

Fly away with me

This challenge is driven by efforts to expedite materials data analysis and generate insight into physics and chemistry of industry relevant materials. Ferroelectric lithium niobate (LiNbO_3) is widely used in integrated and waveguides due to its optical, piezoelectric, electro-optic, elastic, photoelastic, and photorefractive properties.¹ This is a human-made dielectric and does not exist in nature; with its ferroelectric properties first shown in 1949.² It is now extensively used in the telecoms market, for mobile telephones, optical modulators, and of surface acoustic wave devices.³ Although lithium niobate is important in numerous broad areas of technological significance, the details, and more importantly the origins of its physical as well as chemical properties remain hotly debated. The purpose of this data challenge is to piece together the chemical behavior of LiNbO_3 from Time of Flight Mass Secondary Mass Spectrometry data as a function of applied electrical bias.

Time of Flight Mass Secondary Mass Spectrometry (ToF-SIMS) is a destructive analysis technique designed to reveal the chemical composition of the sample's topmost layer.⁴ Ions from a primary ion source strike the surface breaking bonds and releasing some material particles and their associated fragments. Fragments produced in the top 2-3 monolayers of the sample will have enough energy to overcome the surface binding energy and leave the sample. A small portion of those will be charged, either positively or negatively depending on their electron configuration. The mass to charge ratio (m/z) of the species are analyzed and yield positive and negative secondary ion mass spectra consisting of the ion m/z versus the number of ions detected at each m/z .

Data generated by ToF-SIMS contains millions of points per spectra. The ToF detector effectively counts every single event, (that is every charged atom or molecule!) as a function of time. This generates sparse data sets containing many single or zero events, with robust peaks containing thousands to million counts. A spectrum is collected at each spatial pixel. There are typically 256×256 or 128×128 pixels per single chemical image. In this data series we contain multiple chemical images as a function of *depth into material, the applied electrical bias, and the distance between two biased electrodes*. This combinatorial approach is already a challenge in sample preparation and data collection; which is further exacerbated by a wealth of extracted information at both global and local scales necessitating a drastic improvement in capability to transfer, store and analyze multidimensional data sets.

In this challenge, contestants will be supplied with a series of 3D chemical image data sets as a function of spatial position, applied electrical bias, and distance between two biased electrodes. Each 3D data set consists of a mass spectrum mass 1 - 500 at each pixel. The challenge is to spatially co-register datasets taken in the same location; offer insight into which elements, or complexes, are most affected by bias; how this effect changes with electrode spacing; and visualize the distribution of key chemical players and their change as a function of bias and electrode spacing.

Challenge Questions

1. Co-register 3D chemical image sets taken in the same location. *Deliverable:* Co-registered data and the transformation matrix.
2. Identify key peaks (m/z values) that show the largest response to:
 - a. Applied bias
 - b. Distance between biased electrodes.

Deliverable: (a) 2D maps of key components and their evolution as a function of bias and distance between biased electrodes, quantification and visualization of this difference.

3. (*Advanced*) Identify inter-relationship between the key components (m/z values). Which elements or fragments are co-dependent? Which are mutually exclusive? How does this behavior change as a function of bias, distance between biased electrodes? *Deliverable:* Visualization of key m/z value behavior as a function of each other and the experimentally varying conditions: bias, distance between biased electrodes.

References

1. Weis, R.; Gaylord, T., Lithium niobate: summary of physical properties and crystal structure. *Applied Physics A* **1985**, *37* (4), 191-203.
2. Matthias, B.; Remeika, J., Ferroelectricity in the ilmenite structure. *Physical Review* **1949**, *76* (12), 1886.
3. Toney, J. E., *Lithium Niobate Photonics*. Artech House: 2015.
4. Belu, A. M.; Graham, D. J.; Castner, D. G., Time-of-flight secondary ion mass spectrometry: techniques and applications for the characterization of biomaterial surfaces. *Biomaterials* **2003**, *24* (21), 3635-3653.