


USE OF THE MATERIALYTICS SEQUENCING SYSTEM (M2S) TO SOLVE COMPLEX GEOCHEMICAL PROBLEMS: THE CASE OF EMERALD PROVENANCE



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Overview

- The Project
- The Samples
 - Database
- The Process
 - System Components
 - Sample Analysis
 - Data Analysis
- The Study
- The Future



The Project - Materialytics

- In the last four years we have invested in samples collection, cataloging and R&D, including:
 - Substantial database, with samples from around the world
 - Plasma spectroscopy configurations for a variety of geomaterial applications
 - Generic pattern matching software that works with a wide range of geomaterials without human parameterization

The Project - Our Team

This was an interdisciplinary effort so thanks to our:

- Catalogers
- Combustion Engineers
- Geochemists
- Logisticians
- Mathematicians
- Optics Engineers
- Photographers
- Plasma Physicists
- Programmers
- System Operators
- Technology Team



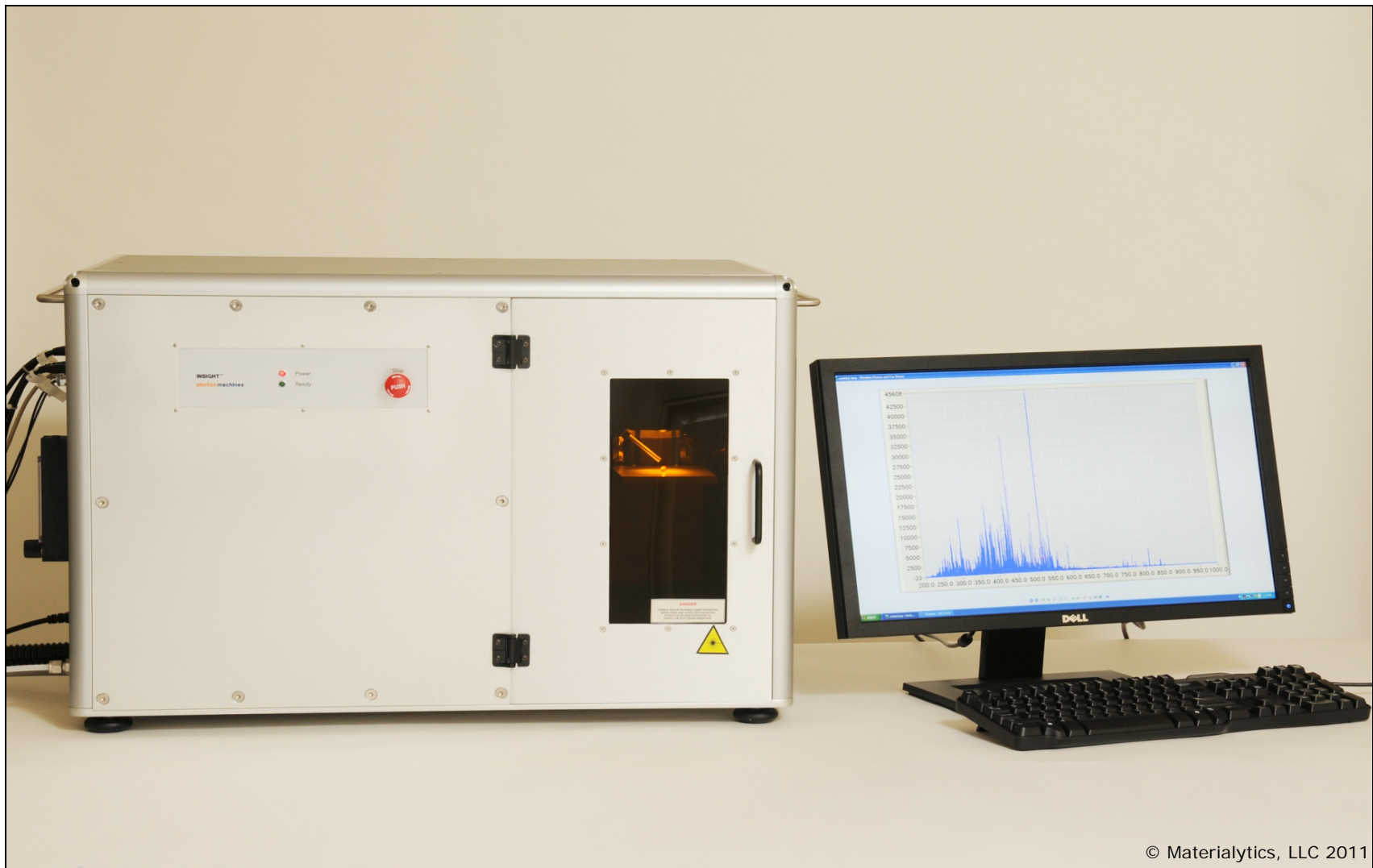
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The Samples - Our Database



