



First in-situ single-crystal structure refinement of a garnet included in diamond

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The study of mineral inclusions in diamond is providing invaluable insight into the geodynamics of the Earth's mantle. A complete characterization of inclusions in diamond is fundamental in order to evaluate the P-T-fO₂ conditions and thus they represent a real "Earth's ultra-deep microprobe". The in-situ investigation of the inclusions using non-destructive techniques remains challenging. One of the potentially most powerful non-destructive methods is single-crystal X-ray diffraction. The application of such technique on inclusions in diamond is hampered by the complicated centering of the X-ray beam on the inclusion single-crystal (Kunz et al. 2002). Because of this experimental problem, in-situ single-crystal structure refinements of inclusions in diamond have never been carried out.

In this work we investigated by X-ray diffraction a diamond-hosted garnet single-crystal from the Jericho kimberlite (Slave Craton, Canada). The garnet, not clearly visible under the microscope due to the irregular shape of the diamond host, had the largest size not greater than 100 microns. We used two STADI-IV STOE single-crystal diffractometers: the first instrument, equipped with a CCD detector, allowed us to collect a large number of diffraction reflections and to obtain an approximate orientation matrix for the garnet. Using this matrix, we mounted the diamond on the second instrument, equipped with a point detector and the software SINGLE (Angel et al. 2000), capable of obtaining an accurate X-ray beam centering through the 8-position centering method (this method is often used in high-pressure, in-situ X-ray studies). Such a procedure allowed us to measure with very high accuracy and precision the unit-cell edge ($a = 11.5826(2)\text{\AA}$). Then we mounted back the diamond with the perfectly centered garnet on the first diffractometer and collected a complete X-ray intensity dataset in order to obtain complete structural information. We collected 410 unique reflections up to $2\theta = 86^\circ$ and refined anisotropically the crystal structure obtaining an agreement factor (R) lower than 2%. Such very high quality data allowed us to refine the occupancies on the X, Y and Z crystallographic sites providing 17.6, 12.9 and 14.0 electrons (errors below 0.1 electrons), respectively. Average bond lengths for X-O, Y-O and Z-O were respectively, 2.313(2), 1.902(2) and 1.634(2) Å. These values indicate a Y site totally occupied by Al and a Z site totally occupied by Si, which suggests that the chemistry of the garnet belongs to the Cr-poor eclogitic or websteritic paragenesis. As Jericho diamonds < 3 mm comprise 90% eclogitic stones and 7% websteritic (De Stefano et al., 2009) there is a high probability that the garnet studied in this work is from an eclogitic source. A similar approach is being adopted for olivines from Siberian diamonds and the preliminary results will be discussed.

References

- De Stefano et al. (2009) Contributions to Mineralogy and Petrology, 158, 295-315.
Kunz et al. (2002) Earth and Planetary Science Letters, 198, 485-493.
Angel et al. (2000) Reviews in Mineralogy and Geochemistry, 41, p. 559-596.