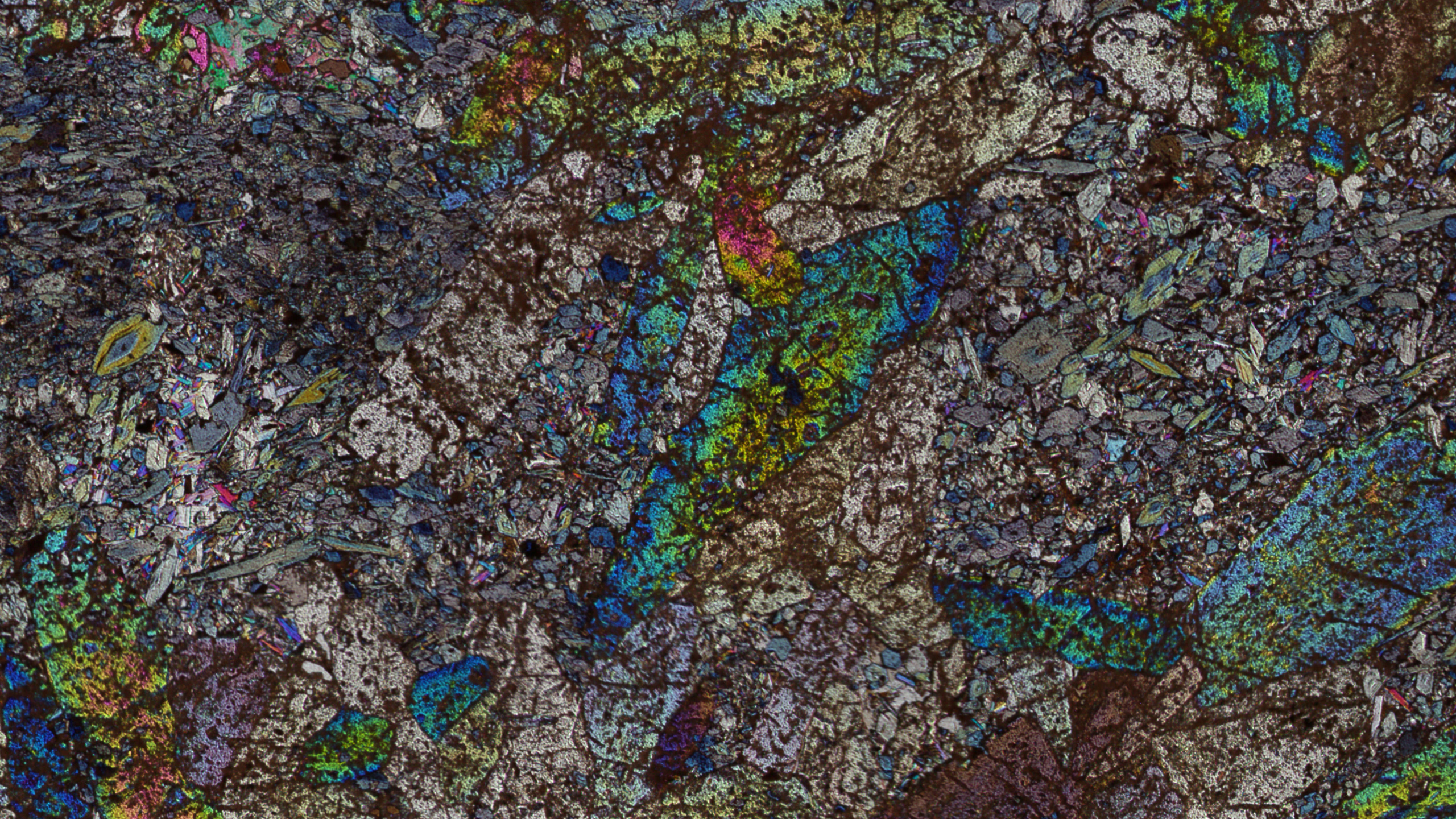
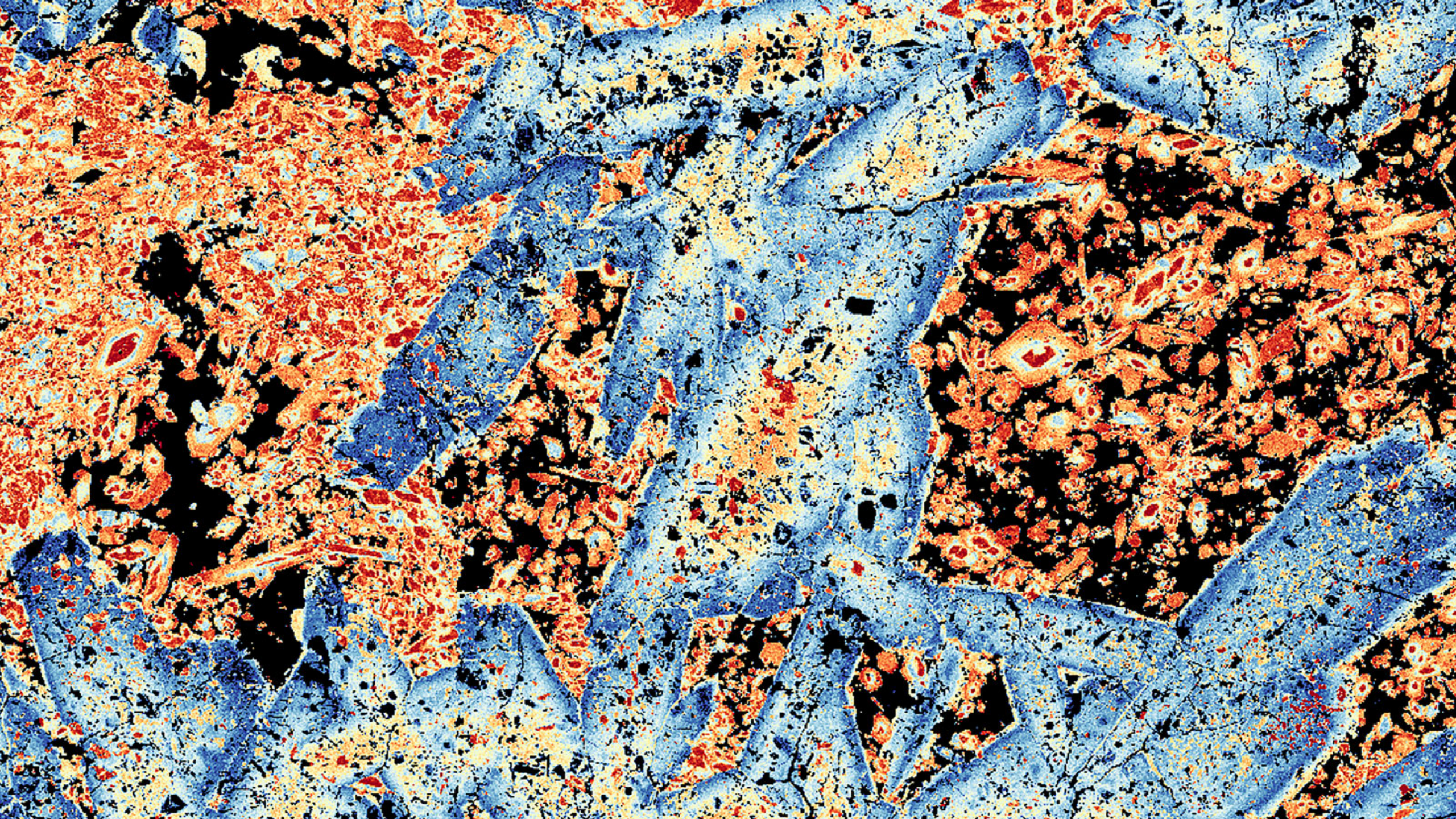
PHASE EQUILIBRIUM MODELING
APPROACHES AND PITFALLS

