Technical White Paper

Spectral Resolution in Dispersive Raman Microscopy

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Spectral resolution in Raman microscopy:

Selecting the right spectral resolution is of decisive interest to all Raman users. This applies to the purchase as well as the daily work with a Raman microscope. In most cases, the user's application and studied materials determine the final choice in spectral resolution.

For example, narrow Raman lines, such as those found in highly crystalline materials or gases, require higher spectral resolution. In contrast, high resolutions are not required for the identification of amorphous solid material or liquids.

➔ If you want to catch up with the basics of Raman spectroscopy please take a look at our introduction website.

The definition of spectral resolution:

The ability of the spectrometer to separate two adjacent spectral lines is called spectral resolution. Among other factors, the spectral resolution of a dispersive Raman instrument is mainly affected by the following parameters:

- **Focal length of the spectrograph**
  (the longer the focal length the higher the spectral resolution)
- **Optical grating**
  (the higher the groove density the higher the spectral resolution)
- **Excitation wavelength of the Raman laser**
  (the longer the wavelength the higher the achievable spectral resolution)

How spectral resolution is determined:

The best way to evaluate the spectral resolution of a Raman spectrometer is to measure a real sample which shows Raman lines which are significantly narrower than the spectrometer would be able to resolve. A suitable example is liquid nitrogen which shows extremely narrow bands.

To evaluate the spectral resolving power of the SENTERRA II Raman microscope it was compared with a high performance FT-Raman instrument as reference (see Figure 1). The line width of the N-N stretching vibration was determined as 1.2 cm^{-1} for the compact Raman microscope SENTERRA and 0.2 cm^{-1} for the FT-spectrometer.

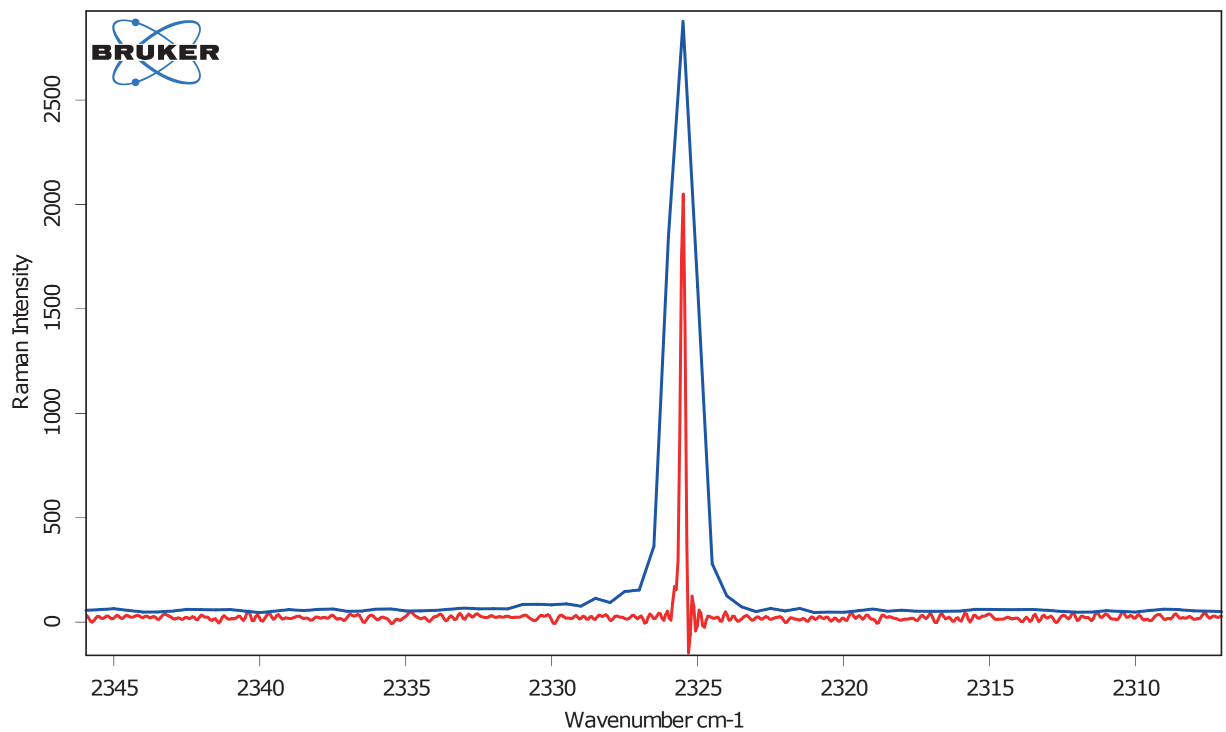


Figure 1: Raman spectra of the N-N stretching vibration of liquid nitrogen recorded with the dispersive Raman microscope SENTERRA II (blue spectrum, laser 785 nm) and the VERTEX/RAM II FT-Raman instrument (red spectrum, laser 1064 nm).