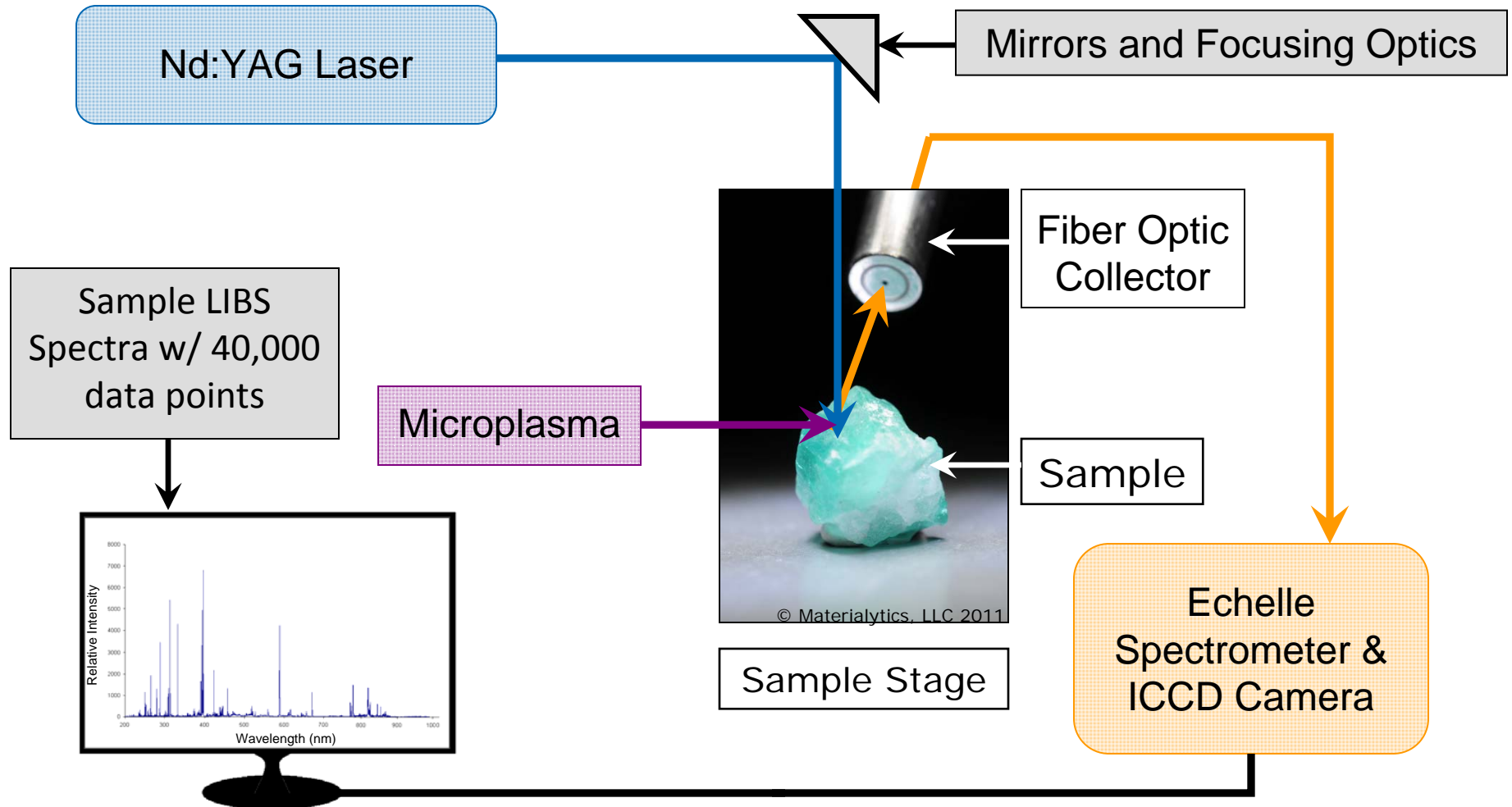
- Over 50,000 samples
- Over 60 countries on 6 continents
- 330 unique locations

