



# UV-VIS-NIR Spectroscopy in Gem and Mineral Identification

GL Gem Spectrometer UV-VIS-NIR  
GL Gem Spectrometer NIR PL405

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## The Gemmologist's "Tripod"



whom

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cure.

Source: Meiji Techno, Eickhorst



Over 75 years ago Basil Anderson, whom we consider "The Father of Gemmological Spectroscopy" wrote: The spectroscope is the third leg of the tripod of instruments in which modern determinative gemmology rests secure.

Here is the first one - a diffraction grating type spectroscope.

Can you name the other instruments? There's the refractometer and then of course the microscope. And if money doesn't matter- an immersion scope which we have in our lab for serious gem identification.

## Current Status of Advanced Gem Testing with Low Cost Spectrometers

- Hand Spectroscope vs. Spectrometer
- Transmission Spectrometry (GL Gem Spectrometer)
- Photoluminescence Spectrometry (NIR PL405)
- Vibrational Spectroscopy (GL Gem Raman PL532)

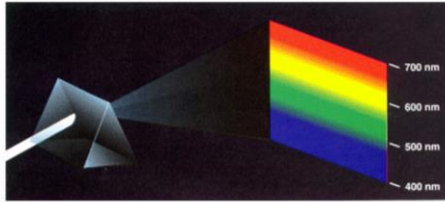


Gem testing instruments have varying degrees of usefulness. Some are being used by the practicing gemmologist on a daily basis; some are used less often because they are difficult to use. Spectroscopes are one of them.

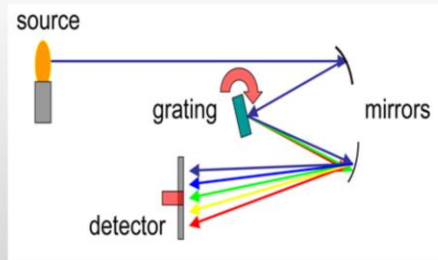
In several video clips I will demonstrate how the GL Gem Spectrometer works and how reference databases are used to identify certain spectral characteristics.

At the end I will briefly discuss several advanced testing instruments.

## Development of Spectrometry



- **Prism Spectroscope**  
(Dispersion)



- **Spectrometer**  
(Diffraction Grating)

Source: Wikipedia

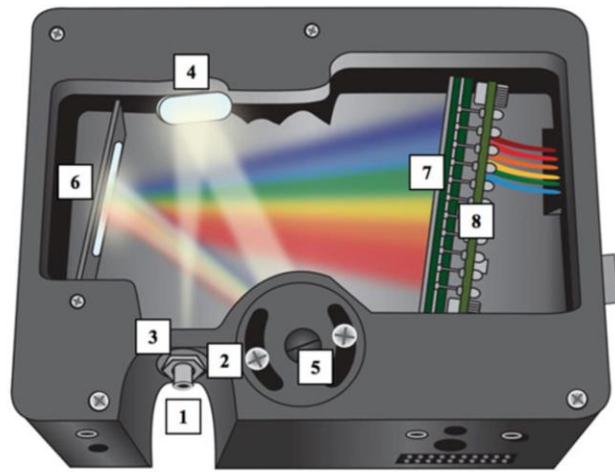


We all know how a prism spectroscope is built and understand the optical property called “dispersion” - the splitting of white light into its rainbow spectrum.

Today, most gemmologists are using a diffraction grating spectroscope. It was introduced 35 years ago as the so called OPL spectroscope and has replaced the prism spectroscope because it can be made at a lower price.

Similarly, the modern spectrometer does not use a prism anymore but a grating as you can see in the simple drawing.

## Miniature Spectrometer



- 1 SMA 905 port
- 2 Fixed Entrance Slit
- 3 Long pass Filter
- 4 Collimating Mirror
- 5 Grating
- 6 Focusing Mirror
- 7 Collection Lens
- 8 Detector

Optical Bench: UV-VIS-NIR: 200 – 1100 nm range

Source: Ocean Optics USB 4000



The GL Gem Spectrometer covers a range from 300 – 1,000 nm. The optical bench looks very similar to this illustration.