XMapTools

Pierre Lanari

Virtual workshop, May 10th to 14th 2021

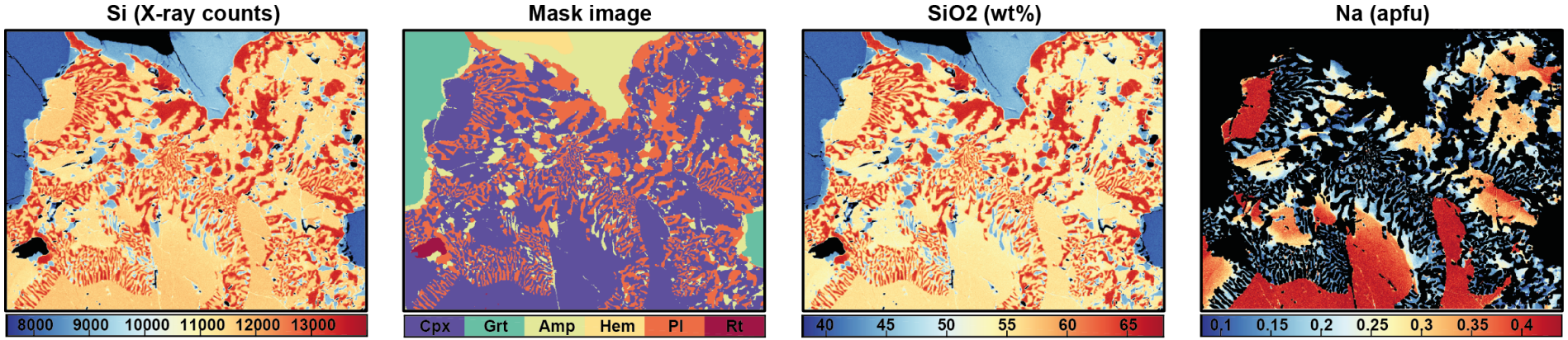




XMapTools

Semi-quantitative

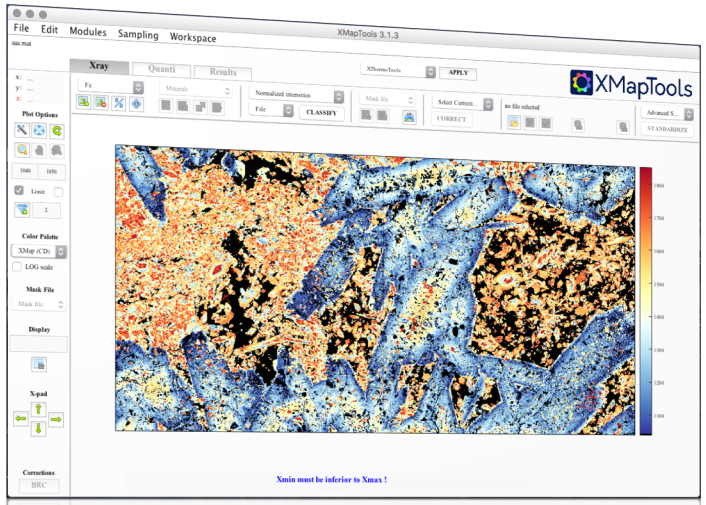
Quantitative



Data from Lanari et al. (2013), Geology

EPMA
X-ray maps
350'000 pixels for 15 elements
10-40 h

Data processing
1-2 h max
Maps of structural formula
Local bulk composition



XMapTools

- ✓ A free (MATLAB-dependent) software solution developed by a petrologist
- ✓ No secret algorithm or obscure data reduction scheme (publications, source code available)
- ✓ Free for academic research; large community of users
- ✓ Largely compatible with EPMA, SEM and LA-ICP-MS data (among other)

Lanari et al. (2014; 2019)

XMapTools

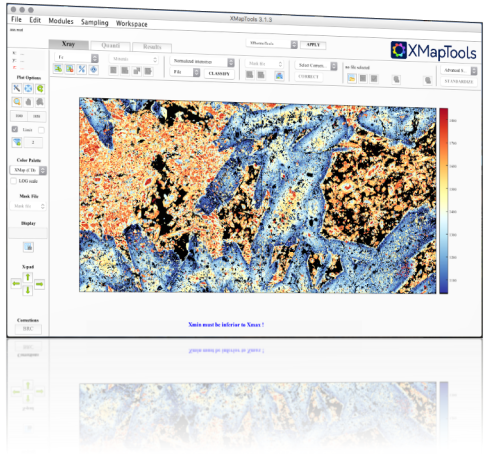
What is XMapTools and what does it do?

Data reduction (EPMA)

Selected examples of application

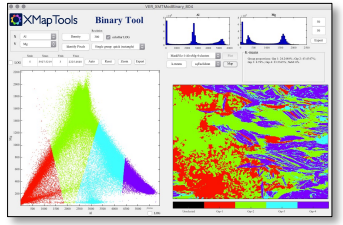
A set of tools for quantitative petrology

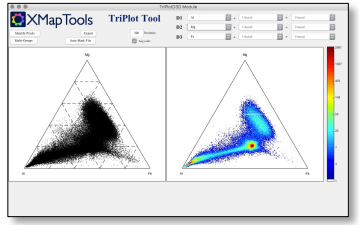
Main GUI

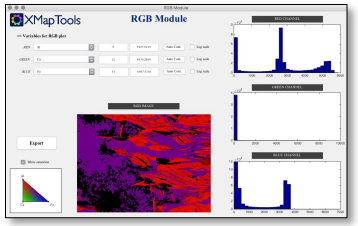


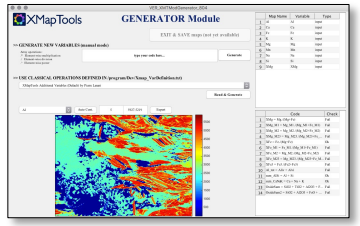
Chemical Modules

Binary, Triplot, RGB, Generator

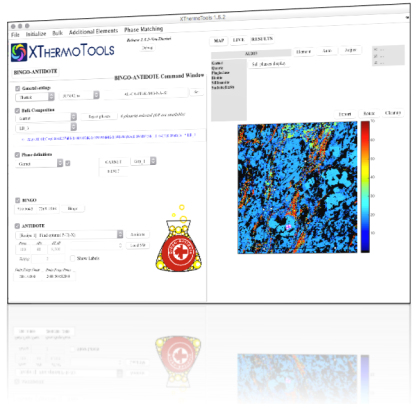








Add-ons



A guided environment for

- ✓ Classification
- ✓ Standardization
- ✓ Normalization
- ✓ Data extraction

- ✓ Data exploration and visualization
- ✓ Manual classification & clustering
- ✓ Generation of new maps

Sign up and give XMapTools a try at www.xmaptools.com

Acquisition of spots (wt%)

Acquisition of maps (counts.s^{-1}) → **Classification** *Image analysis* → **Standardization** *(oxide wt%)* → **Additional calculations** *e.g. Structural formulas*