The Process - System Components



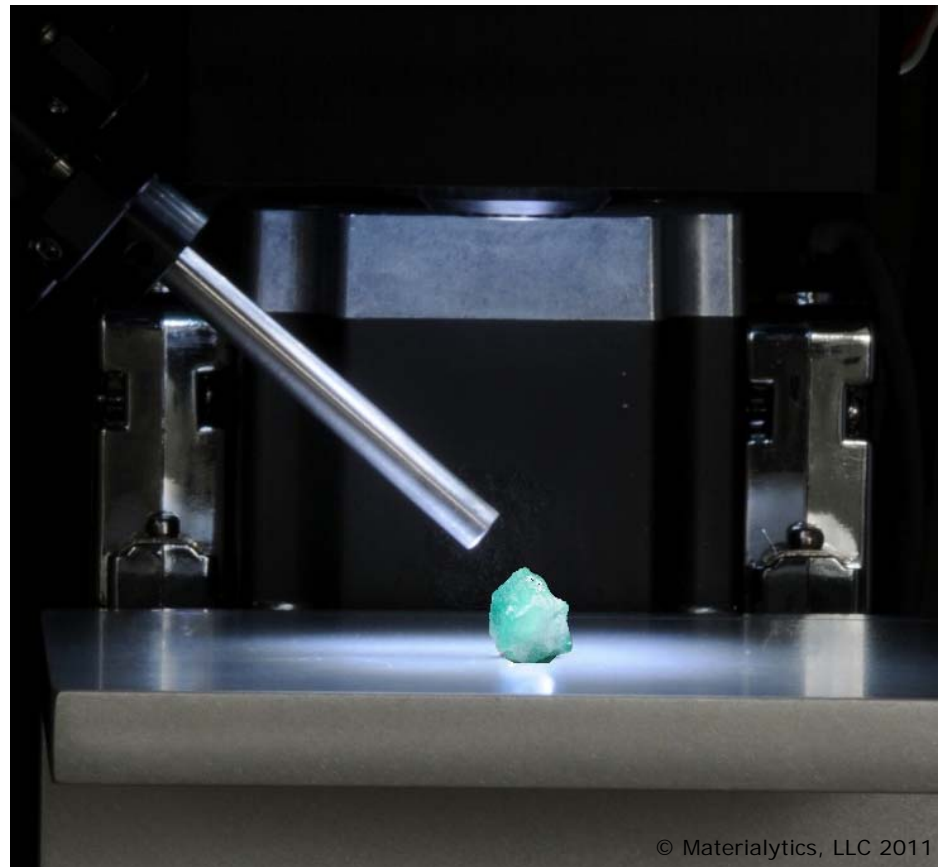
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The Process - System Components



The Process - Sample Analysis

- We clean the sample surface with isopropyl alcohol prior to analysis.
- It is then mounted on mineral tack and positioned within the sample chamber.



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The Process - Sample Analysis

- ❑ For every shot collected we collect tens of thousands of data points.
- ❑ For comparison, LA-ICP-MS collects approximately 30 data points*.
- ❑ We collect tens of shots per sample, for a total of over 2 million data points per sample.
- ❑ We use over 70 million data points to begin to characterize a locality.

*Abduriyim, A. & Kitawaki, H. (2006) Applications of laser ablation–inductively coupled plasma–mass spectrometry (LA-ICP-MS) to gemology. *Gems & Gemology*, Vol. 42, No. 2, pp 98–118