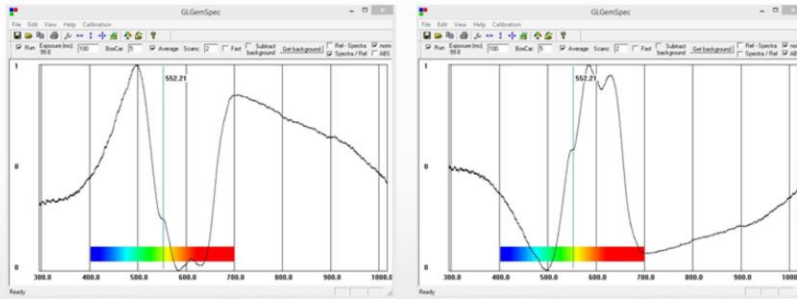
Above the slit is a connector for the light holder or an optic fiber. The slit is usually from 25 – 100 microns in size. *The slit regulates the amount of light that enters the optical bench and controls spectral resolution.*

The entering light is now reflected off a collimating mirror and focused towards the Grating of the spectrometer. *Gratings are available in different groove densities allowing you to specify wavelength*

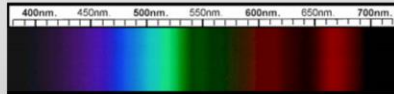
*range and resolution of the spectrometer.*

The light reflected from the Grating focuses now onto the detector plane. *The detector converts the optical signal to a digital signal. Software is necessary to display the data on a computer screen.*

## Transmittance vs. Absorbance

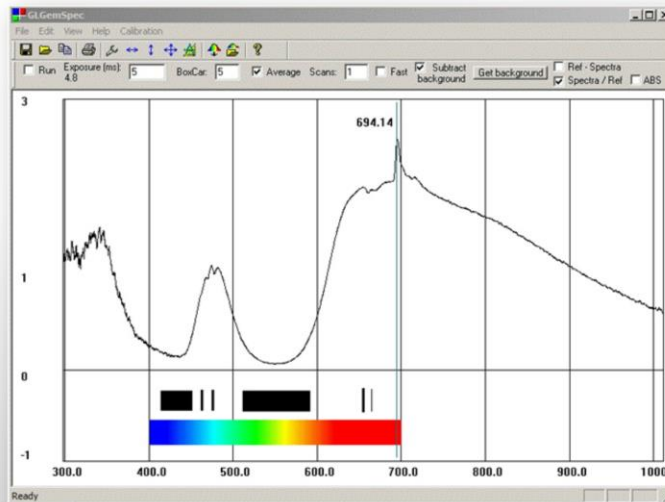


Synthetic Blue Spinel (Verneuil), cobalt bands



Before we move on, let's take a quick look at transmittance and absorbance.

## Transmittance Spectra



Synthetic Ruby, Verneuil (flame fusion)



The GL Gem Spectrometer measures transmission.

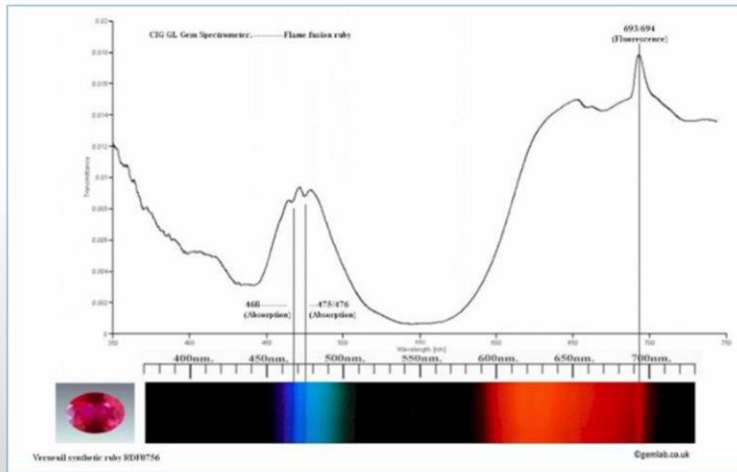
Here is an actual graph illustrating transmittance compared to what you would see in a hand spectroscope.

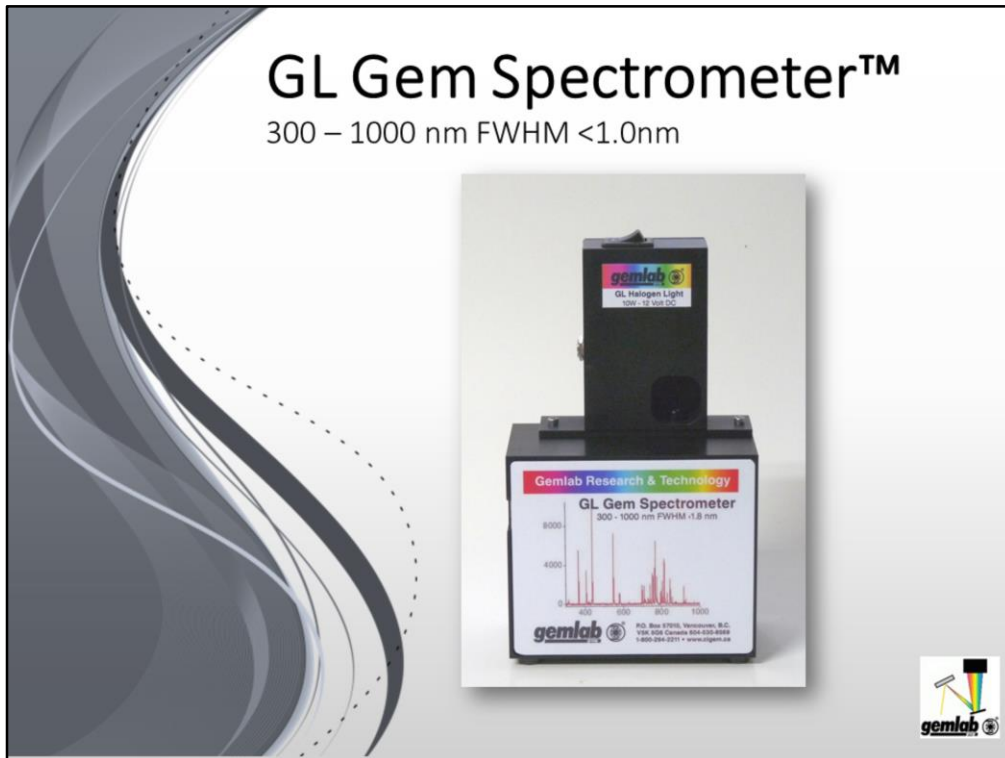
We are looking for peaks, dips or valleys.