EPMA / SEM

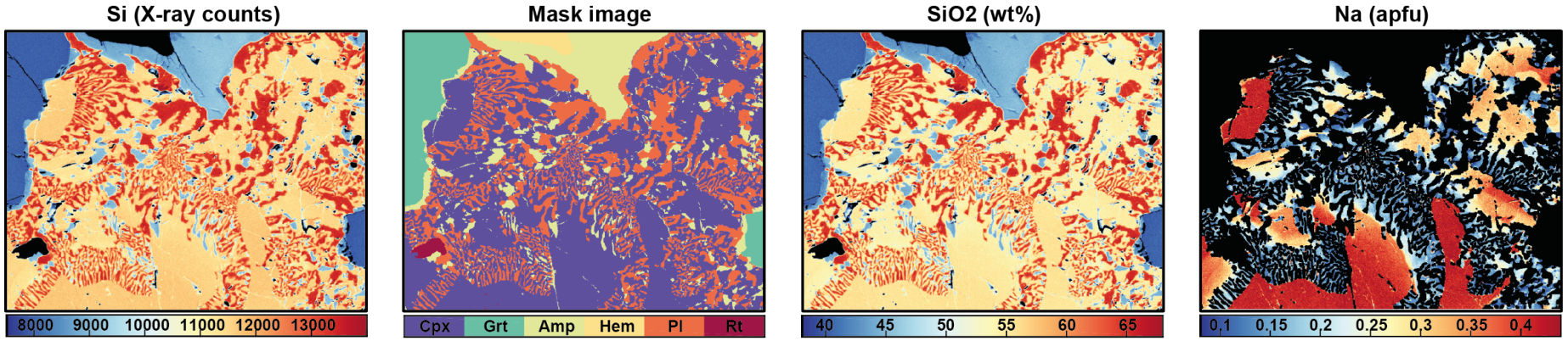
EDS
WDS
BSE / SEI / TOPO

+ corrections

Automated (supervised)
Manual

Internal standards + pseudo background correction

Structural formulas
Binary diagrams
Ternary diagrams
Maps of element ratios
Automated tools



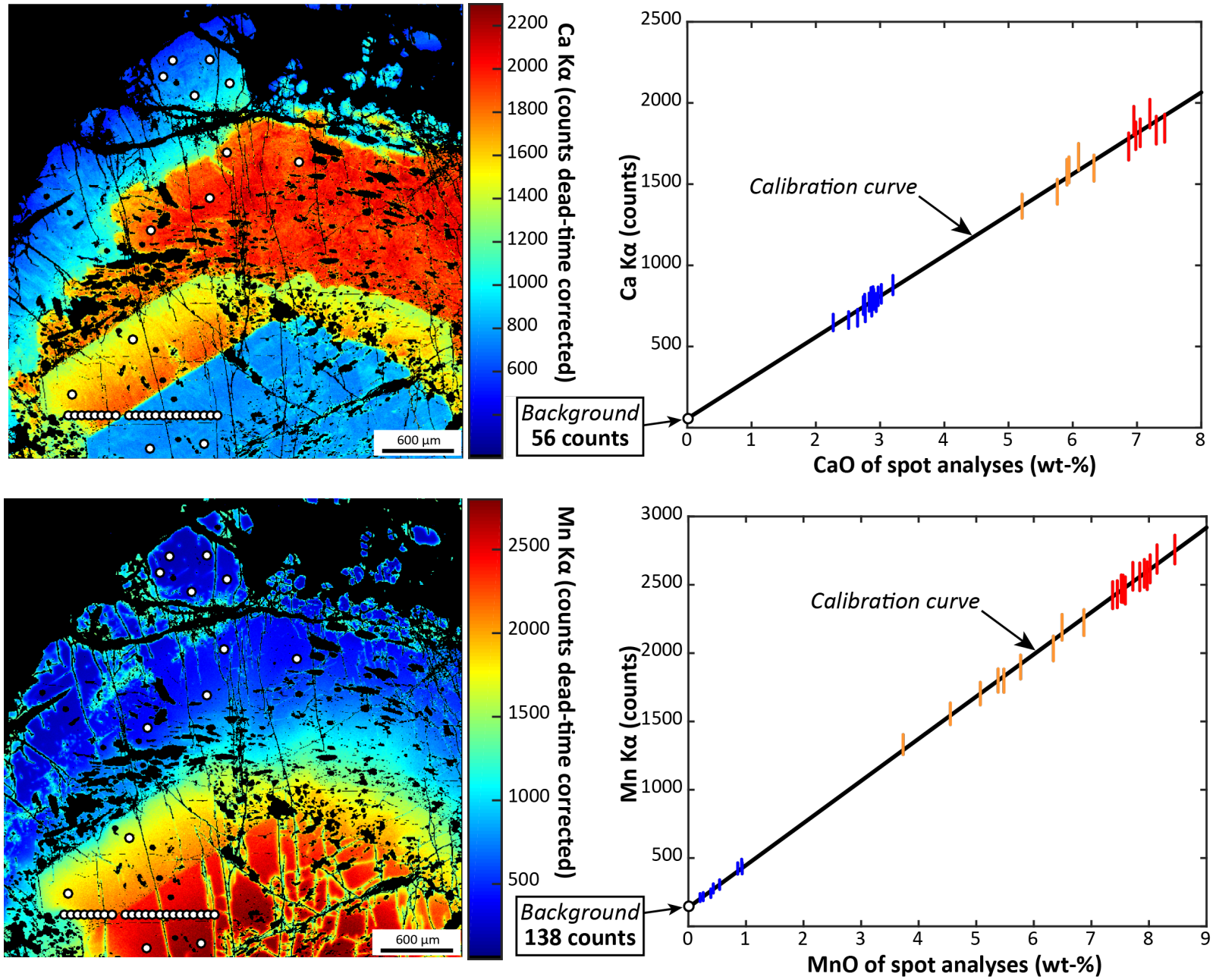
Quick (usually < 30 s)