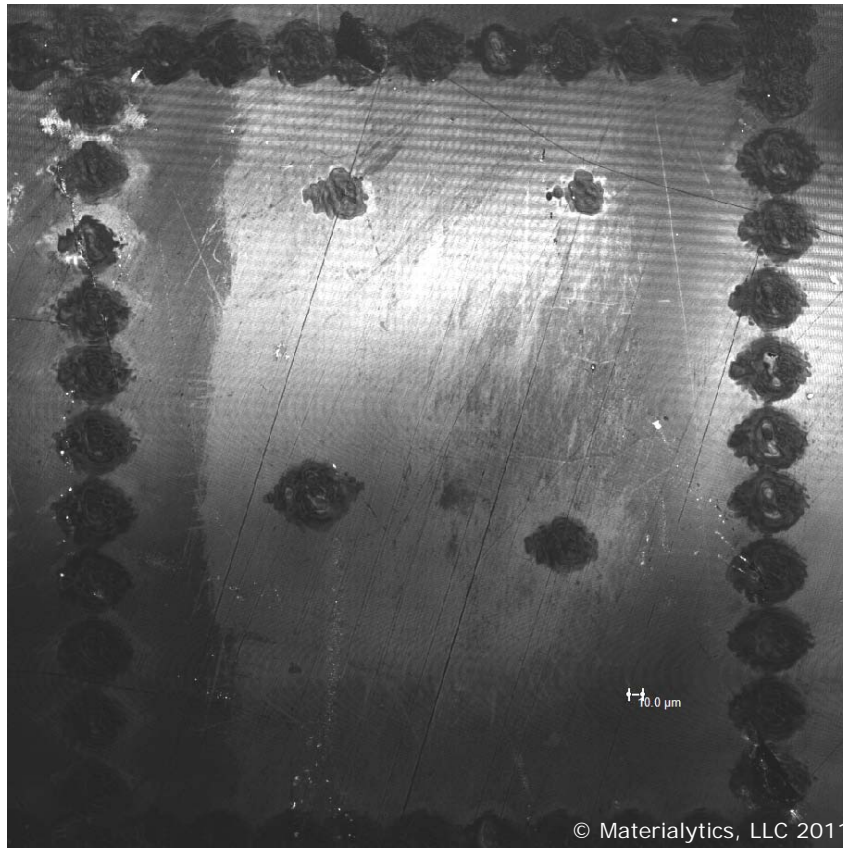
The Process - Traces of Analysis



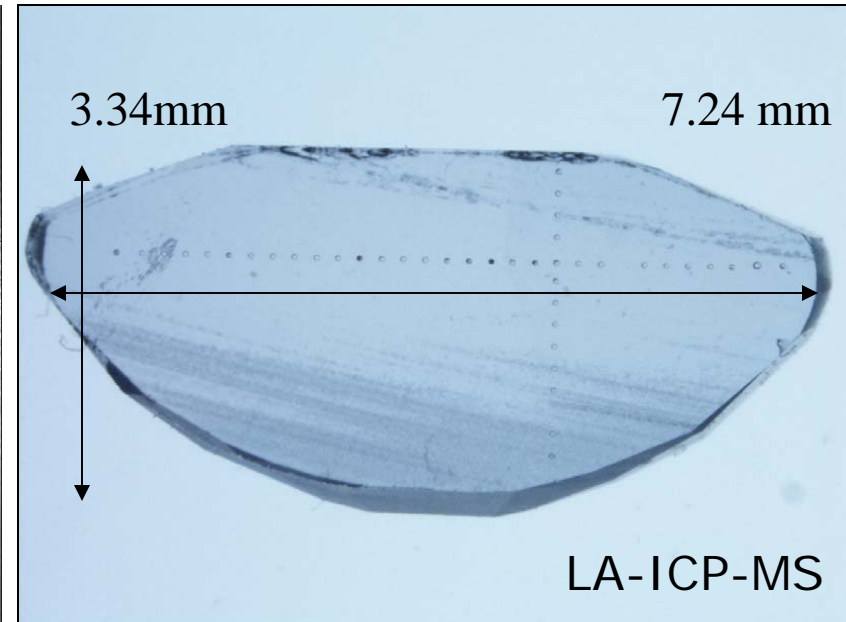
The traces of analysis range in size from sub 10 – 150 microns depending on numerous analytical conditions.

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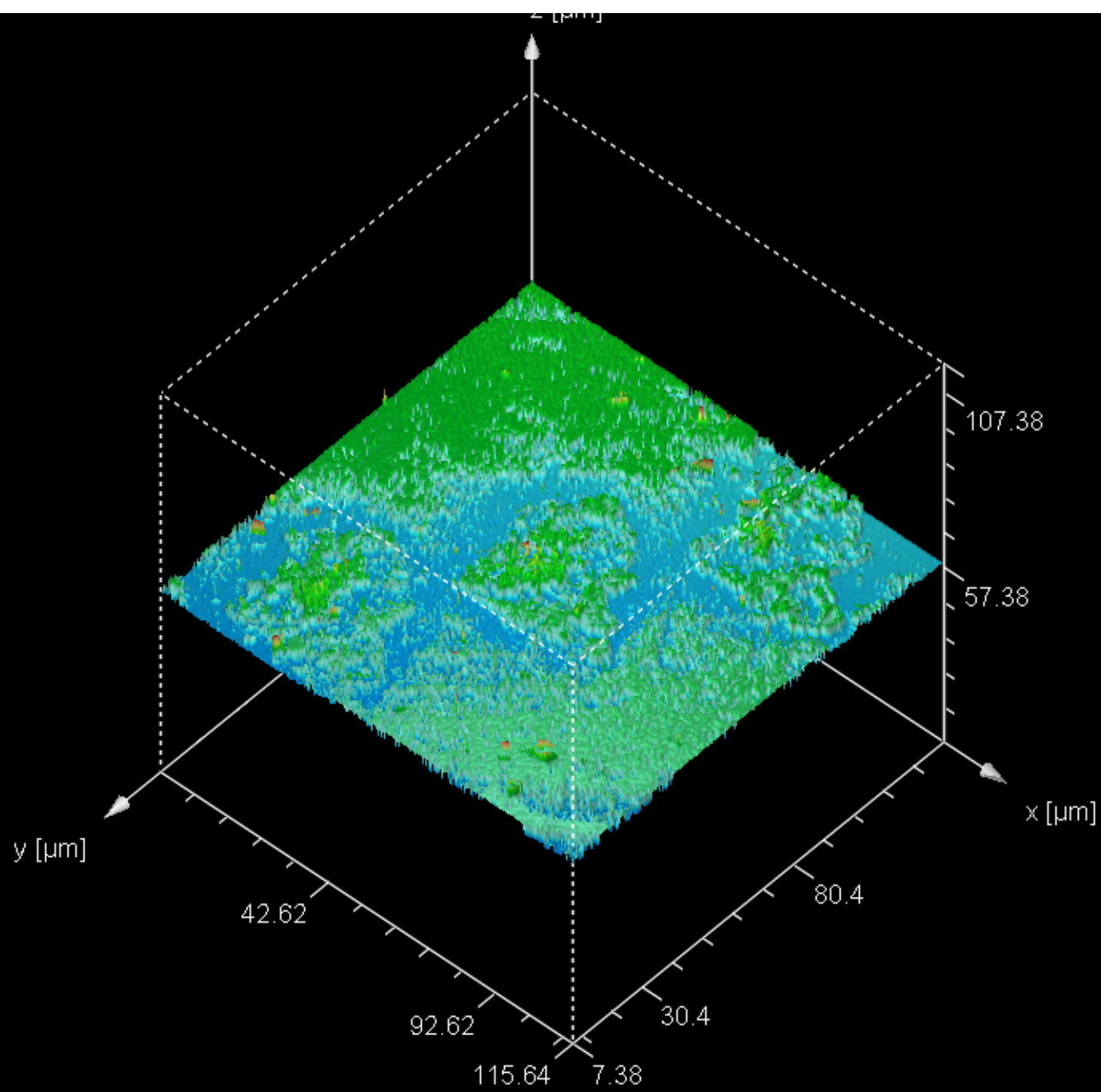
The Process - Traces of Analysis