The dips or valleys represent low transmission or, in other words, areas where more light is being absorbed. In a hand spectroscope you would see black lines or bands in these areas.



# Synthetic Ruby, flame fusion



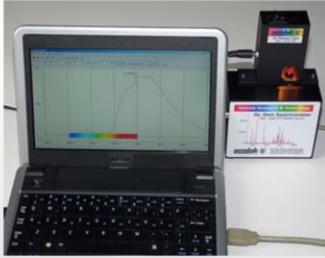


Now let's take a closer look at the GL Gem Spectrometer.

To protect the gemstone the built-in light holder has a cooling fan. It also can be removed if the sample is larger.

Special firmware in the micro-processor optimizes the unit for the near infra-red range (GL Gem Spec NIR PL405) which is of interest to gemmologists.

## Advantages of the GL Gem Spectrometer



- ❖ Easy and Quick Setup (USB Plug & Play)
- ❖ Observe Spectra in Real Time
- ❖ Eyes are protected from strong light
- ❖ Transmission and Absorption Modes
- ❖ Save Spectra for Later Editing
- ❖ Test Rough and Faceted Gems in Bulk

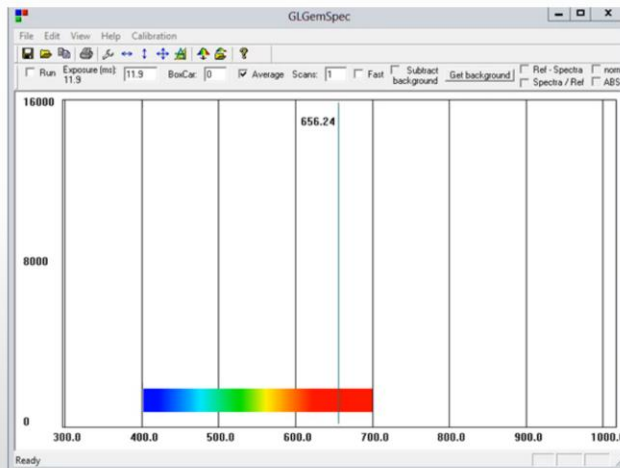


## Getting Ready with Spectroscopy



The sample is placed above the entrance port of the spectrometer; a small cosine connector with a Teflon disk works as a diffuser.

## How to Obtain a Spectrum



This is how the interface of the GLGemSpec program looks when you first start the program.

A spectrometer is similar to a digital camera. You have to make certain adjustments for light conditions, the object and its background.

Exposure time is in milliseconds. For darker stones we will increase the exposure time. BoxCar smoothens the spectral curve at the expense of resolution.

When we click on RUN we will see a wiggling line near zero. Now we click GET BACKGROUND and the box

next to it will lighten up. We click on SUBTRACT BACKGROUND . Next we TURN THE LAMP ON and immediately you will see the bell-shaped curve of the halogen bulb. We are now in SCOPE mode.

Next we click on the rain-bow icon to take a lamp spectrum. Now all the boxes to the right lighten up. Click on [HERE](#) for a transmission spectrum or [ABS](#) to obtain an absorption spectrum.