Assisted calibration for each mineral

Quick and versatile

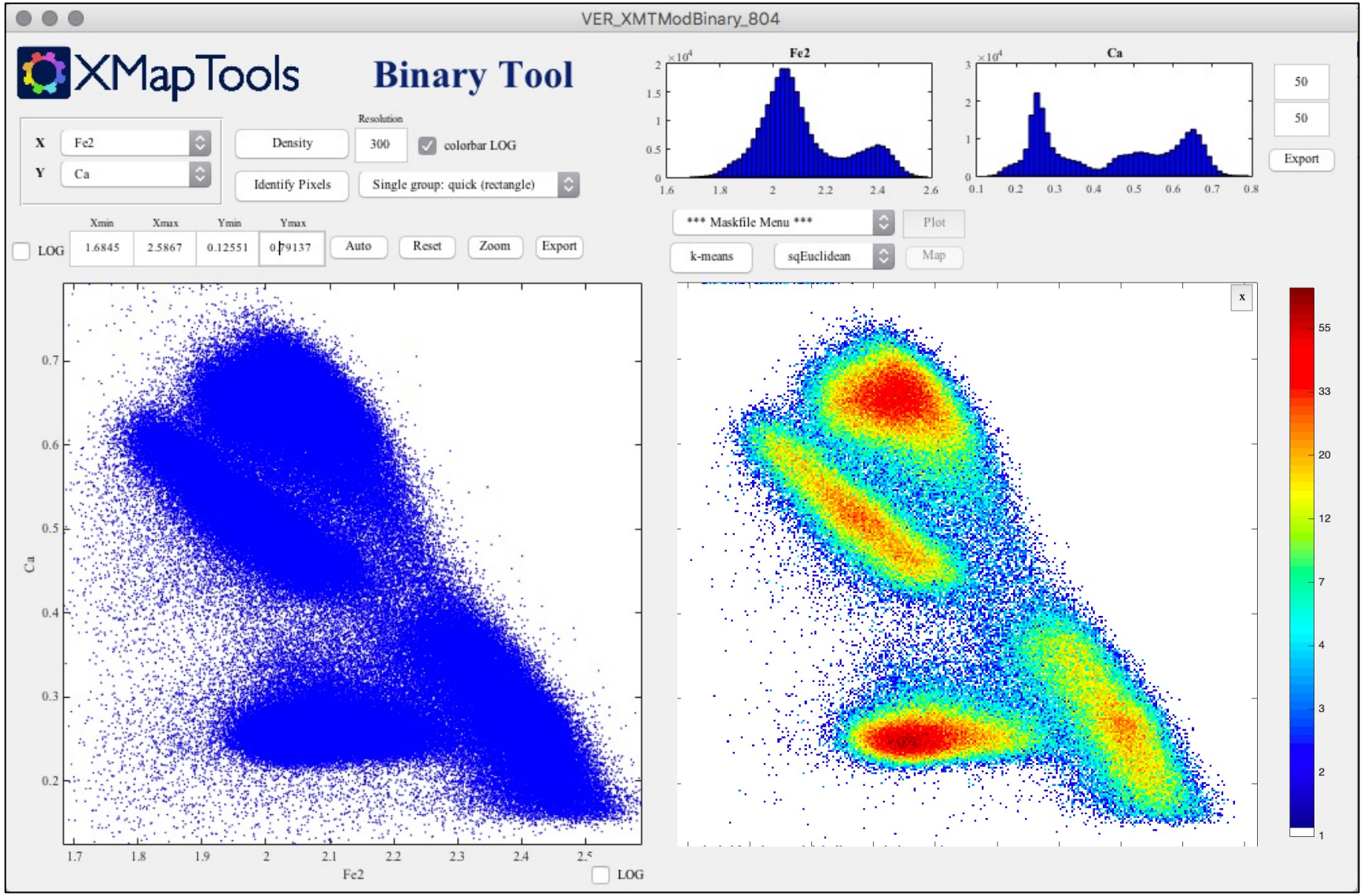
Lanari et al. (2014; 2019)

Map calibration using internal standards and a pseudo-background correction



XMapTools

Map calibration using internal standards and a pseudo-background correction



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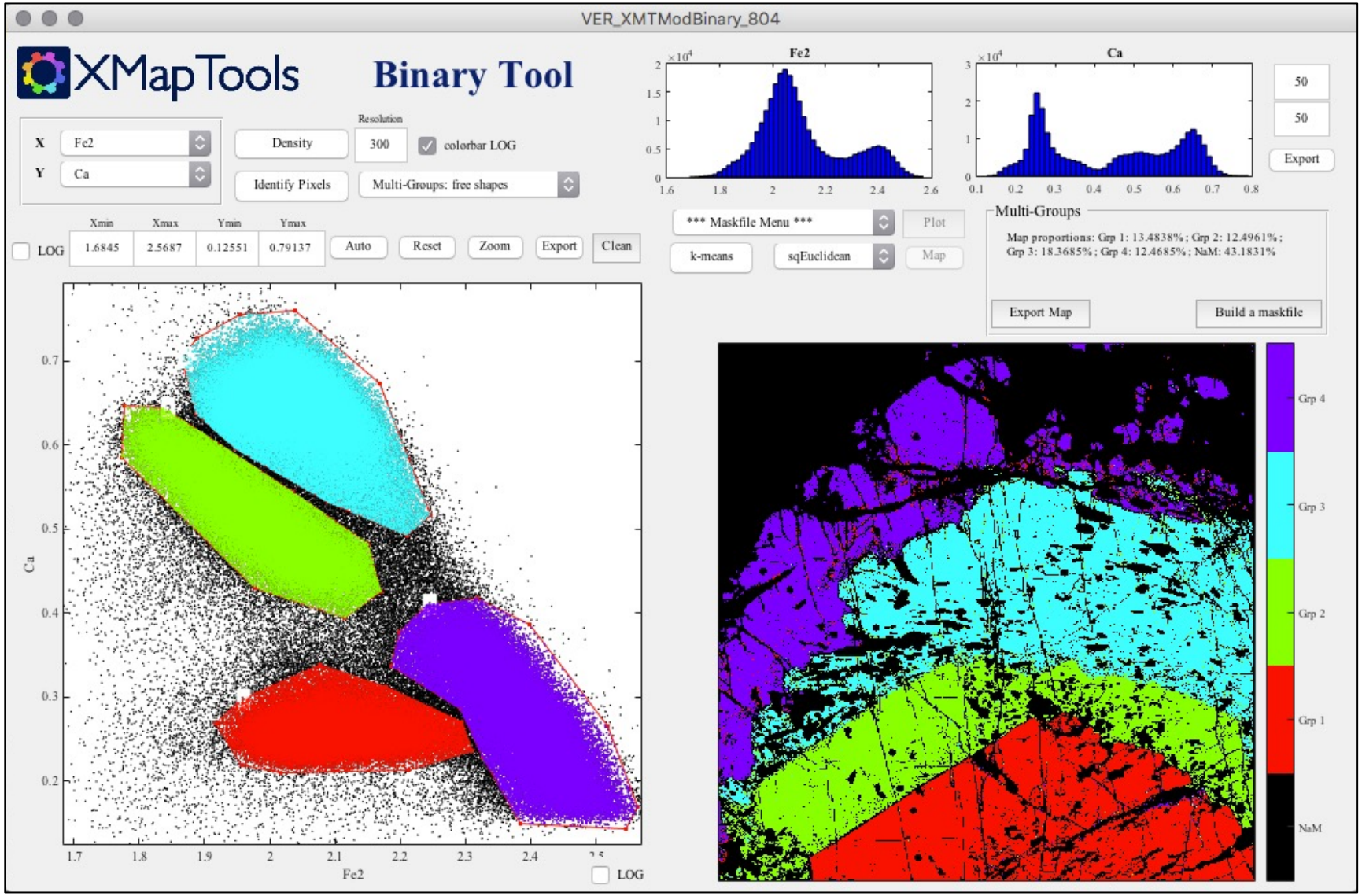
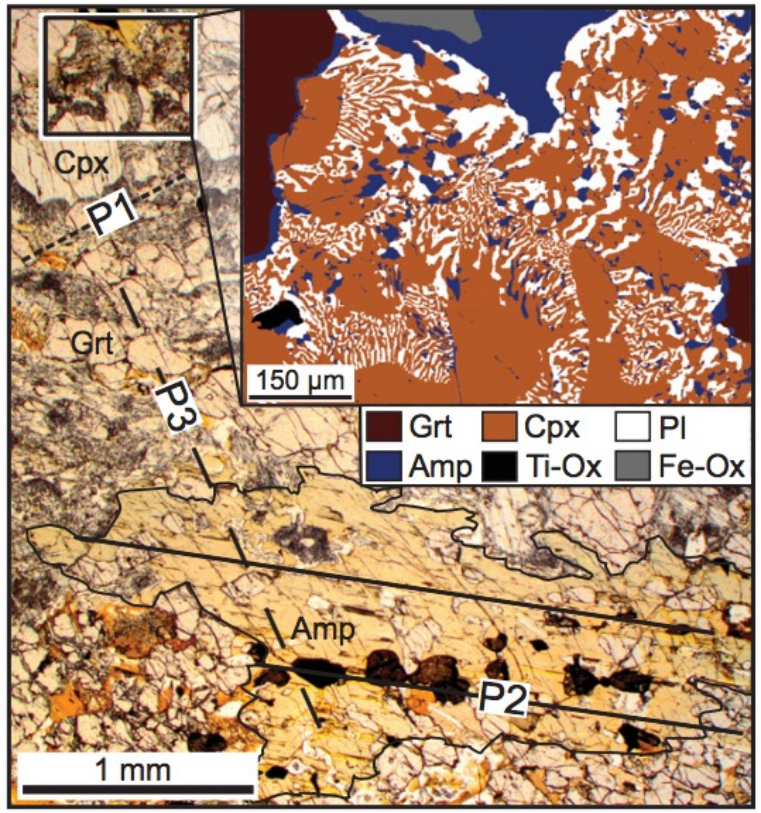