Confocal Microscope Image of M2S Analyzed Sample



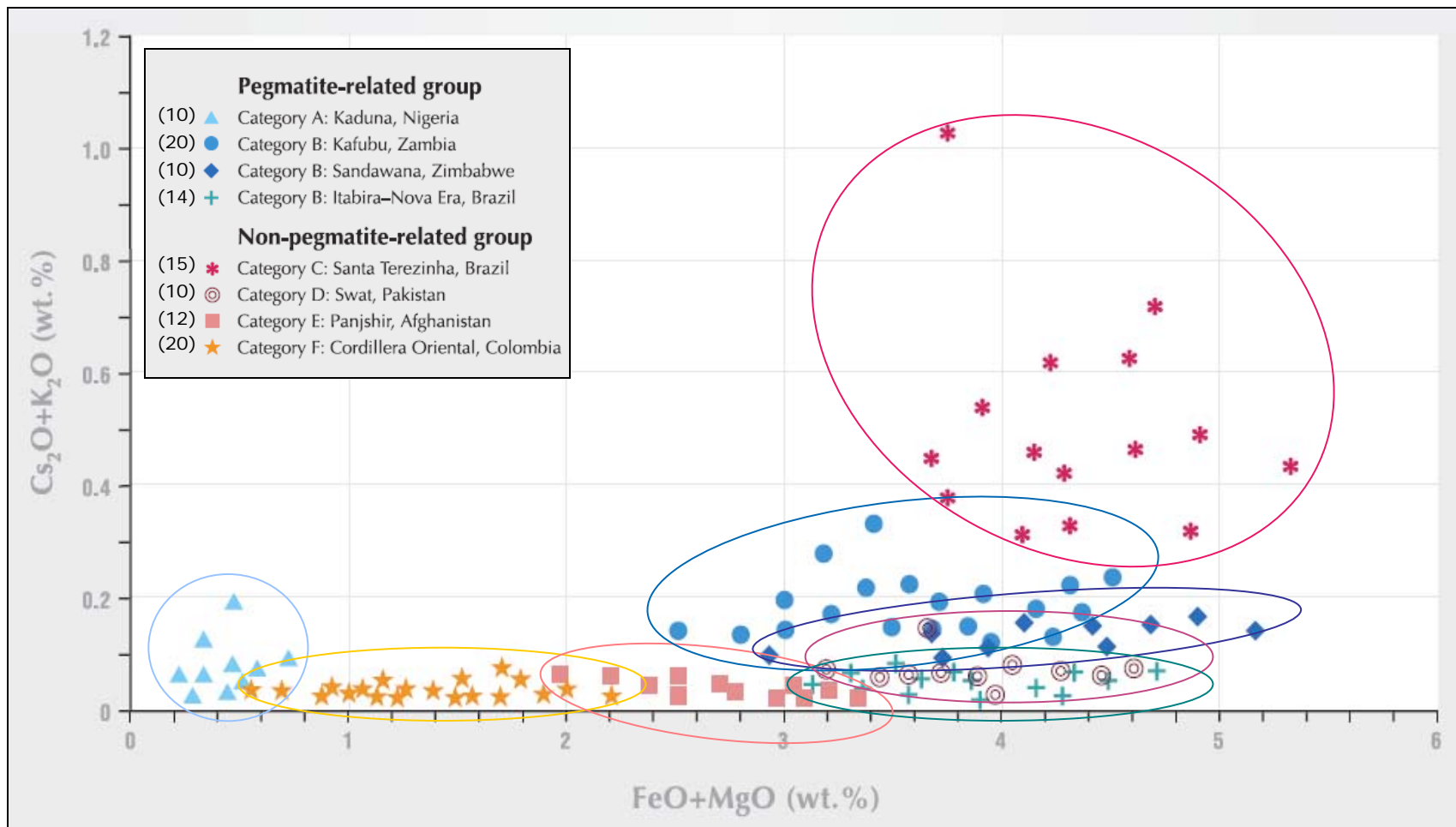
DuToit, G., Thanachakaphad, J., Scarratt, K. (2009) Beryllium Treated Blue Sapphires: Continuing market observations and update including the emergence of larger size stones. June 25th 2009. *On-going Research*, <http://www.giathai.net/lab.php>



