Multi Modal Materials Analysis (MMoMA)

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Proposers' Day

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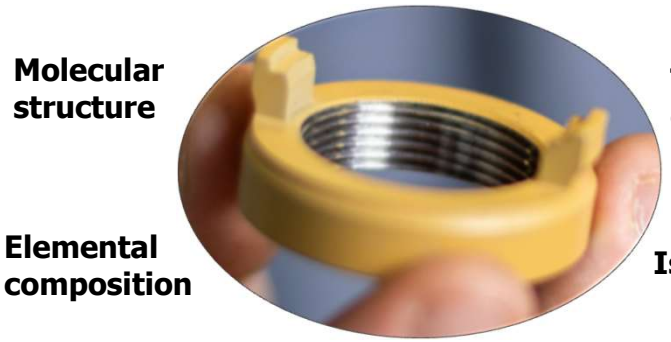
Multi Modal Materials Analysis (MMoMA)

Multi-modal signatures (molecular structure, elemental composition, trace elements, and isotopes) can identify things and provide unbreakable provenance.

Program Objective:
- Explore innovative methods that use a single continuously tunable excitation source to conduct multi-modal materials analysis
- Extract the maximum amount of information from a sample
- Surface and bulk analysis of molecular structure, elemental composition, trace elements, and isotope ratios
- Under ambient conditions and without the need for special sample preparation.

Vision:
Rapid and reliable identification of materials and things for:
- Supply chain integrity
- Tagging and tracking
- Tamper detection and authentication
- Forensics and attribution
- Prospecting (including in space)



Surface and bulk analysis

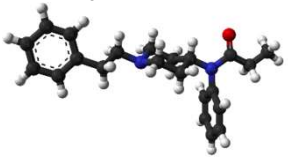
Where did it come from ?
Who made it ?
Was it altered ?

https://www.metal-am.com/articles/beyond-the-digital-warehouse-whats-really-driving-the-additive-manufacturing-of-spare-parts-in-2025/

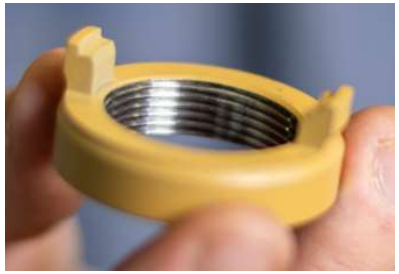
MMoMA Objective:
Establish capability and value of multi-modal analysis

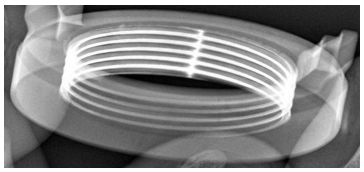
Supply chain integrity: Is this what we ordered ?

Surface residues:
~1 ppm
e.g. $C_{22}H_{28}N_2O$, fentanyl



Coatings:
~0.1 atomic %
ceramics (ZrN, …)





Molecular structure:
≤ 1 ppm

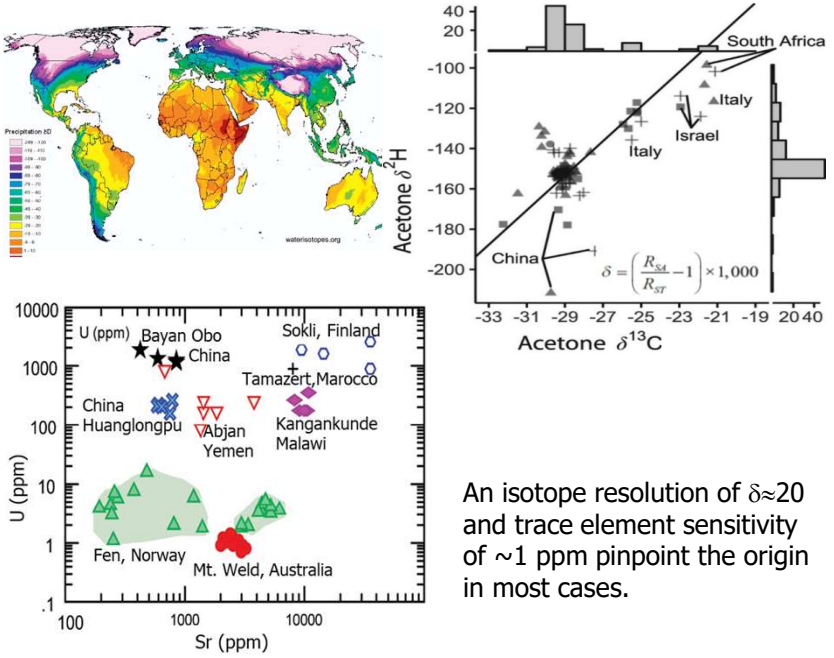
Atomic composition:
~0.1 atomic %, Ti 90%, Al 6%, V 4%