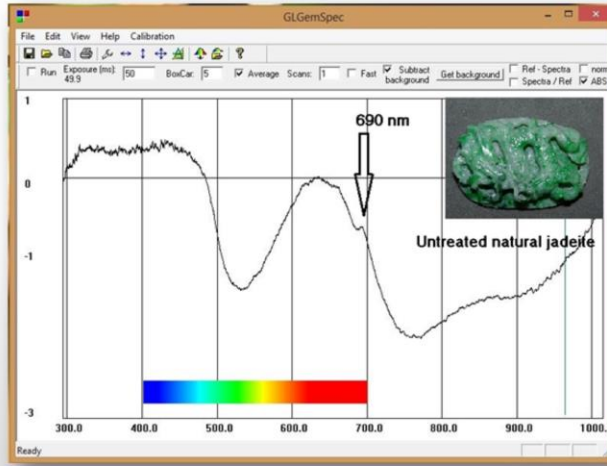
Let's watch.

## Removing the GL Light Holder



- Remove the light holder and put some "blu-tack" to level the sample with the entrance port
- Place the sample area over the entrance port
- Shine the GL Xenon Flashlight from above onto the sample and observe the spectral graph

## Jadeite – Natural or Dyed?



- Jadeite, Burma – Naturally Coloured with Typical Absorption Lines at 437 nm, 630 nm, 655 nm and 690 nm  
(Edited in Spekwin32)

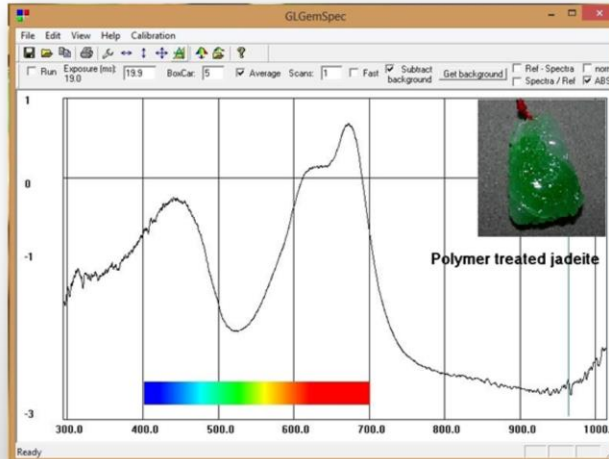


This study is based on research by the National Gem Testing Center of China and was published in the Journal of Gemmology in 2012.

In a survey with 3,000 samples of untreated jadeite all had the same characteristic absorption peaks.



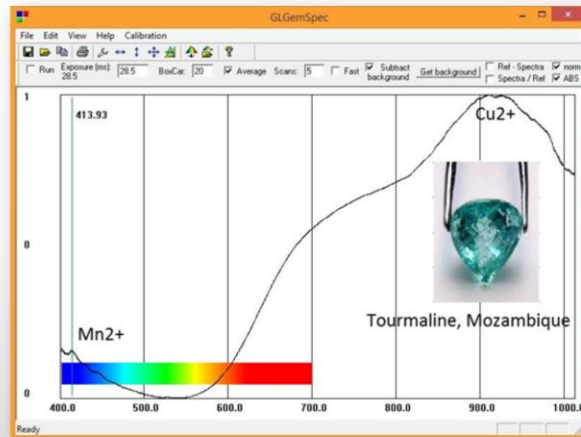
## Jadeite – Natural or Dyed?



- The 690 nm peak is missing. The jadeite could be treated by dyeing (use Chelsea filter) or polymer treatment (use GL Gem Raman PL532 or GL Analyzer PL405)



## Detection of Chromophores

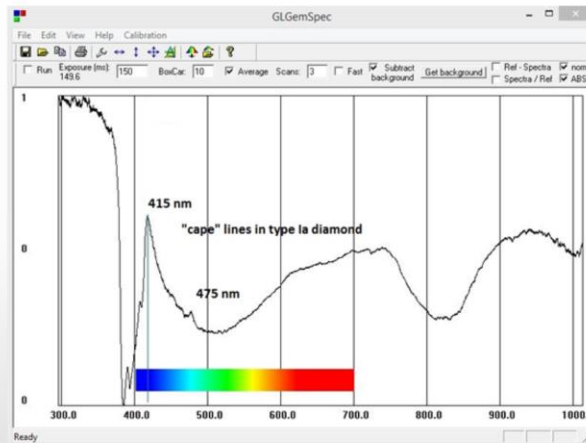


- Typical Absorption in the 920–940 nm Range of Blue Copper Bearing Tourmaline



The GL Gem Spectrometer allows quick checking for certain features.

