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An automated technique for detailed μ-FTIR mapping of diamond and spectral deconvolution

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Since the original classification of diamonds based upon their absorption in the one-phonon region of the mid-infrared (IR) range was first introduced, a vast amount of research has been carried out in this field. The result today is that IR analysis has become the principle tool for classifying diamonds based upon the concentration and aggregation state of nitrogen, the most common impurity found within their crystal lattice. These studies have shown that diamonds can contain a large range of nitrogen, from nominally nitrogen free i.e. below detection limits (termed Type II) to nitrogen rich (termed Type I) with up to 5000 ppm. It has also been shown that the nitrogen concentration, aggregation and distribution in an individual stone can be either homogeneous or heterogeneous.

Nitrogen has been shown to reside within diamond in three different aggregation states. The first is in the form of single substitutional nitrogen atoms, known as C centres. Diamonds that contain nitrogen only in this form are termed Type Ib. The second aggregation state is pairs of nitrogen atoms forming A centres (termed Type IaA diamonds) and the final state is four nitrogen atoms tetrahedrally arrange around a vacancy, forming a B centre (termed Type IaB). The sequence of aggregation has been shown to progress from C centres to A centres to B centres and is a function of time and temperature. As such it is a commonly used tool in the geological study of diamonds to gauge their mantle residence time / temperature history. The first step in the sequence is thought to occur relatively quickly in geological terms; the vast age of most diamonds therefore makes Type Ib samples rare in cratonic diamond deposits. The second step takes considerably more time, meaning that the A to B centre conversion may not always continue through to completion. So diamonds containing a mixture of both A and B centres are commonly termed Type IaAB. IR analysis of diamond also has the capability of identifying other commonly found defects and impurities. Whether these are intrinsic defects like platelets, extrinsic defects like hydrogen or boron atoms, or inclusions of minerals or fluids.

Recent technological developments in the field of spectroscopy allow detailed μ-FTIR analysis to be performed rapidly in an automated fashion. The Nicolet iN10 microscope has an integrated design that maximises signal throughput and allows spectra to be collected with greater efficiency than is possible with conventional μ-FTIR spectrometer-microscope systems. Combining this with a computer controlled x-y stage allows for the automated measuring of several thousand spectra in only a few hours. This affords us the ability to record 2D IR maps of diamond plates with minimal effort, but has created the need for an automated technique to process the large quantities of IR spectra and obtain quantitative data from them. We will present new software routines that can process large batches of IR spectra, including baselining, conversion to absorption coefficient, and deconvolution to identify and quantify the various nitrogen components. Possible sources of error in each step of the process will be highlighted so that the data produced can be critically assessed. The end result will be the production of various false colour 2D maps that show the distribution of nitrogen concentrations and aggregation states, as well as other identifiable components.