Friday's topics

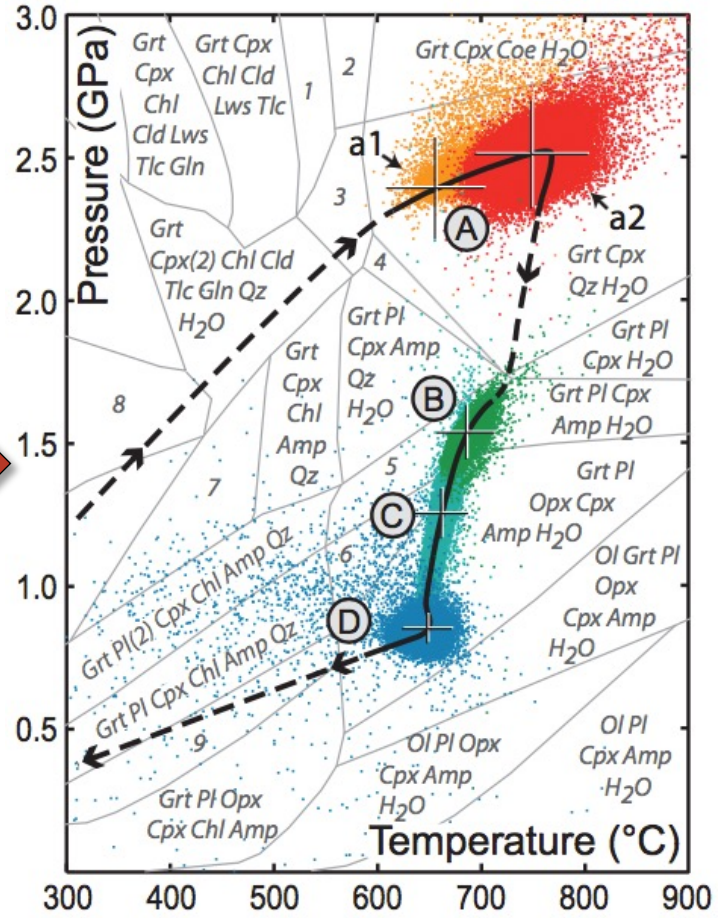
- *What is XMapTools and what does it do?*
- *Data reduction (EPMA)*
- *Selected examples of application*

Mineral compositions in a microstructural context



Lanari et al. (2013), Geology

Petrological modeling



Peak conditions:

Temperature: Grt+Cpx (Ravna 2000)
Pressure: Grt+Cpx+Ph (Waters & Martin 1993)

Retrograde conditions:

Temperature: Amp+Pl (Holland & Blundy 1994)
Pressure: Cpx+Amp+Pl (Waters 2002, 2003)

Mineral compositions in a microstructural context

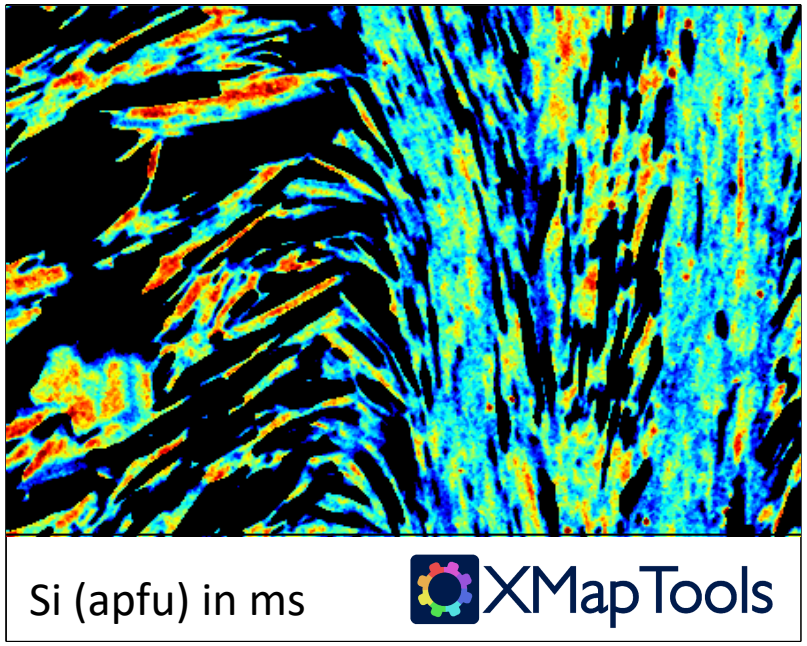
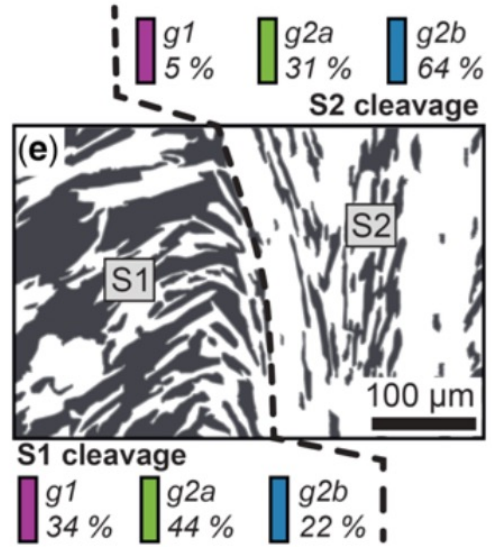


