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Attom Note **NA10**

Attolab Time Resolved Analysis (TRA) Software for Accessory Integration and Data Handling

Introduction

The ICP-MS technique has become a powerful tool for a growing set of applications including isotope ratio and elemental determinations in a range of samples through laser ablation ICP-MS or the use of ICP-MS as an element specific detector for chemical speciation work with a variety of chromatography techniques. Compared to quadrupole ICP-MS, magnetic sector instruments offer generally better signal-to-noise ratios along with flat-topped peak profiles that yield much better measurement precisions, especially when dealing with signals that are not at steady state as seen with laser ablation and chromatography applications.

To take the best advantage of the instrumental benefits provided by the fast scanning, flat topped or fully resolved peaks available from AttoM, a variety of software tools have been developed and integrated into the TRA (Time Resolved Analysis) capabilities of the AttoLab software suite. This technical note will describe these tools in more detail.

Data Acquisition

The fast scanning capability of the AttoM has been described previously for high precision isotope ratio measurements using flat top peaks with minimised mass bias effects in Note NA05. The same fast scan optics can be used with peaks resolved from interferences for applications such as chromium speciation using ion chromatography or combined with continuous magnet scanning in LinkScan mode to give full mass range coverage for the fast transient signals that can be seen with laser ablation ICP-MS. For all of these applications, users need to see data in real time, with fine time resolution so they can judge quickly whether optimum data is being obtained from precious samples which may have taken weeks to collect and prepare. AttoLab gives the user flexibility to define methods utilising optimised data collection using the fast scan capability of the AttoM and then visualise the data being collected in real-time with the standard TRA module as shown in Figure 1.

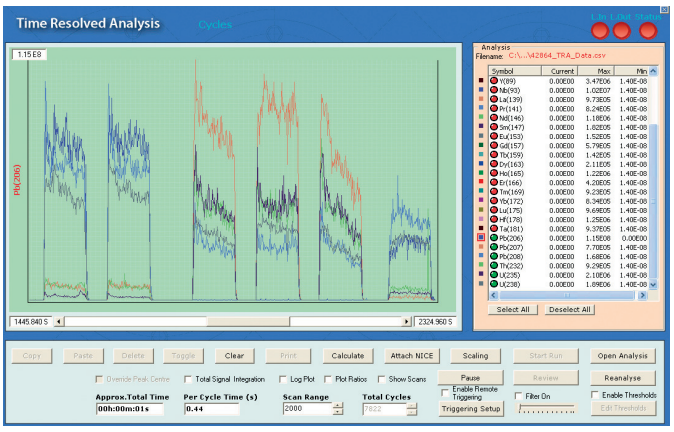

Figure 1: Showing LinkScan data for a wide range of masses whilst ablating multiple single spots in different minerals.

Data Filtering

As part of the method development for data acquisition, the user often has to determine the best compromise between precision of data collection and the time resolution of data. AttoLab allows the user to collect the data at the fastest possible rate to minimise the effects of fractionation and sample introduction flicker, before applying a filter to the data to help remove spikes and improve the precision as can be seen in Figures 2a and 2b for the same data set.