Trace elements:
<1 ppm, B, Sr, Pb, …

Isotope ratios: ~1%
$^{46\text{-}50}Ti$, $^{11/10}B$, $^{86/87}Sr$, $^{13/12}C$, $^{238/235}U$, delta ~20

Bulk analysis:
radiography, elemental composition, trace elements, and isotopes.

Example: origin of acetone and rare earths from isotopes and trace elements



An isotope resolution of $\delta \approx 20$ and trace element sensitivity of ~1 ppm pinpoint the origin in most cases.

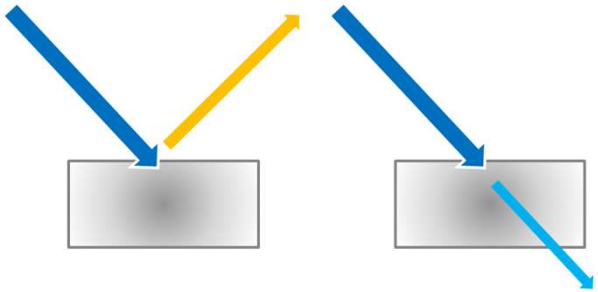
Hypothesis: Spatiotemporal correlations in multi-modal signatures tell a more complete story and provide a lot more useful information than the sum of the parts from SOA sequential analysis.

D. Howa, "triacetone triperoxide isotopes and worldwide acetone variation" (2018).
Liu, X., et al. "Mineral to Metal Traceability" (2024). Waterisotopes.org

R_{SA} (R_{ST}): isotope ratios in analyte (standard), 1 ppm: 1 part per million
Monazite (Ce, Nd, …)-PO_4, acetone: $(CH_3)_2CO$

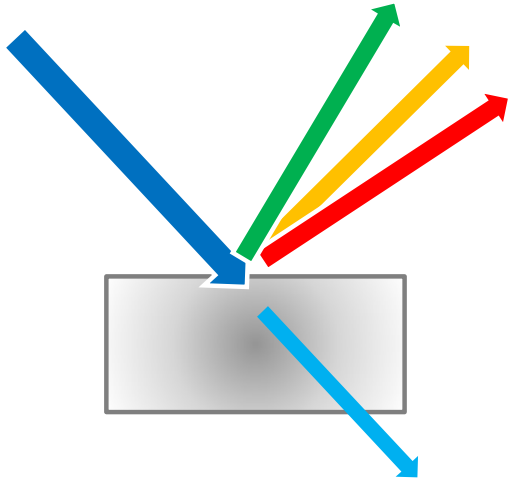
From single mode sequential analysis to multi-mode parallel analysis

Traditional single mode analysis



- Today, we have many instruments that are optimized for detection of one signature
- Different instruments for surface and bulk analysis
- Full picture can be stitched together from data collected in several instruments, which takes a while and correlations get lost

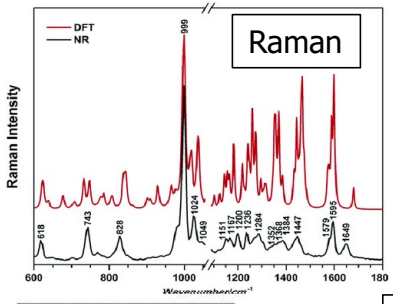
Novel parallel multi-mode analysis

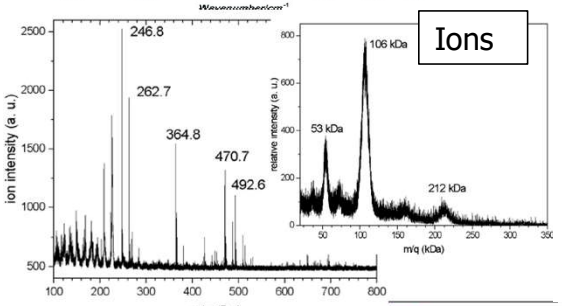


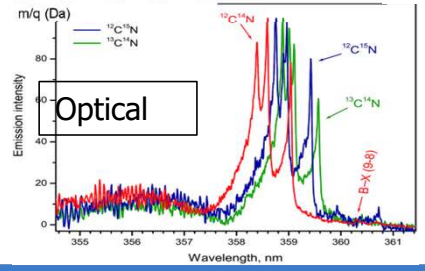
- MMoMA: Explore multi-modal materials analysis with one tunable excitation source for surface and bulk analysis
- Prove the power of multi-modal analysis, implement data fusion, explore novel signatures from correlations
- Long term vision is a transportable instrument

