



# Application Note AN M121

## Analysis of Gemstones and Diamonds in Jewelry with the FTIR Microscope LUMOS II

#### Introduction

Since the late 1800s synthetic gem-crystals are available and the production processes were more and more refined. Later, starting in the 1950s, also diamond was available via different kinds of syntheses and can now be produced in gem-quality with individual masses of one carat or more. In parallel many different methods were developed for the quality improvement of natural gemstones and diamonds like fracture filling, color improvements via physical and chemical methods and so forth. Thus, the knowledge about the stone's genesis and history has become crucial and has substantial economic implications.

Fourier-Transform-Infrared spectroscopy (FTIR) is one of the most significant analytical techniques and the method of choice when it comes to the identification and classification of diamonds and gemstones. However, the analysis of mounted stones which are very small or very close to other stones is often very challenging since the commonly used reflection techniques do not provide the necessary spatial resolution for such difficult specimens. The FTIR microscope LUMOS II allows analyzing mounted stones of almost any size. Due to the high working distance of the LUMOS II also such stones can be analyzed that are inaccessible to macroscopic IR-measurement techniques like for instance sunk-in stones.

| Keywords                      | Instrumentation and Software |
|-------------------------------|------------------------------|
| IR Microscopy                 | LUMOS II FTIR Microscope     |
| Gemstone identification       | Opus Software                |
| Jewelry analysis              |                              |
| Diamond type<br>determination |                              |



Figure 1: LUMOS II FTIR microscope

#### Instrumentation

The FTIR microscope LUMOS II stands out due its full automation and ease-of-use combined with sample visualization and infrared spectroscopic performance of excellent quality. Mounted stones can be inspected with the aid of a special sample holder vice that allows fixing all kinds of jewelry. The vice allows tilting the sample up to a certain angle in order to precisely position different measurement points without the need to remove the sample.

Besides the automated hardware the software provides a very elegant wizard based operating concept. The user is guided through the whole measurement procedure by the dedicated OPUS video-wizard, a user interface that always provides the appropriate functions for the current measurement step. Although the LUMOS II is designed to be operated by non-experts for routine applications, its exceptional sensitivity makes it also very suitable for high demanding applications.



Figure 2: Diamond ring fixed in the sample holder vice on the LUMOS II stage.

#### **Example: Diamond ring**

Figure 2 shows the sample holder vice with a diamond ring. The whole ring is shown in the picture inset; the single diamond stones are very small and mounted very closely together which makes it difficult to analyze them separately with macroscopic IR-measurements. An example measurement of one of the stones is shown in figure 3 together with the visual image. The IR-spectrum allows drawing direct conclusions about the crystal lattice of the



Figure 3: Diamond spectrum of one of the stones from the ring.

diamond, impurities like nitrogen, boron or hydrogen can be easily detected. Furthermore it is possible to get information about the configuration of the nitrogen impurities like the presence of isolated nitrogen atoms or clusters of two or four nitrogen atoms. The y-axis of the IR-spectrum shows the absorption and the x-axis the reciprocal value of the wavelength in cm<sup>-1</sup> (i.e. how many waves exist over one cm) which is a unit commonly used in IR-spectroscopy. Nitrogen impurities typically show absorptions between ca. 500 and 1500 cm<sup>-1</sup> and boron impurities show typical peaks around 2800 and 2460 cm<sup>-1</sup>. The strong and broad bands between ca. 1600 and 2700 cm<sup>-1</sup> are so called two phonon bands and characteristic for all diamonds. They are an excellent marker than can be used to differentiate between diamonds and imitates. Furthermore, depending on the type and configuration of foreign atoms, it is possible to assign a specific type to every diamond. This type information helps to differentiate between natural and synthetic stones. The spectrum shown in figure 3 is typical for diamonds of type IaA which proves the natural origin of the stone. Typically for diamonds in jewelry the spectrum shows additional signatures from organic contaminations like for instance from skin fat. The double peak below 3000 cm<sup>-1</sup> results from the C-H stretching vibrations that are typical for organic substances.

#### **Example: Gold ring with gemstones**

This example presents the analysis of different stones mounted in the gold ring shown in figure 4. Amongst others the ring has three very small sunk-in colorless stones that are very difficult to access. Figure 5 shows a visual image together with the IR-spectrum of one of the clear stones. The spectrum clearly shows that the stone is a diamond from type IaAB which means that it is of natural origin. Again the spectrum shows additional bands from fat and protein that are superimposed on the regular diamond spectrum.

Additionally spectra were measured from a representative green, blue and red gemstone mounted in the ring. The spectra can be seen in figure 6; two upper spectra are typical reflection spectra of corundum and stem from the blue and red gemstone which can thus be identified as sapphire and ruby. The spectrum of the green stone is shown on the bottom of figure 6 and shows bands that are typical for beryl. Thus the stone is identified by the spectrum and its green color as an emerald.



Figure 4: Gold ring with diamonds and green emerald.



Figure 5: Image and spectrum of one of the diamonds from the ring pictured above.



Figure 6: Spectra of gemstones in the gold-ring. From top: Blue, red and green stone.

#### Summary

The FTIR microscope LUMOS II allows to examine, identify and classify even very small mounted diamonds and gemstones and can handle also sunk-in stones. Small stones that are in close proximity to others can be measured with a very high selectivity. The spectral data allows drawing conclusions whether the stone is synthetic or treated and thereby assessing its true value.

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