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TM014 – Multi-file data analysis (univariate)   WiRE™ 5

This document aims to show the WiRE™ 5 user how to analyse multifile Raman data (linear/area) to create profiles or images based on a simple single value variation. It assumes that the WiRE™ 5 software has been installed correctly with the required passwords and that the inVia instrument has an encoded mapping microscope stage.

Creating images

Once data has been collected as a mapping type measurement (see modules TM8, TM9, and TM10) Raman images can be created. Data is required to be in a multifile format and can represent a variety of external experimental variables. These can range from multi-dimensional spatial information such as surface line, depth, or area, or one dimensional variables such as temperature, time, and humidity.

The data can be used in various ways to create profiles and images. Images can be derived from:

- Raw data
- Curve-fitting
- Other

The choices available are:

Intensity at a point	Peak area	Chi squared
Signal to baseline	Peak position	FocusTrack value
Signal to axis	Peak width	Percent Gaussian
	Peak intensity	Ratio map

Multivariate image creation methods are also available (see module TM15).

Of these, the first three (red) use the raw data, and the 'peak' images (blue) require curve-fitting. If FocusTrack was used during data collection, the data stored by the computer can be used to generate a topography map. The Chi squared option allows the variance in 'fit quality' to be analysed. The Percent Gaussian allows the profile of the band(s) fitted to be expressed spatially.

Ratio maps can be generated through direct selection of any two previously generated maps.
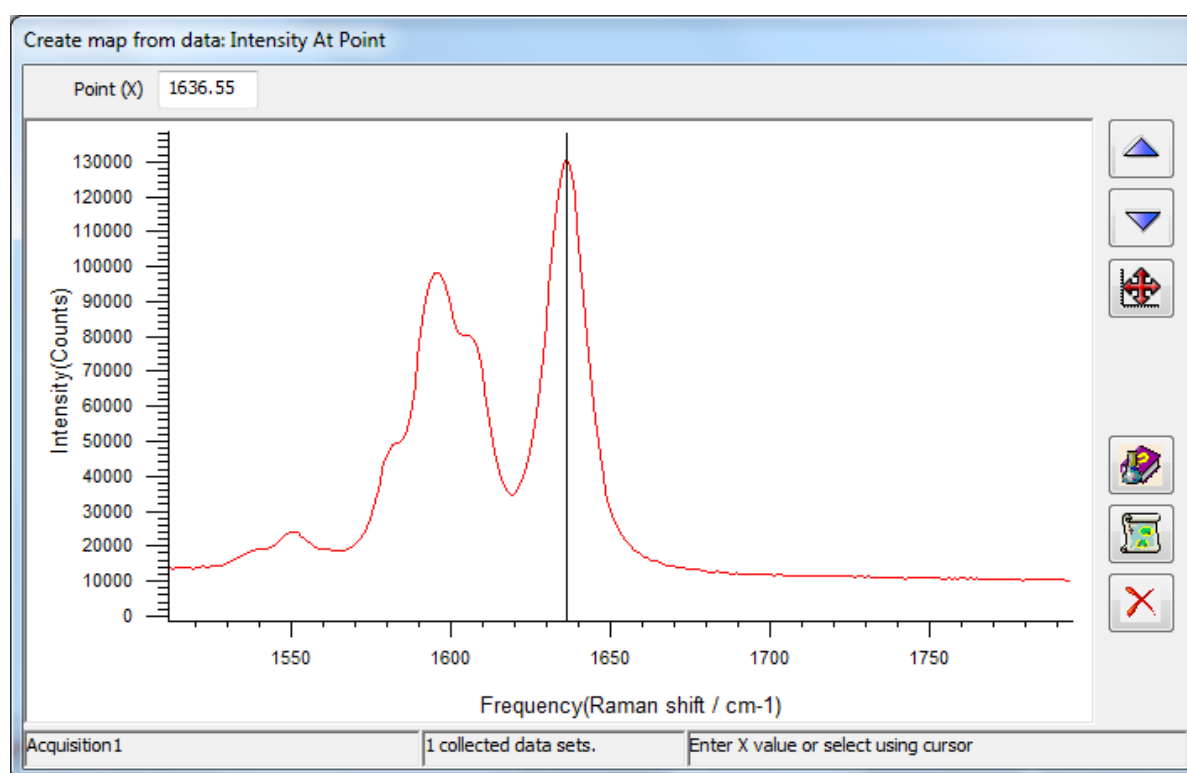
An example of creating a map follows and the principle for creating the others is similar:

- From **File…Open in new window** select the mapping data .wxd file. A Spectrum Viewer will open and display the first subfile in the dataset.