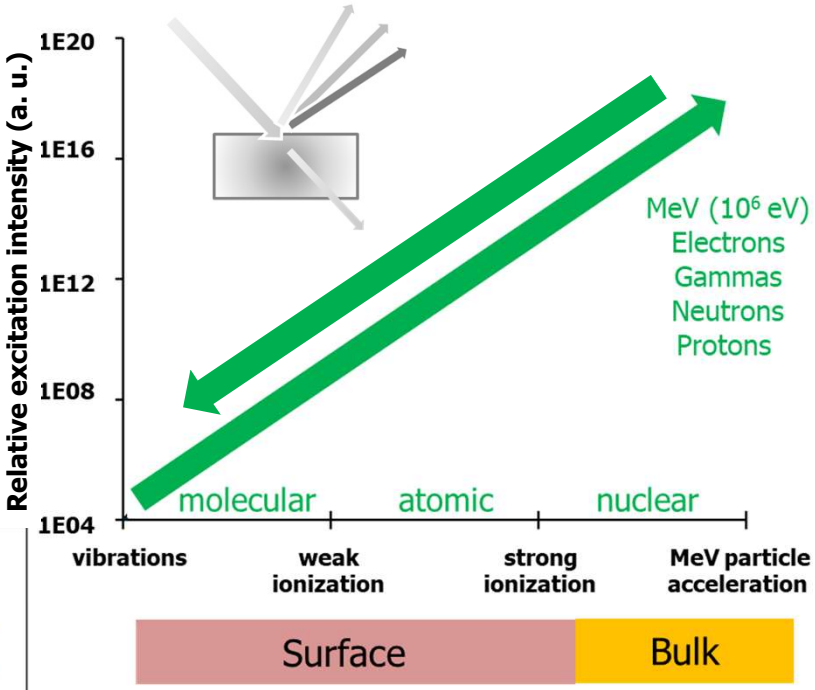
e.g. https://www.eag.com/techniques/

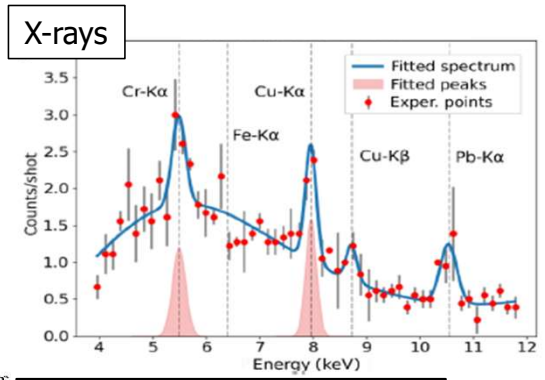
Scan the excitation intensity, collect multi-modal signatures, observe spatiotemporal correlations with in-situ feedback

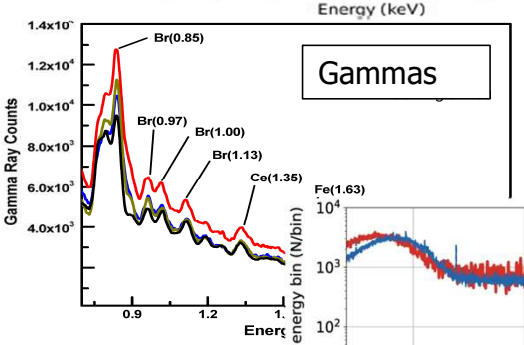


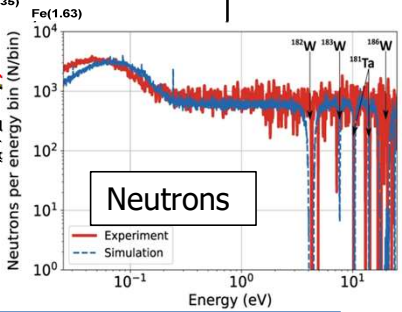












Performers will analyze data in situ for adaptive feedback loops to maximize the information they can extract from correlated (x, t) molecular, compositional, trace elemental and isotopic signatures.