Image analysis



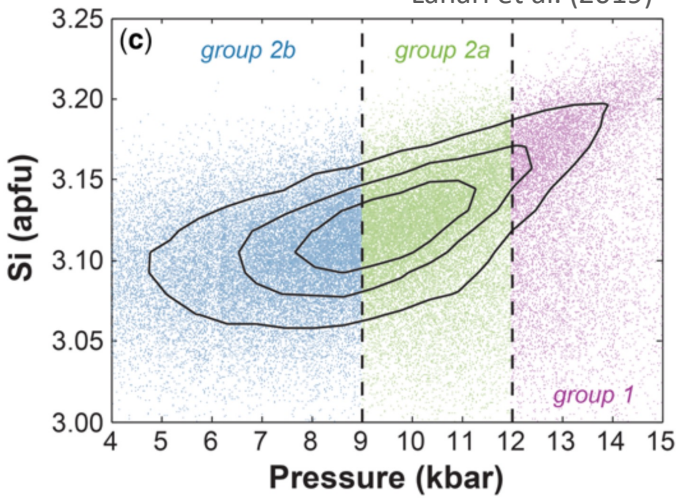
Airaghi et al. (2017), Lithos

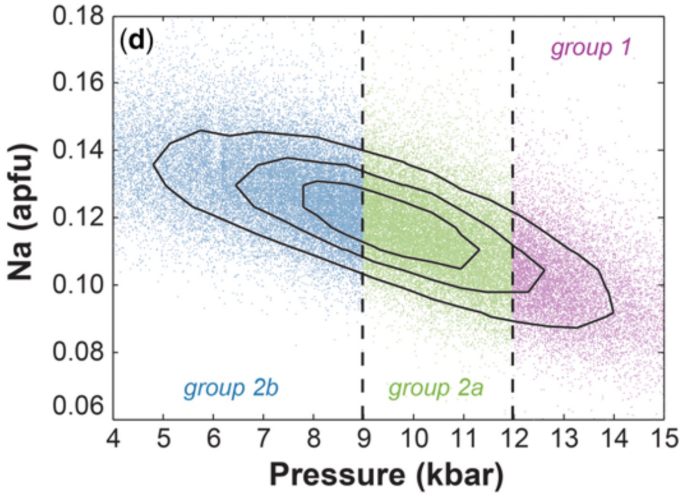
Multi-equilibrium thermobarometry using advanced inverse models:

Ph+Qz+H2O

Dubacq et al, (2009)

Lanari et al. (2019)





XMapTools

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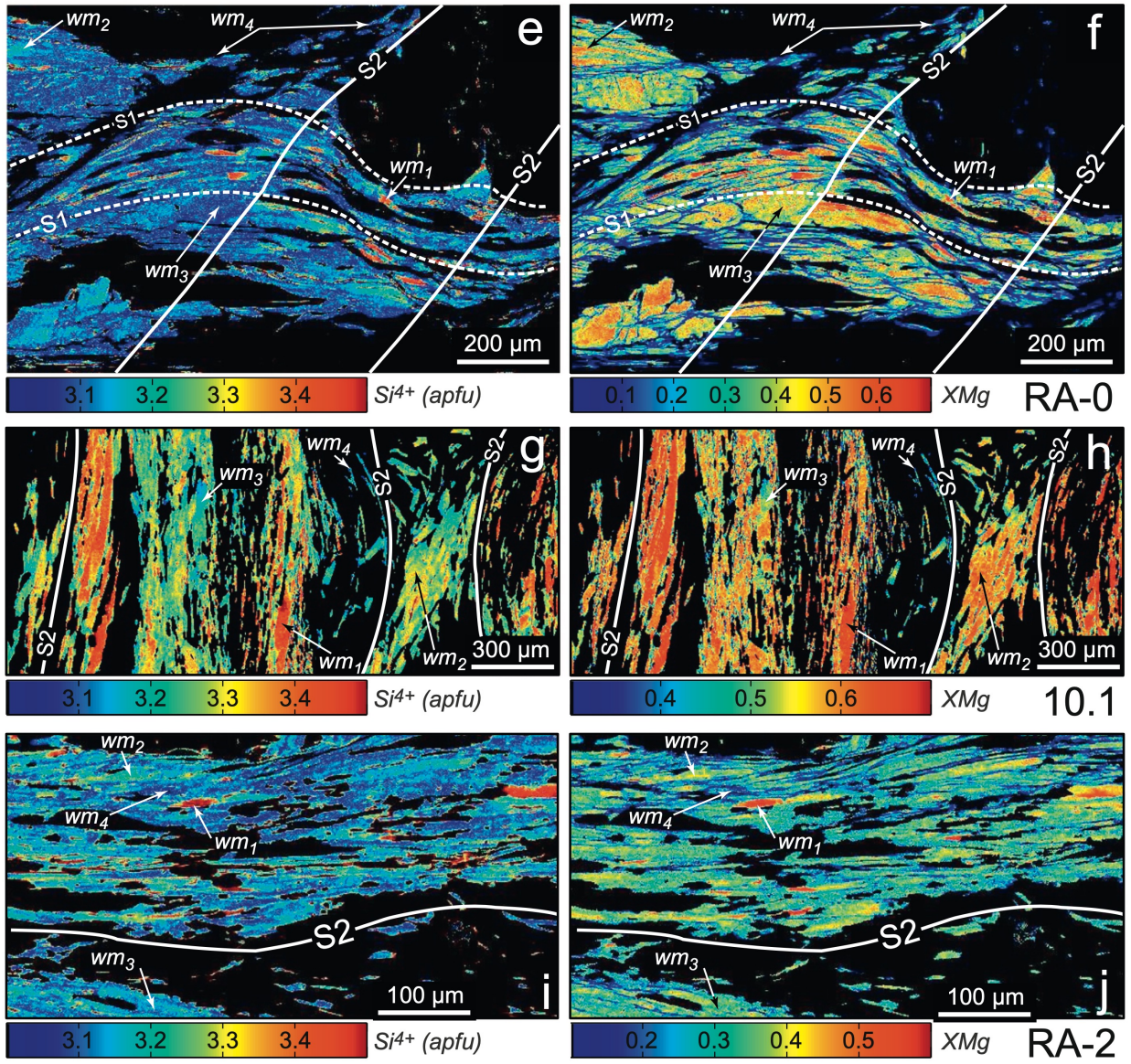
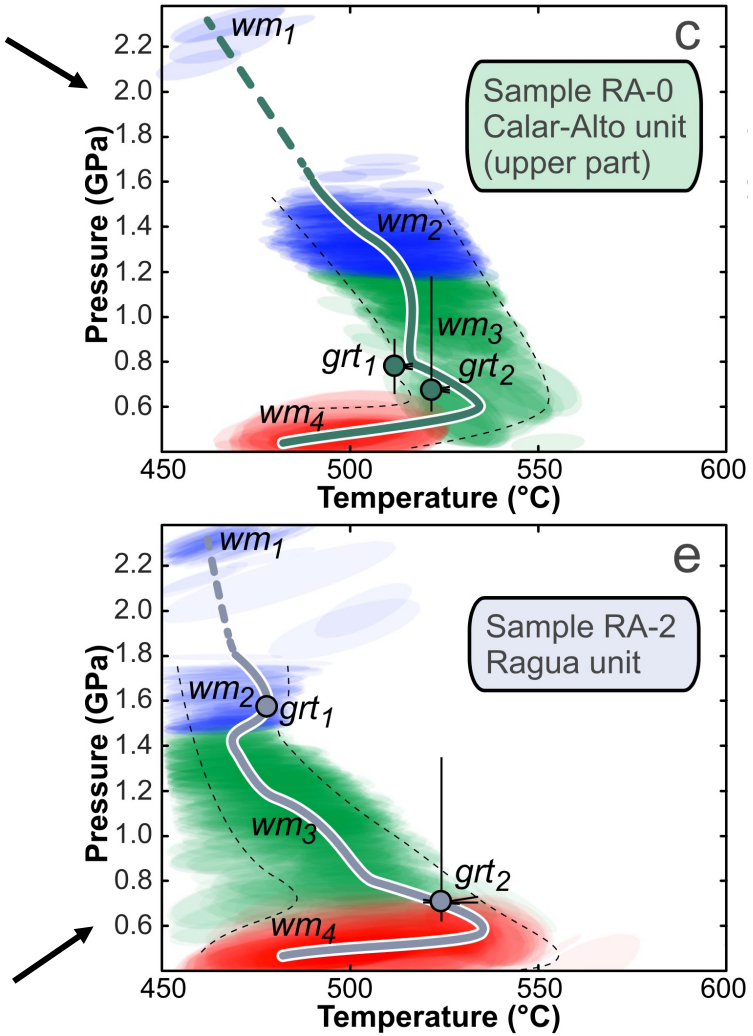
Selected examples of application