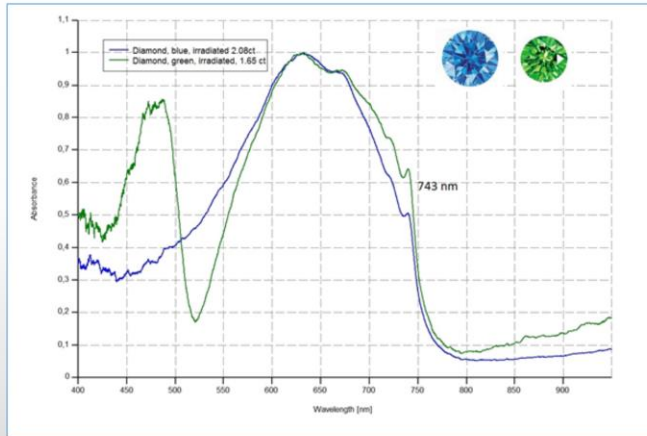
## Diamond Characterization



- Typical 415.5 & 475 nm Peaks for Cape Type Ia Diamond (edited in Spekwin32)
- Recently (October 2013) the GIA Research Lab in New York reported several Type Ia diamonds to be treated by HPHT.



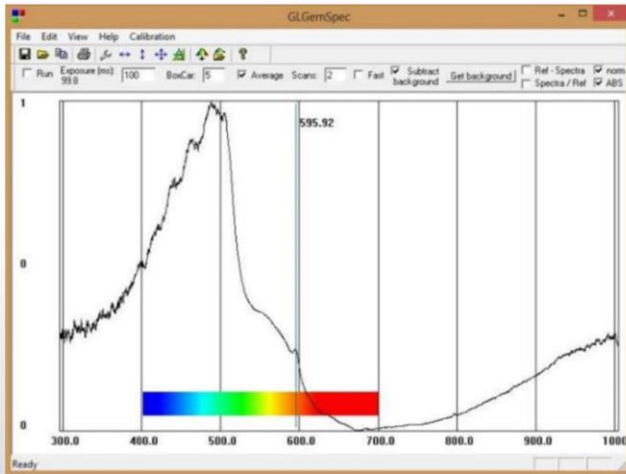
## Diamond: Irradiated



Irradiated Diamond with Typical GR-1 Band at 743 nm



## 595 nm band, Reddish Diamond

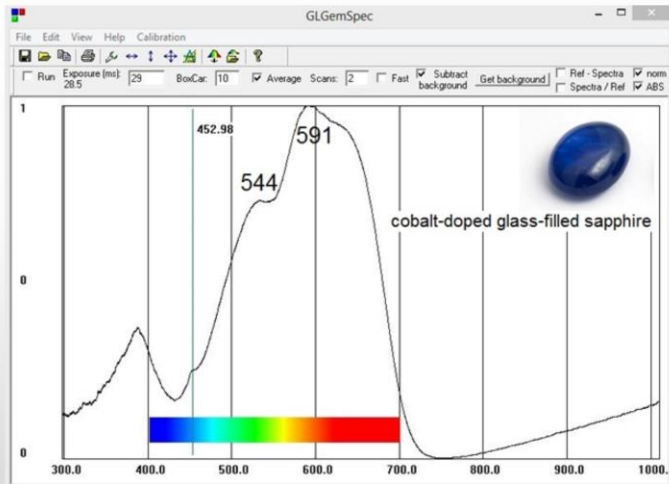


Nitrogen-related defect of uncertain structure commonly associated with irradiation and annealing of the diamond.

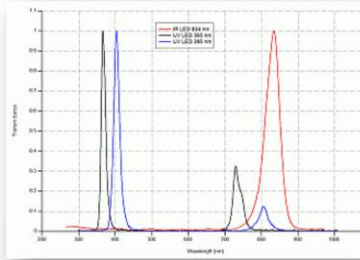


This band is a nitrogen-related defect of uncertain structure. It is commonly associated with laboratory irradiation and annealing of diamond.

# Sapphire, treated

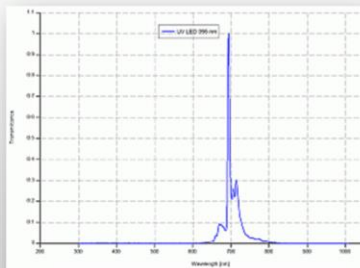


## Emission Spectra UV-LED Excitation



- Emission Spectrum of UV LED 365 nm (Nichia, black), LED 395 nm (blue), IR LED 835 nm (red)

Note second-order effects from diffraction at 750 and 800 nm: 2015 model has built-in diffraction order sorting filter



- Synth. flame fusion ruby, scope mode with emission peaks

Source UV LED 395 nm



Several people have experimented with UV-LEDs and believe that emission spectra are helpful in gem identification. There has been very little work done in this area; most studies of the past use obsolete mercury lamp as an excitation source.