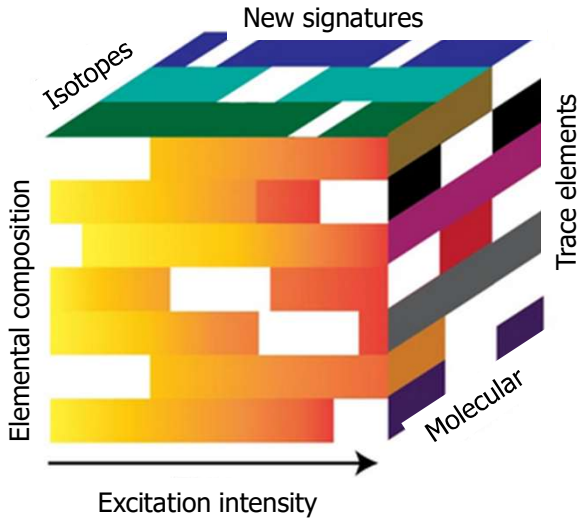
F. Mirani *et al., Sci. Adv.***7**,eabc8660(2021), L. Tian et al., J. Food Qual. 1308645 (2022)
T. Schenkel et al. Appl. Phys. Lett. (2023); Zimmer, M., et al., Nat Commun 13, 1173 (2022)

AlMisned, G.; et al., Appl. Sci. 2022, 12, 3714; A. Bol'shakov et all, J. Anal. At. Spectrom., 2016, 31, 119; J. Leonard, J Raman Spectrosc. 2017;48:1323

Data fusion for in-situ feedback and discovery of correlations in multi-modal data

	Signature
Molecular structure	IR, optical photons, ions, …
Elemental composition	Optical photons, x-rays, gammas, ions, …
Isotope ratios	Optical photons, gammas, ions, …
Trace elements	Optical photons, x-rays, gammas, ions, …
New signatures	**Exploration of new x-t correlations and patterns in multi-modal data**

AI/ML tools for data fusion, in situ feedback and exploitation of spatiotemporal correlations in multi-modal data



Velten, B., et al, Nat Methods **19**, 179 (2022)

Performers will explore multi-modal data fusion for in-situ adaptive feedback and to discover correlations in N-dimensional data.

MMoMA program structure

<table>
<tr><th colspan="4">Phase 1 Metrics</th><th colspan="3">Phase 2 Metrics</th></tr>
<tr><td colspan="4">Learn how much information we can extract from a sample by multi-modal analysis vs. SOA. Enough to warrant further evaluation of multi-modal analysis ?</td><td colspan="3">Determine if multi-modal analysis is superior across a range of high impact use cases in lab demos and warrants in-field demonstrations.</td></tr>
<tr><td rowspan="5">Data Generation</td><td rowspan="5">Achieve required sensitivity, initial inter-lab studies

Initial analysis of path to field capability (van scale)</td><td>Signatures</td><td>Required sensitivity, selectivity for potential applications</td><td rowspan="6">Demonstrate Effectiveness of Multi-modal Analysis</td><td rowspan="6">Inter-lab, round-robin comparisons of multi-modal data fusion for <u>DARPA selected</u> challenge problems (with transition partner input)

Answers equal or exceed performance of SOA serial analysis in <5 h (sample received to answer)</td><td>Cover >90% of use cases with >95% confidence</td></tr>
<tr><td>Molecular structure</td><td>m/dm>1000 optical: ~0.1 nm, ~1 cm^{-1}</td><td rowspan="5">Example challenge problems:

• Do these components match the expected composition, structure, processing history ?</td></tr>
<tr><td>Atomic composition</td><td>≤0.1% (1E-3)</td></tr>
<tr><td>Nuclear, isotope ratios</td><td>Delta +/-20</td></tr>
<tr><td>Trace elements</td><td><1 ppm (1E-6)</td></tr>
<tr><td>Data Analysis</td><td>Multi-modal data fusion</td><td colspan="2">Sets with ≥4 signature components, correlation analysis</td></tr>
<tr><td>Samples</td><td>Universal</td><td colspan="2">Solid or liquid, ~0.1 mm to 10 cm scale, any composition, analysis under ambient conditions of pressure and temperature, no sample preparation required</td><td>Samples</td><td>Universal</td><td>Any composition, ~0.1 mm to 10 cm, ambient conditions, no sample prep</td></tr>
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MMoMA Program Schedule