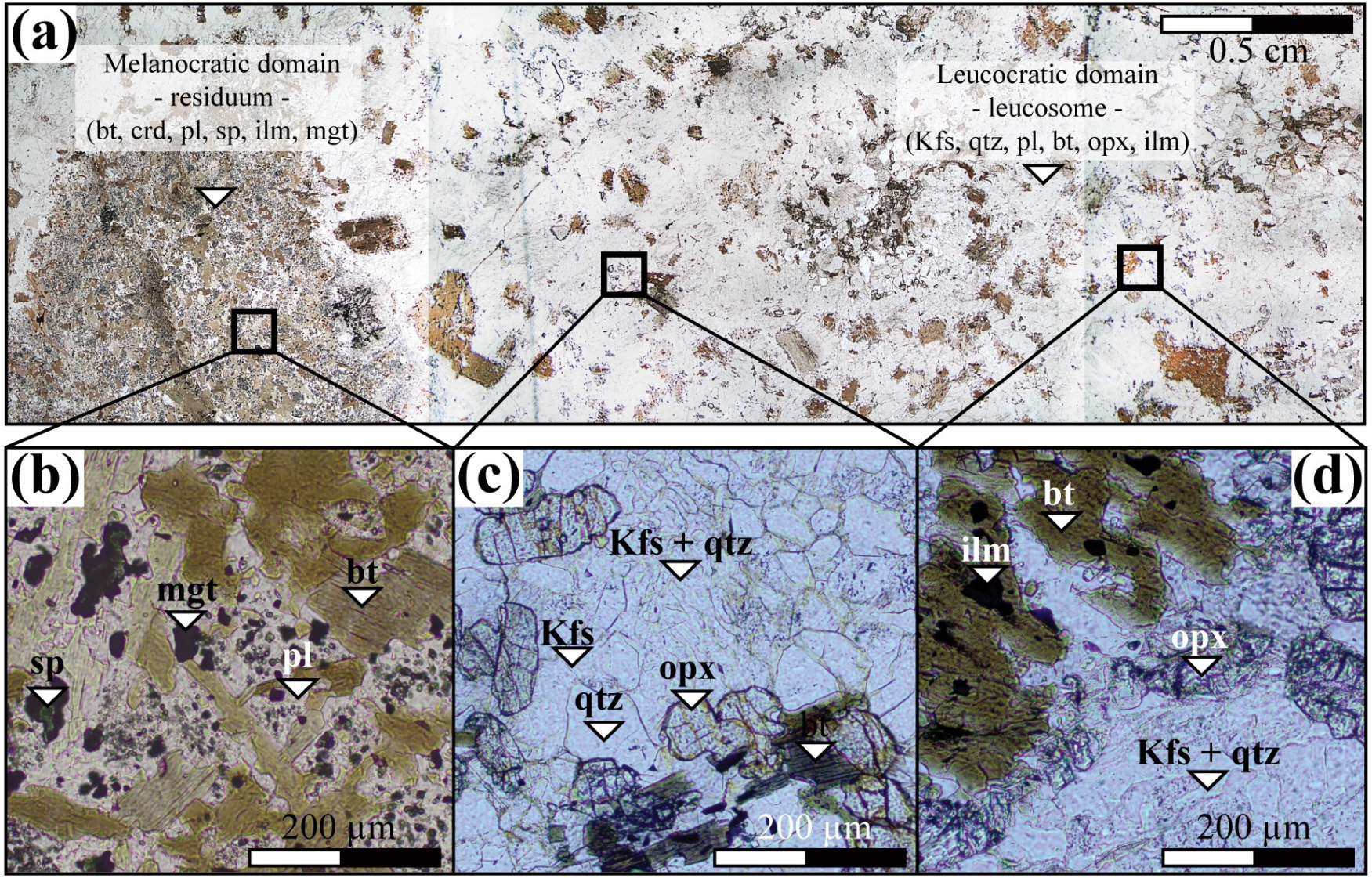
Mineral compositions in a microstructural context





Santamaria-Lopez et al. (2019), Tectonophysics

Mineral compositions in a microstructural context



Unpublished data from Lanari & Riel

PHASE EQUILIBRIUM MODELING

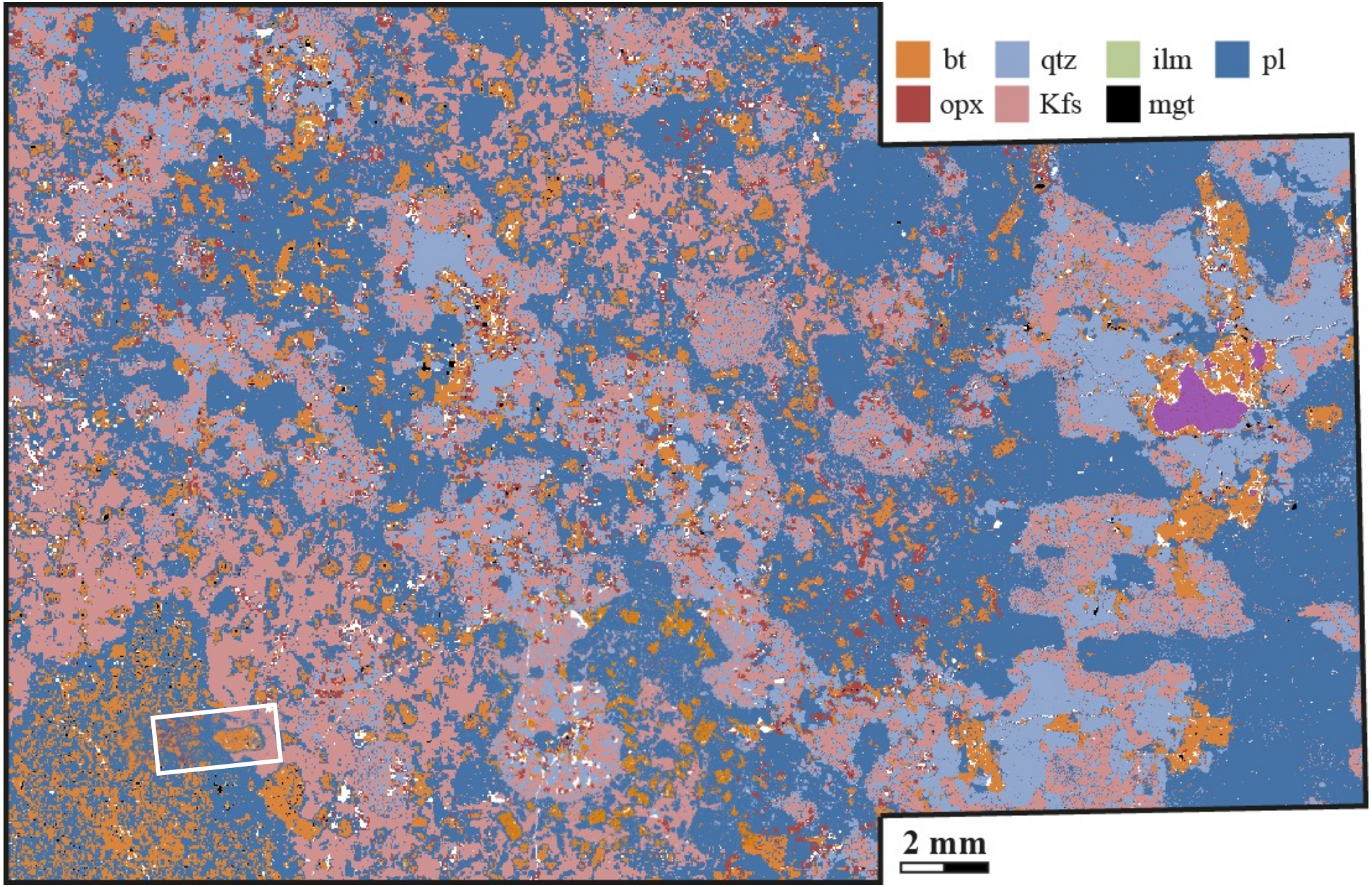
AN INTRODUCTION TO PETROLOGICAL MODELLING