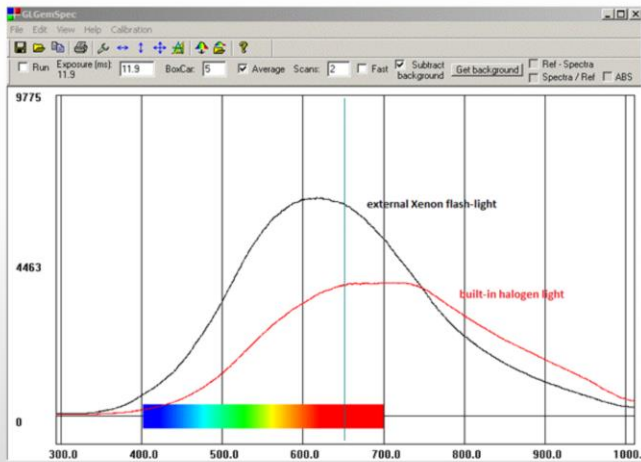
Emission behaviour of a gemstone depends largely on the excitation source. We found that a just slight change in wave-length of the LED lead to unexpected emission patterns.

A proper graph recording these spectra must be 3-dimensional because an array of light sources must be

used. Educating people on how to interpret these results could be a challenging task.



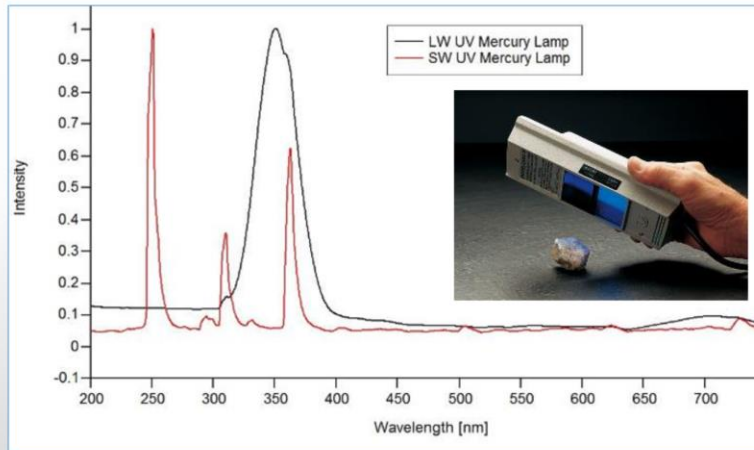
# Comparison of Halogen and Xenon Light Sources



Xenon light has better performance in VIS than halogen.



## Problems with mercury lamps



Both short-wave and long-wave mercury lamps do not emit monochromatic radiation: NOT RECOMMENDED



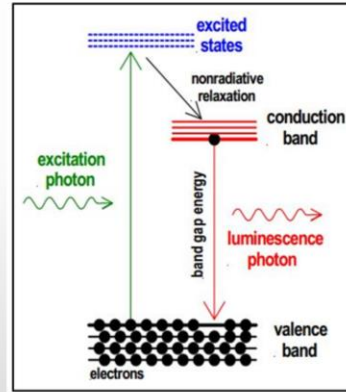
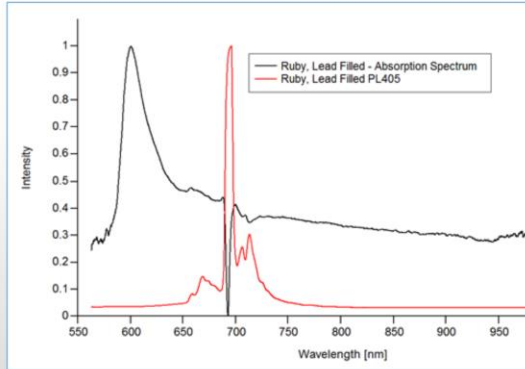
# Photoluminescence and VIS-NIR Spectroscopy

The GL Gem Spectrometer can be used for PL studies using a laser or UV LEDs; a long wave band pass filter is recommended.

Many fluorescent gemstones can be identified based on their Cr<sup>3+</sup> PL response.



Photoluminescence (PL) is light emission from any form of matter after the absorption of photons (electromagnetic radiation)



Cr<sup>3+</sup> Excitation Source Blue Laser (405 nm)