- To view the white light image, if any, select **View….View map data**.

- Use the toolbar arrows to scroll through the collected data or click on the image to select the spectrum at that point.
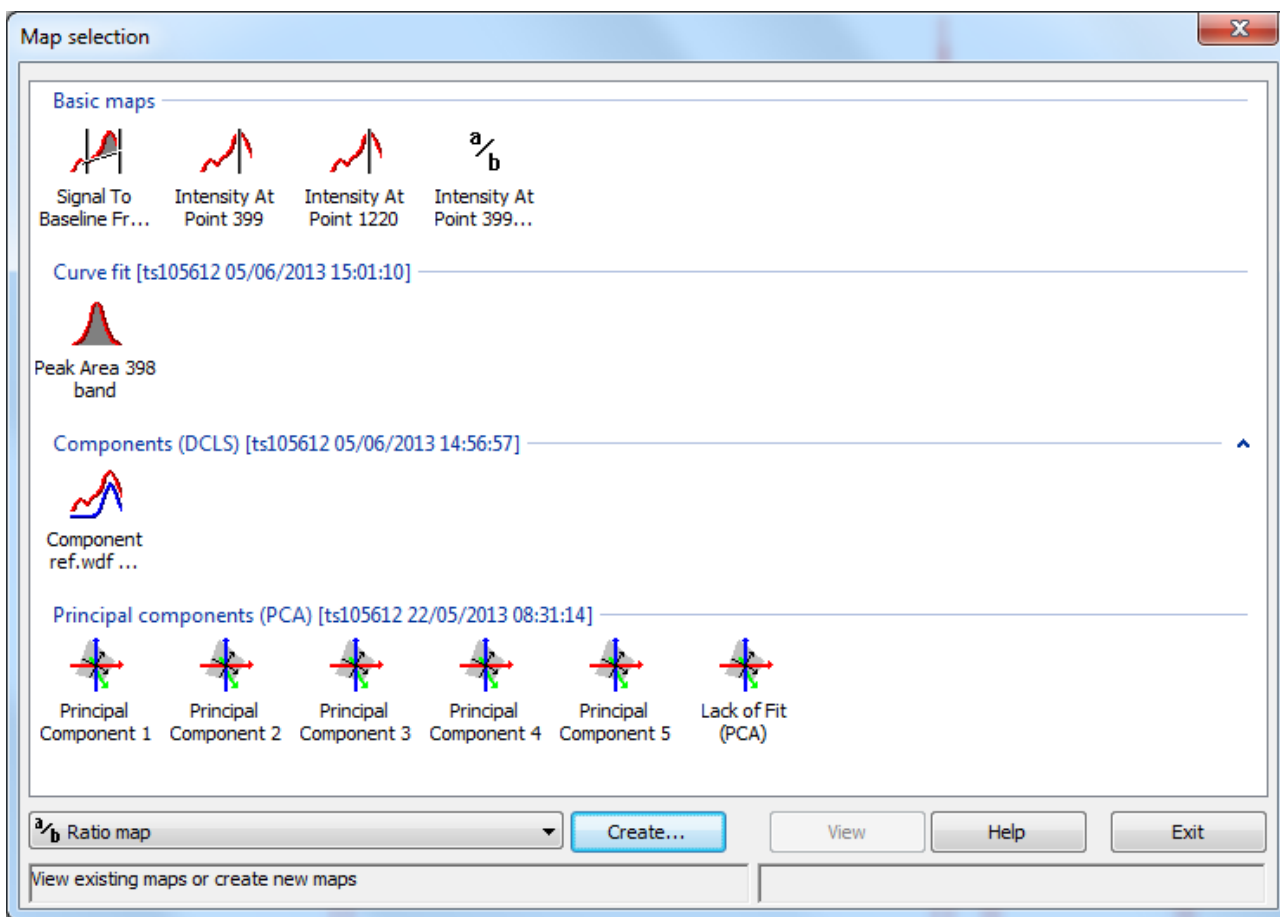
- Use the Data tab in the Navigator to view different subfiles.

- Select the [image] button to create a new map / image.

- From the dropdown, select the type of map you wish to produce (default to intensity at a point), then press **Create**.

- The 'Create map from data' window appears for the raw data-based maps, the 'Create map from curve fit results' window appears for the curve-fit based maps.

Raw data maps

For the 'Intensity at a point' mapping the cursor is used to select the frequency of the Raman band to map. It is possible to 'zoom in' on the spectrum to more accurately place the cursor or to enter the wavenumber location directly.