The Process - Data Analysis

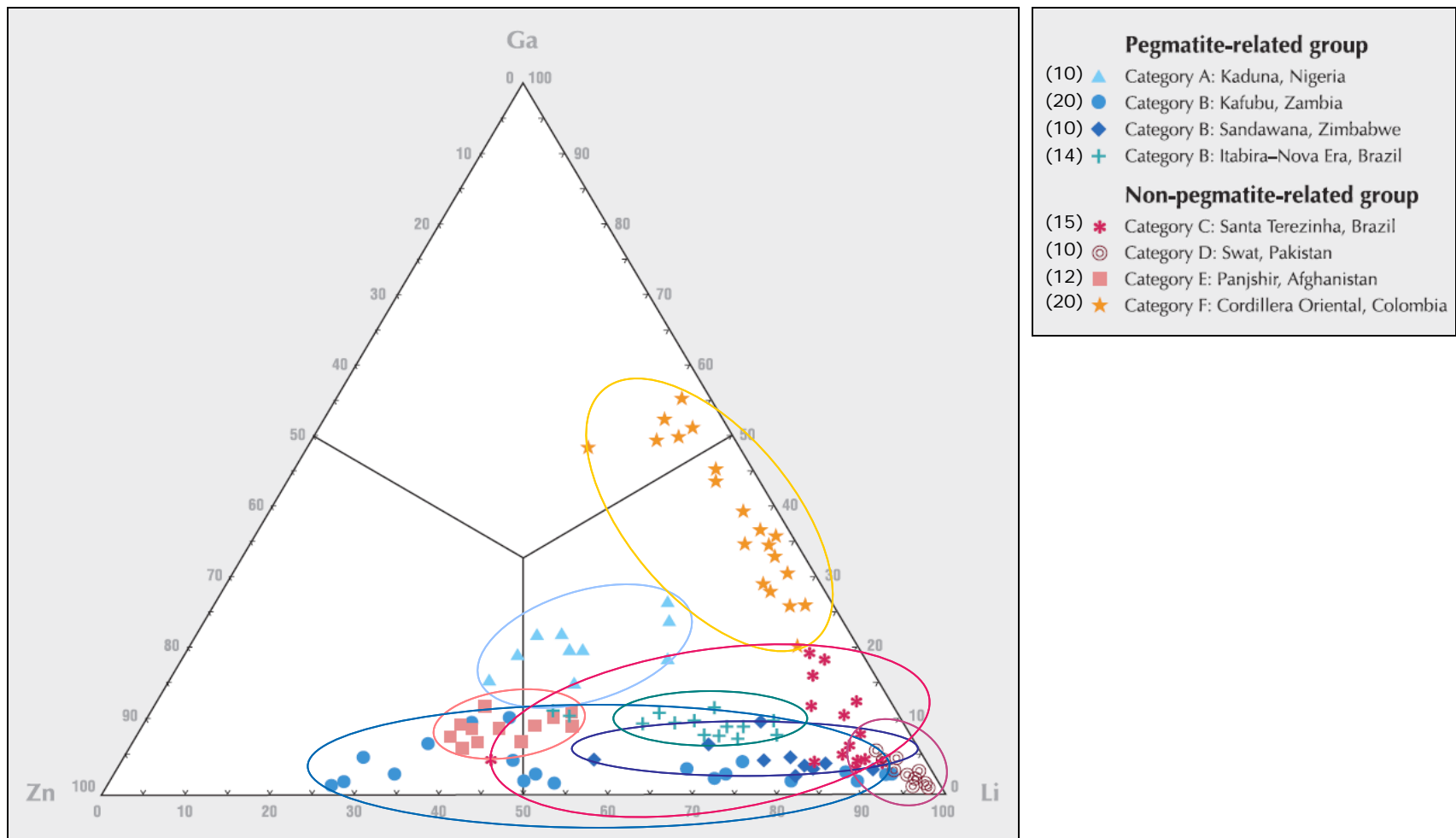
- Traditional Geochemistry
- Non-Traditional Geochemistry
 - Chemometrics
 - Signal Processing

Traditional Geochemistry-2 Variables



(Abduriyim, A. & Kitawaki, H. (2006) Applications of laser ablation–inductively coupled plasma–mass spectrometry (LA-ICP-MS) to gemology. *Gems & Gemology*, Vol. 42, No. 2, pp 98–118)

Traditional Geochemistry-3 Variables



(Abduriyim, A. & Kitawaki, H. (2006) Applications of laser ablation–inductively coupled plasma–mass spectrometry (LA-ICP-MS) to gemology. *Gems & Gemology*, Vol. 42, No. 2, pp 98–118)

