Coesite Inclusions: Microbarometers in Diamond

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Mineral inclusions in diamond provide valuable information for decoding their thermobarometric, mechanical, and mineralogical conditions during and after diamond formation deep within the earth's mantle. Coesite, a polymorph of silica (SiO_2), shares the same chemical composition as quartz but has a different crystal structure and a higher Mohs hardness Anthony et al., 1990). Coesite forms at pressures greater than 2 GPa (i.e., 20,000 times atmospheric pressure). It has been found in high-impact meteorite craters and as inclusions in minerals and diamonds in ecologites in ultrahigh-pressure metamorphic terrains (Sobolev et al., 1999).

Mineral inclusions in diamonds record the physical and chemical history of diamond formation; consequently, they provide a window to processes occurring in the deep interior of the mantle. Microscopic Raman spectroscopy is a very effective "fingerprint" technique for identifying unknown materials such as inclusions in gems, because Raman spectral features closely correlate to the crystal structure and chemistry of a material. Furthermore, this technique is nondestructive and requires virtually no sample preparation.

We recently examined a suite of high-quality pink diamonds set in a bracelet. These stones were type Ia and exhibited gemological and spectral characteristics typical of the rarest group of high-quality Argyle pink diamonds (refer to table 2 in Shigley et al., 2001). A cluster of mineral inclusions were present in a 0.21 ct marquise in the intense to vivid purple-pink color range (figure 1).

Raman spectra were collected with a Renishaw inVia confocal Raman system interfaced with 488, 514, 633, and 830 nm laser excitations. For the purposes of mineral identification, spectra were obtained in the lattice vibration region of the electromagnetic spectrum, which occurs between 1500 and 100 cm^{-1}. A representative Raman spectrum collected in-situ from the inclusions is shown in figure 2. The sharp peaks are uniquely attributed to coesite, and the included crystals in the image (figure 1) were identified as coesite. The broad peak at 689 cm^{-1} is due to fluorescence commonly observed in pink Argyle-type diamonds at a laser excitation of 633 nm. Note that fluorescence spectral features are often much stronger than Raman peaks.

Diamond, the strongest naturally occurring material, is capable of sustaining high internal confining pressure on its inclusions. These particular coesite inclusions provide a rare in-situ probe for investigating the internal pressure in the diamond. A systematic shift in Raman peak positions is observed in these included coesites as compared to peak positions of coesite at ambient pressure. An internal confining pressure of 2.7 (±0.2) GPa can be reliably established from this peak shift (Hemley, 1987). The uncertainty in the pressure estimate is calculated from the variation among the pressure estimates determined for each included crystal.

Diamonds are commonly believed to have formed at depths greater than 150 km, which corresponds to a pressure of ~5 GPa and a temperature of about 1000°C, based on the earth's geotherm, or temperature distribution with depth. Minerals such as coesite can be captured as inclusions during the formation of diamonds and subsequently carried to the earth's surface. At 1000°C, coesite is stable at pressures between about 3 and 9 GPa (Mirwald and Massonne, 1980; Zhang et al., 1996), which is the same pressure range in which the host diamond formed. On ascending to the surface during exhumation, the pressure on the host diamond gradually decreased; however, the pressure of 2.7 GPa is preserved within the included coesite crystal in this diamond at ambient temperature.