When the cursor is positioned on the band whose intensity you would like to map, press [image] to create the map or [image] to abort. A progress bar indicates the process of building the map. When the map has been created, highlight the icon in the 'Map selection' window that corresponds to the map you just created.

In the 'Map selection' window maps are grouped depending on the type.

Basic maps (generated from the raw data) are always displayed at the top with newer maps being added to the right.

More complex maps, which often result in the generation of multiple maps from the same analysis operation, are grouped below for each analysis operation. The map type, user, time and date are shown. Newer maps are shown at the top of the list, under any 'Basic maps' which have been generated.

Maps can be selected individually using the mouse left click or collectively using:

- Left mouse area drag
- Left mouse click in conjunction with the keyboard shift or Ctrl keys
- Left mouse click on the group title to select all of that group

Maps can be renamed by clicking on the map and clicking on the text.

Curve-fit maps

Subtle variations, for example stress in wafers, can be mapped more accurately using curve-fitting compared to raw data. A wxc curve file is required, and can be produced in several ways.

1. Press 'Load Curves' to load in a previously saved and applicable .wxc file
2. Press 'Edit Curves' to create a new curve fit using the wizard (the wizard is identical to the one used to under **Analysis…Curve fit…Curve Fit Properties**).

Loading a pre-defined curve allows the user to 'test' the curve fit prior to applying to the map data. This is achieved by curve-fitting the same curve to different spectra, such as the extremes of the spectra collected in the mapping data. Generating a new curve fit from the mapping window will apply this to the whole map data without allowing prior testing on specific single spectra.
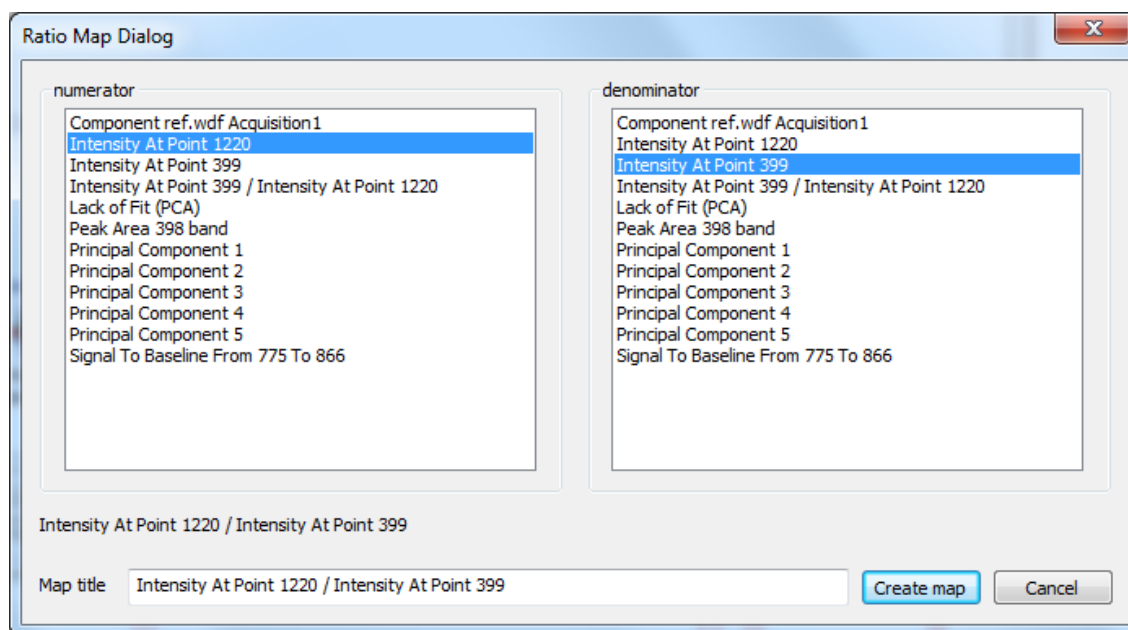
Refer to the curve-fitting section of TM12 – Data processing for further information.

You can fit complex band systems with multiple curves in a single curve-fit; any of these bands can be used to create a map. Use the 'Curve Name' text box to label the curves as this will make it easier to use when creating maps. Use the 'Perform fit' button to initiate the curve fit.

When the curve fit has completed (there is a progress bar), press to create the map. **View** the map as described previously. Once a curve fit has been performed on mapped data you can create other maps without the need to re-perform the curve fit (e.g. peak position, peak width).

Ratio maps

A simple ratio of two maps can be created using the 'Ratio map' option from the drop down menu. The two individual maps must first be created. All generated maps are then available for selection.

The ratio map is automatically titled, but this can be changed by the user.