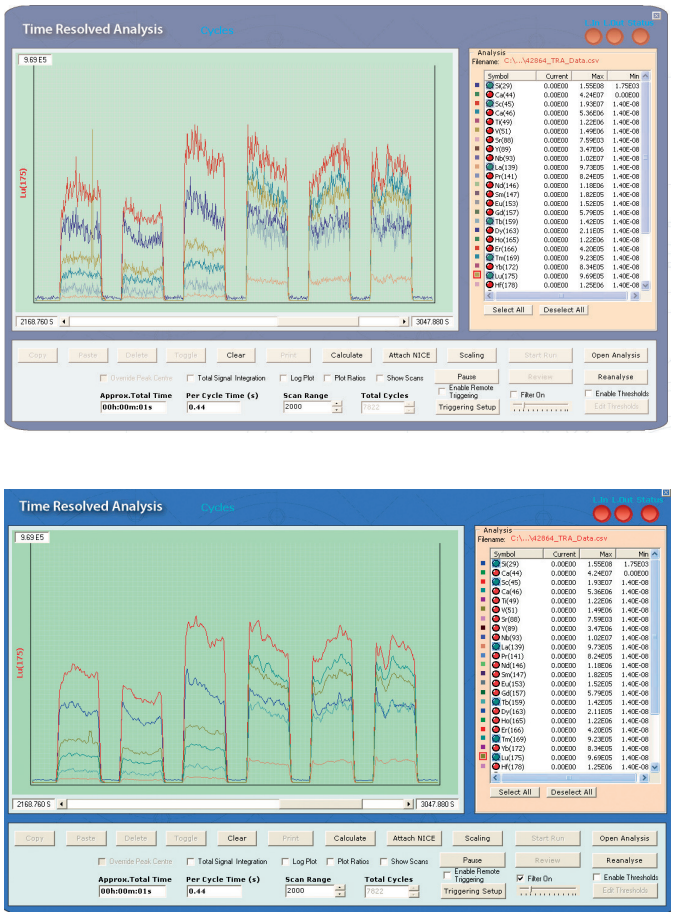

Figure 2: 2a (Raw) and 2b (low level Filtered) of the same ablation craters showing the ability to simply smooth the data for easier data interpretation.

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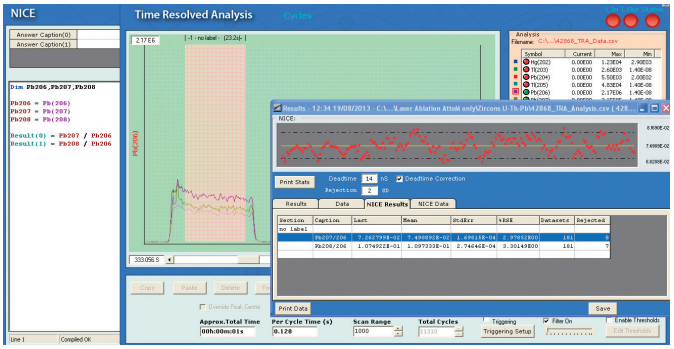
Data Reduction

AttoLab allows users to attach a Nu Instruments Calculations Editor (NICE) file to TRA data which permits simple and sophisticated corrections using normalisation from internal data and externally applied correction factors as can be seen in the example in Figure 3. Regions in the time-resolved data are defined by simple mouse drag operations and the reduced data is then shown for each region with the same graphical and tabulated display as used for other AttoLab data. The data reduction tools can be used on data files as they are being acquired or post-run using the “Reanalyse” facility.



It is possible to start collecting data in TRA mode and then use the laser or chromatograph to introduce samples into the ICP-MS storing the data into a single file which can be later processed into the individual samples. However, many users prefer the convenience of having individual files for samples which requires some form of coordination between the sampling accessory and the ICP-MS data acquisition. AttoLab provides a highly flexible hardware interface with a signal in (>2.3V for trigger OK) and signal out (contact closure) as well as a configurable trigger setup to accommodate the widest variety of devices as shown in Figure 4.

The flexibility permits either the sampling device or the ICP-MS to determine the time taken for data acquisition; this is useful for laser ablation where different patterns may take different times to acquire. The bi-directional nature of the triggers also allows for coordination between devices where for example a chromatograph may provide a trigger to start data acquisition when the sample is injected but then puts the next sample on hold until it receives a release signal from the ICP-MS after the data acquisition has completed.

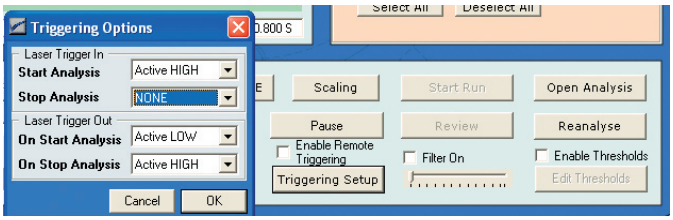


Figure 4: Flexible triggering setup allows coordination of data acquisition with a variety of 3rd party devices.

Third Party Software Compatibility

Whilst AttoLab has a powerful data reduction capability, many users have a body of calibration data from other instruments and historical work which they might want to compare with newly acquired data. To this end, Nu Instruments has coordinated with other organisations to provide simple data exchange with a wide variety of other data formats. These include the most popular geochemical packages Glitter (http://www.glitter-gemoc.com/), Iolite (http://www.iolite.org.au/Iolite.html) and the international standard for chromatography data the AIA netCDF format (Anal. Chem., 1993, 65 (3), pp 133A–133A).

Summary

The TRA module of AttoLab makes full use of the advanced hardware of the AttoM high resolution ICP-MS and enables the user to collect data that is optimised for laser ablation and chromatography applications. The tools provided for data reduction allow fast analysis of the data acquired, even in real-time, so precious samples can be preserved and improving productivity. The bi-directional hardware triggers and compatible data formats also provide the highest level of integration with third party accessory devices and software.