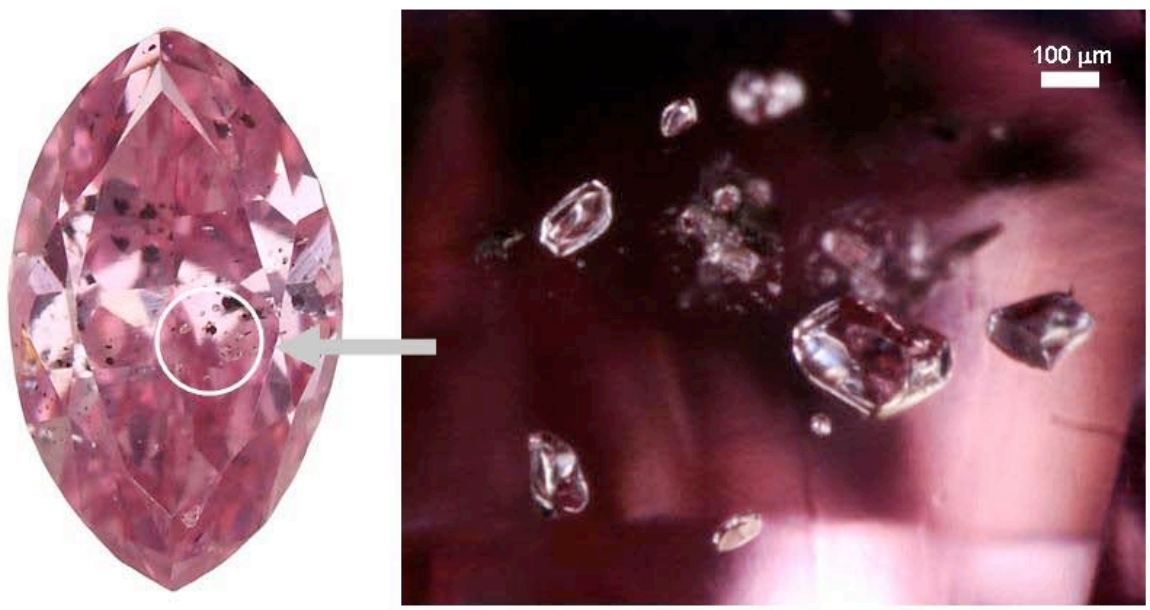

Figure 1. Microscopic examination of this 0.21 ct pink diamond shows a cluster of well-crystallized coesite inclusions. This diamond shows characteristics typical of Argyle diamonds. Raman microspectroscopy was used to identify all the included crystals as coesite. Images by Jian Xin (Jae) Liao.

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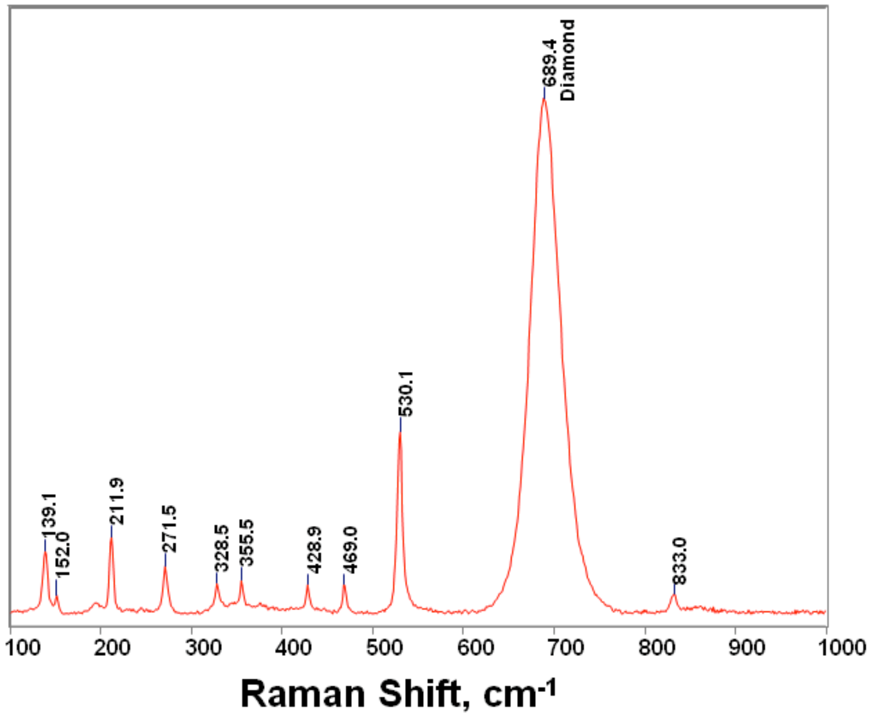

Figure 2. Representative in-situ Raman spectrum collected from the inclusions in the diamond. The small, sharp peaks belong to a pattern uniquely identified as coesite. The strong, broad peak at 689.4 cm^{-1} is due to fluorescence commonly observed in pink Argyle-type diamonds at 633 nm laser excitation.

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