## GL Analyzer Kit 405nm or “do-it-yourself” from parts



Cut-off for red filter around 600 nm



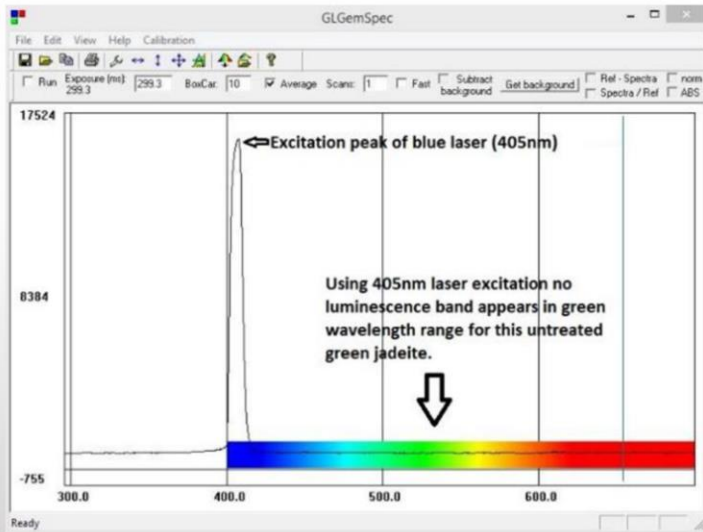
No transmission under 600nm

## Setup of GL Gem Spectrometer for PL 405 Spectroscopy

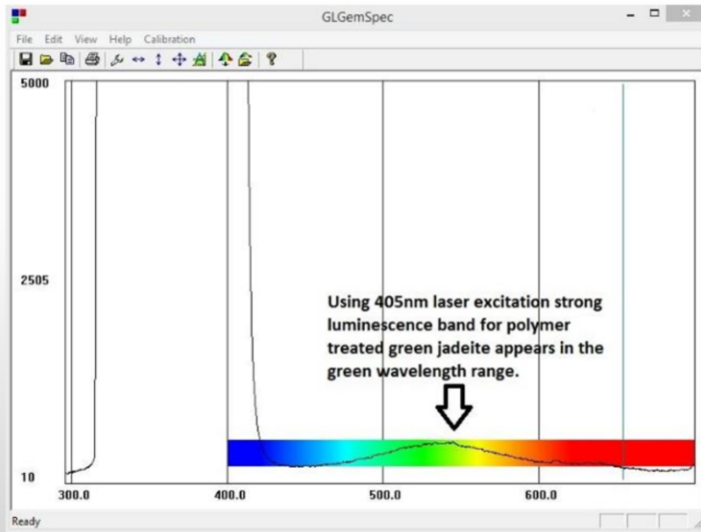


In this setup the green jadeite is tested whether it is polymer treated.

# Untreated Jadeite PL405



# Polymer Treated Jadeite PL405



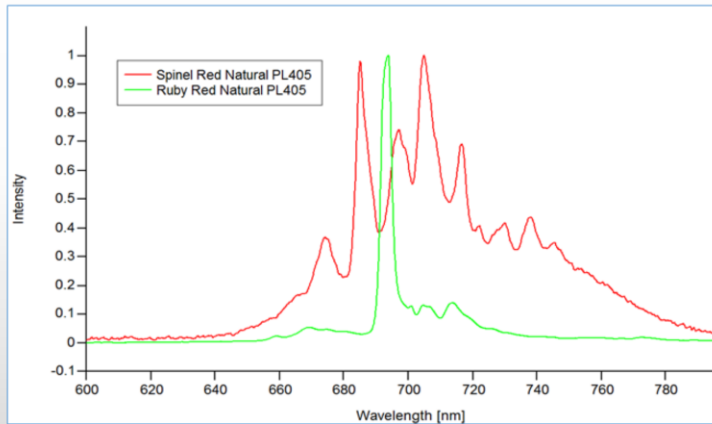


## NEW FOR 2015

The GL Gem Spectrometer NIR PL405  
- a dedicated dual purpose instrument



## Quick separation of natural ruby from natural spinel PL405

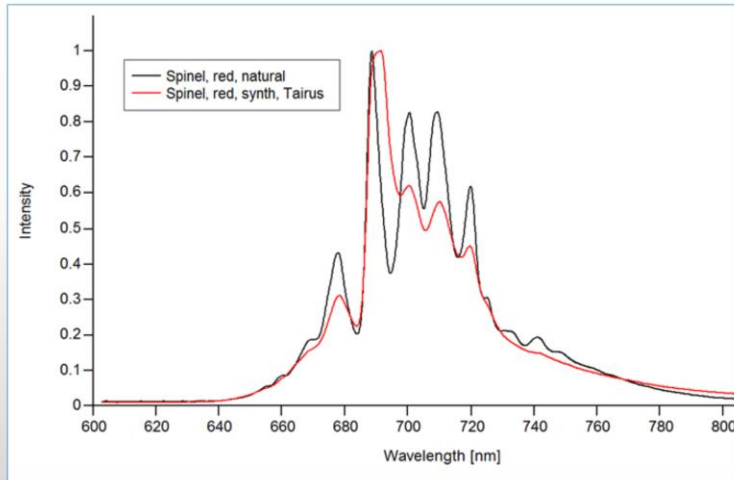


Cr<sup>3+</sup> Excitation Source Blue Laser (405 nm)



Shape and position of CR+3 bands differ between natural and synthetic samples. In natural spinel they are sharper and in synthetic and heat treated spinel they are wider due to disorder.