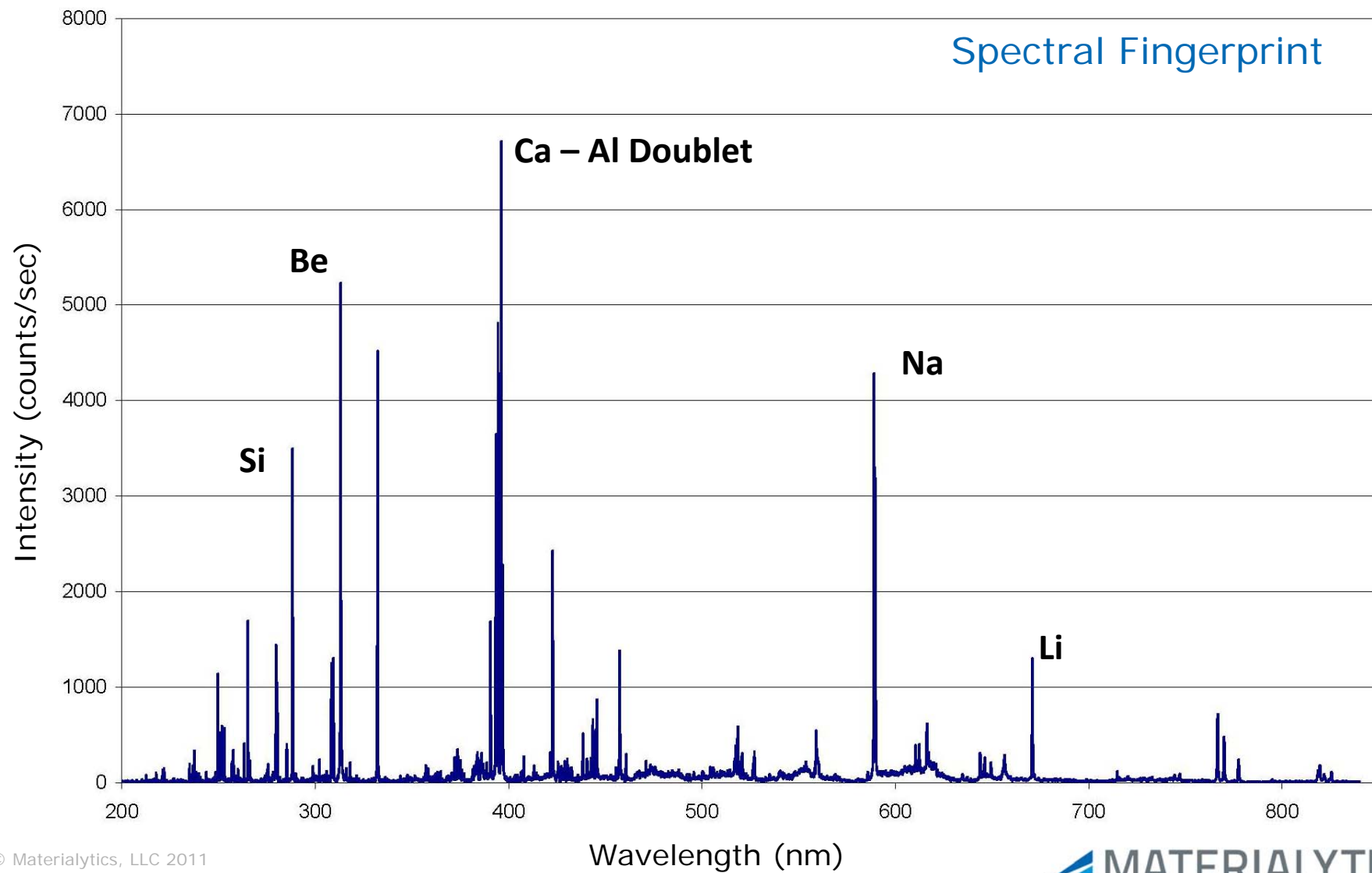
Chemometrics

- Unpublished initial results on beryl using solely chemometrics were unsuccessful.
- In light of recent advances, by Multari et al. (2010) and Yetter et al. (2011) for example, it could be interesting to revisit the research from this angle.