Friday's topics

What is XMapTools and what does it do?

Data reduction (EPMA)

Selected examples of application



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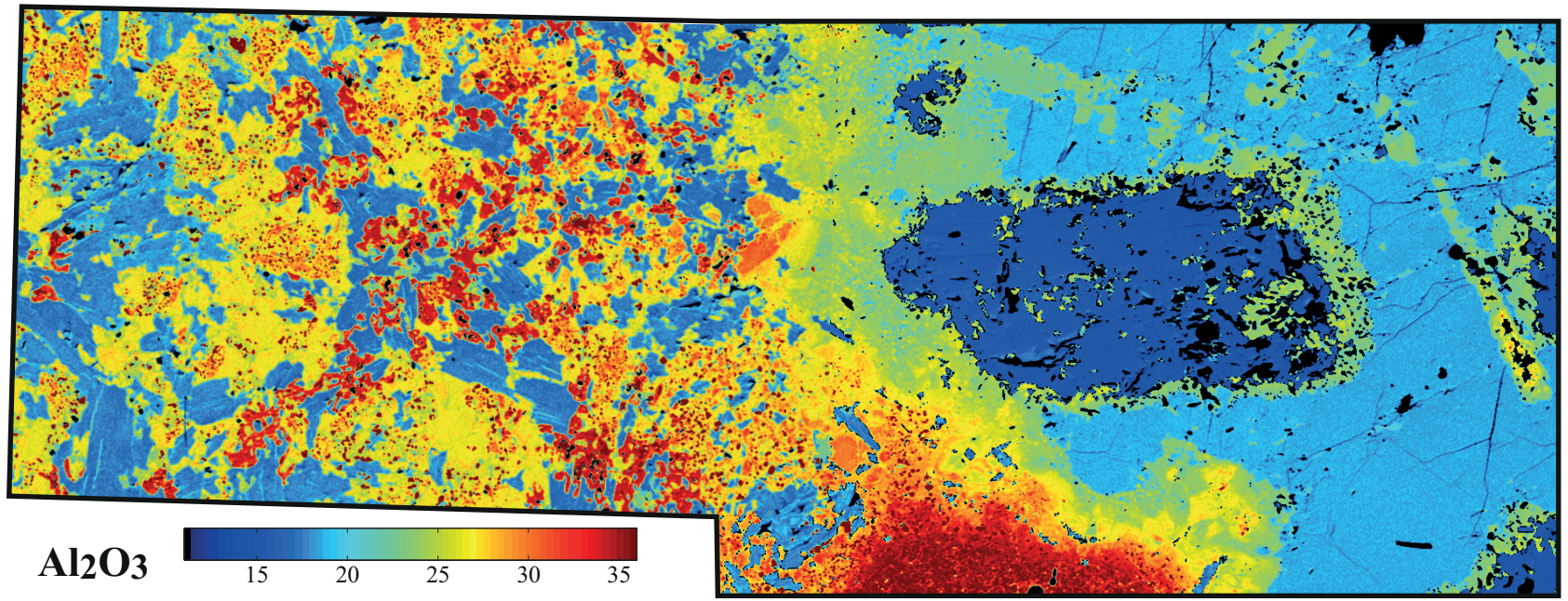

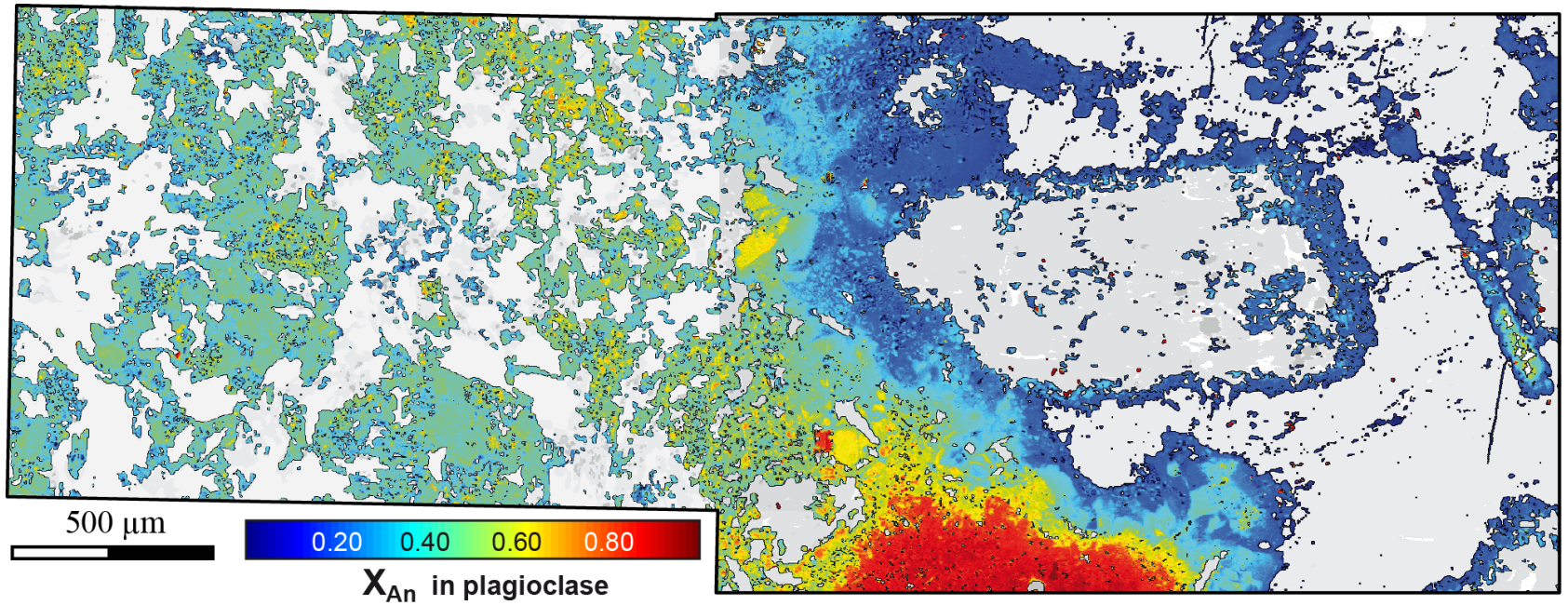

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