Why spectral resolution is so important:

Simply said: High spectral resolutions can reveal more details of the sample. Figure 2 shows the spectra of Triptycene at standard (4 cm^{-1}) and high spectral resolution (<1.5 cm^{-1}) recorded with the Raman microscope SENTERRA II. Obviously, the Raman spectrum with higher spectral resolution exhibits much more spectral details.

High spectral resolutions are not always better:

The acquisition of the high-res spectrum required at least three times more measurement time. This is because of the reduced spectral coverage of the high-resolution grating (1200 gr/mm) making it necessary to acquire several spectra and merge them into a single spectrum for covering the entire spectral range. Additional measurement time may be necessary to compensate the higher noise level of the high-resolution grating.

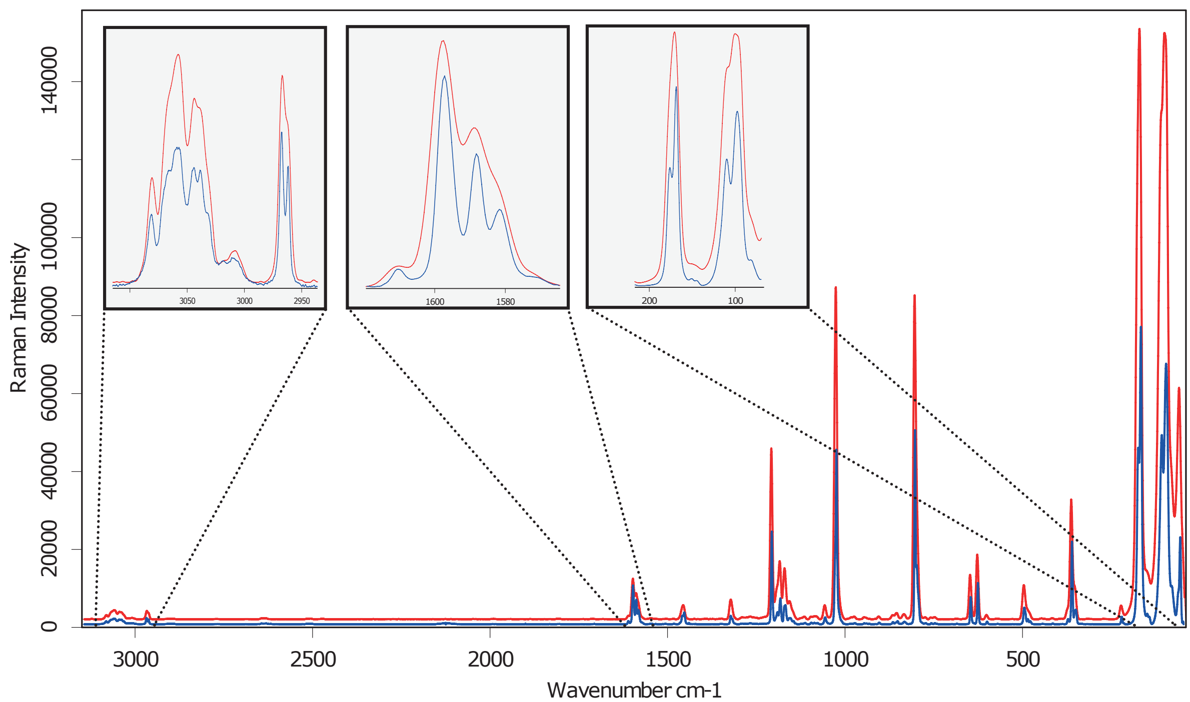


Figure 2: Raman spectrum of trypticene collected with full spectral range with the standard grating (4 cm^{-1}, red) and the high-resolution grating (1.5 cm^{-1}, blue). The highlighted areas show the obvious differences between the spectra.

In fact, spectral resolution comes at a price:

You should be aware, that there is a frequent trade-off between spectral information and acquisition time. Especially with Raman images, this becomes painfully obvious as measurement time is a key factor. Therefore, the spectral resolution should be kept at a sweet spot, where prominent spectral features are still easily recognized, but the measurement time remains feasible.

The best resolution for each application:

As we have seen, higher spectral resolutions are not necessarily the better choice. For routine analysis such as sample identification with digital reference libraries a spectral resolution of 4 cm^{-1} or less is quite sufficient.

If, however, you want to perform structure analyses and study polymorphic materials and molecular interactions, a high spectral resolution of smaller than 2 cm^{-1} is mandatory. Fortunately, only high-end research applications require resolutions of better than 1 cm^{-1}, for example to resolve the rotational and vibrational fine structure of gases.