Signal Processing

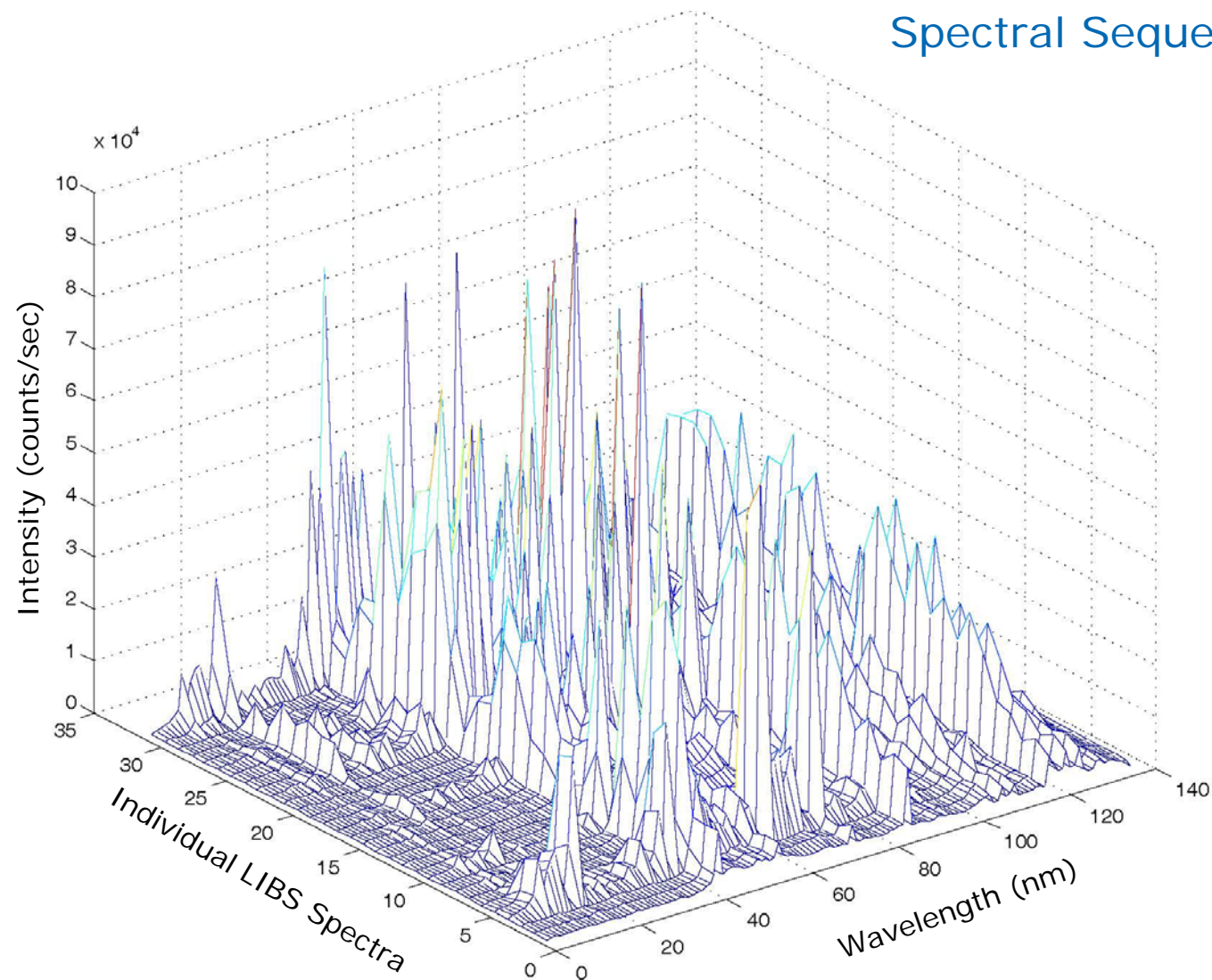
- Spectral fingerprint = spectral data in a single LIBS shot
- Spectral sequence = array of spectral fingerprints

Signal Processing



Signal Processing

Spectral Sequence



The Process - Data Analysis

- ❑ Evaluation of the data indicates that the signals are both linear and non-linear.
- ❑ In many cases, multiple signals are embedded within each spectrum.
- ❑ Our processing system (M2S) is three phased.
- ❑ Leave-One-Out Cross Validation is employed, and a variety of mathematical analysis techniques from PCA to non-Bayesian networks are used based on the complexity of the data.
- ❑ The following results are achieved using signal processing techniques.

The Study

300 Emerald Samples from 10 Locations

Afghanistan	AFG	Khenj Mine, Panjshir Region
Brazil	BRA	Carnaiba Mine
Columbia 1	COL1	Chivor Region
Columbia 2	COL2	La Pita Region
Mozambique	MOZ	Unknown
Pakistan	PAK	Pocket #3, Swat
United States	USA	Crabtree Mine, NC
South Africa	ZAF	Gravelotte, Mpumalanga
Zambia	ZMB	Copper Belt, Kalolusha, Fwya Fywa
Zimbabwe	ZWE	Sandwana

The Study - Results

Country	% False Positive	% False Negative	Accuracy
AFG	0.5%	2.0%	98%
BRA	0.6%	1.5%	98%
COL1	0.0%	0.0%	100%
COL2	0.0%	0.0%	100%
MOZ	0.6%	1.2%	98%
PAK	0.3%	1.9%	98%
USA	0.3%	0.2%	100%
ZAF	0.0%	0.7%	99%
ZMB	1.6%	3.0%	95%
ZWE	0.9%	2.3%	97%

In Conclusion – 98%

- ❑ It takes an interdisciplinary team to answer the question “can the source of an emerald be determined only by analyzing the stone?”
- ❑ Scaling up is hard to do; it takes a great deal of time, money, and attention to detail.
- ❑ It is possible to determine the country of origin of an emerald with 98% accuracy.
- ❑ There are indications that it may be possible to source a sample back to its host mine.

The Road Ahead

- Diversifying our Database
 - We need more samples from more locations to complete the study – Antarctica please!
- Improving our LIBS system
 - We have used and abused our LIBS system in ways the designers never could have thought of until you have put as many hours on the laser and miles (yes, miles) on the sample stage as we have.
- So far, M2S has been able to successfully analyze every material we've attempted; we're excited for what will come across our sample stage next.



For more information please visit: www.materialytics.com