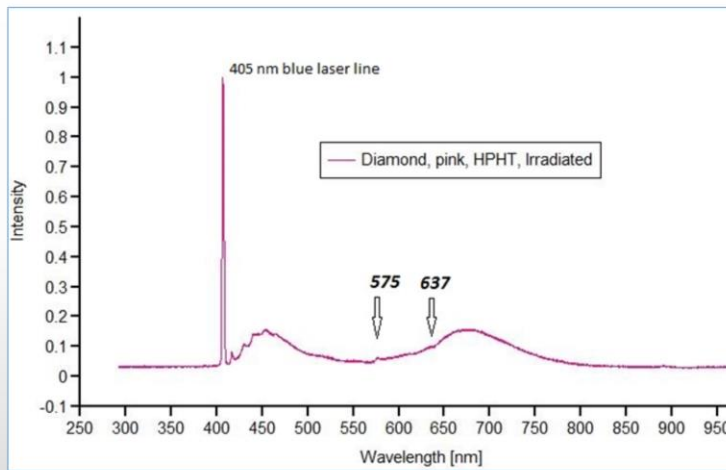
## Separation of synthetic spinel from red natural spinel PL405



PL spectrum of natural spinel shifted to the left



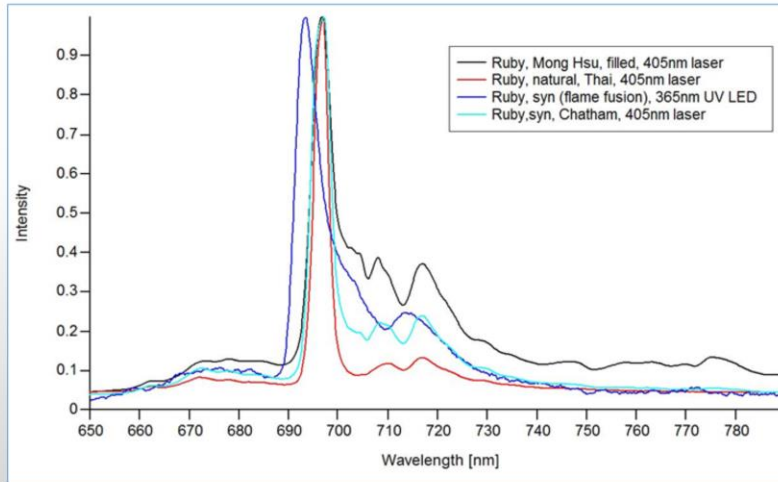
## Diamond Characterization PL405



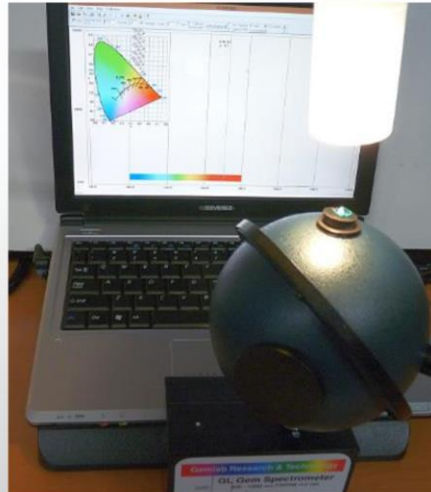
Determination of diamond treatments is difficult because it is often a multi-step process; research is ongoing.



## Ruby Characterization with 365nm UV LED (Nichia) and 405 nm Laser



## Other Applications: XYZ Chromaticity Measurements



For experimentation we offer a firmware modification which allows calculating chromaticity coordinates from spectral power distribution.

The blackbody locus represents the chromaticities of blackbodies having various (colour) temperatures.

The best setup is with an integrating sphere.

## Cryogenic Applications (under development)



Low cost LN (liquid nitrogen) Accessory (Prototype)



GL LN (liquid nitrogen) Accessory for experimental diamond luminescence studies.

This is work in progress.



## SUMMARY OF THE GL GEM SPECTROMETER

- ❖ Low Cost System for Gemmological Laboratory
- ❖ Require Some Training and Experience
- ❖ Various Reference Sources Available
- ❖ Compliments Other Gem Testing Tools
- ❖ Non-destructive and Ideal for Bulk Testing



The computer is a necessity in the daily work of a gemmologist. My GemSpec instrument is plugged in all the time and I often use it when I would have traditionally used a refractometer first.

Another important part of our project is the creation of a reference data-base. A number of GemSpec users have already contributed to the on-line data-base and others are available for reference on the internet.



## ACKNOWLEDGEMENTS

- Dr. Bill Hanneman for including the GL Gem Spectrometer in his book “Pragmatic Spectroscopy for Gemologists”.
- Bill Wise for allowing use of spectral images from his “Gemology Tools Professional” software.
- John Harris from Gemlab.UK



QUESTIONS?



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