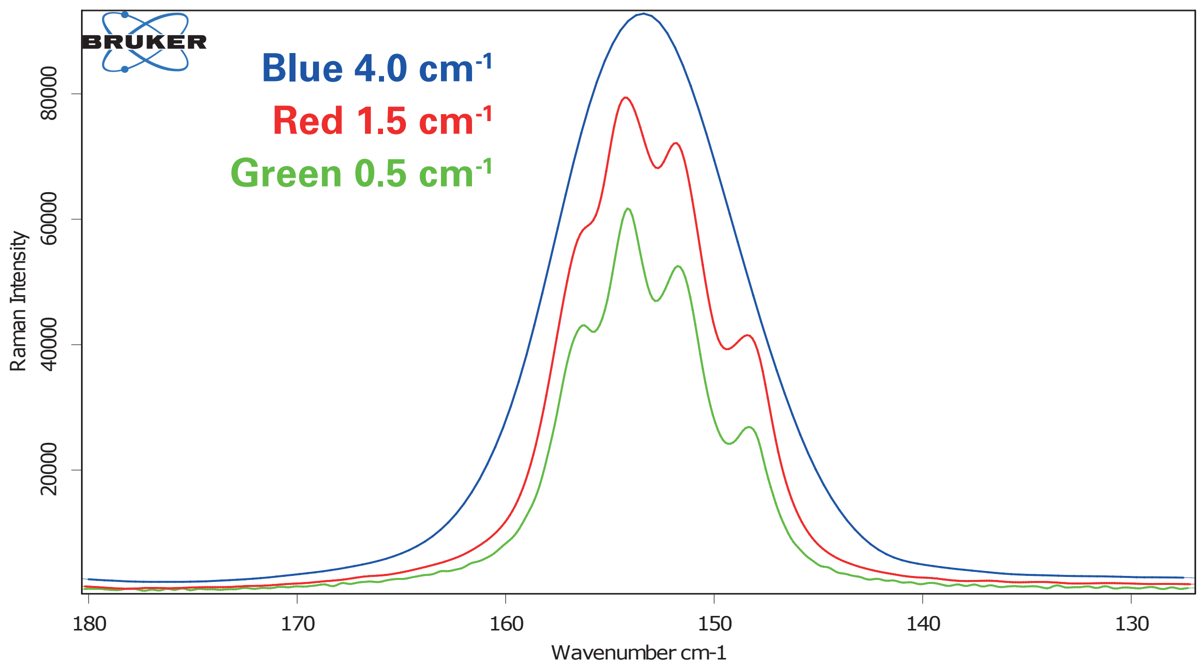


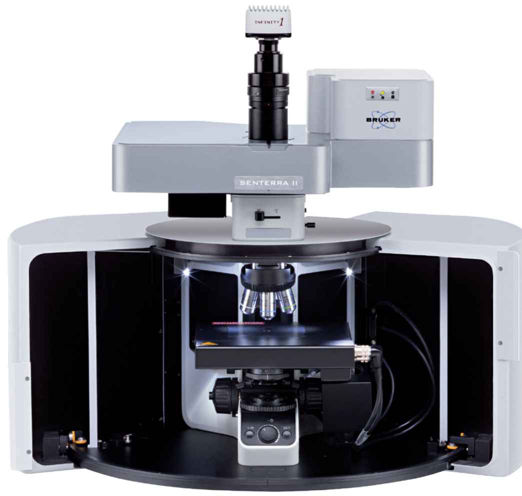
Figure 3: The Raman line of Sulfur at 153 cm^{-1} acquired at different spectral resolutions with different instruments: Blue: 4.0 cm^{-1} by SENTERRA II, 532 nm, grating: 400 gr/mm; Red: 1.5 cm^{-1} by SENTERRA II, 532 nm, grating 1200 gr/mm; Green: 0.5 cm^{-1} by MultiRam FT-Raman, 1064 nm.

This is how you select the optimal resolution:

It should be noted that it is not always required to resolve Raman bands to their full extend. Figure 3 shows the Raman line of sulfur at 153 cm^{-1} at different spectral resolutions. While with the lowest resolution grating only a single line can be observed, at a resolution of 1.5 cm^{-1} all bands are already present. While a resolution of 0.5 cm^{-1} resolves all bands completely, still only four peaks are visible, making a resolution of 1.5 cm^{-1} the optimal choice.

The conclusion:

It has been shown that the spectral resolution required for dispersive Raman microscopy depends on the intended application and the sample material. A Raman microscope must be capable to provide both, full spectral range at 4 cm^{-1} as well as high resolution lower than 2 cm^{-1}. The first for routine tasks like sample identification and the latter for the evaluation of spectral fine structures as required for the study of polymorphism.



Are you interested in more information or would you like to take Raman microscopy to the next level?

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