The Raman Estimation of the Composition of Clinopyroxene Inclusions in Natural Diamonds

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Clinopyroxenes (Na,Mn,Ca,Fe²⁺₁₋₂(Mg,Al,Fe³⁺₁₋₂)[(Al,Si)₂O₆] are common inclusions in natural diamonds of either peridotitic or eclogitic paragenesis. The variety of the composition of pyroxene inclusions in diamonds records the chemical and the physical conditions of the mantle. New approach based on Raman spectroscopy data on 43 pyroxene inclusions in diamonds from Yakutian province (the Siberian craton) and their chemical analyses are provided in this study.

Raman spectroscopy is a high-resolution and non-destructive method used to detect the compositional and the structural characteristics of materials and minerals including high-pressure crystal inclusions in diamonds. Raman spectra of clinopyroxene inclusions in diamonds were collected by Horiba LabRAM HR800 Raman spectrometer with 532-nm laser. In addition, the compositional analyses were obtained by EPMA (JEOL JXA-8100) to correlate chemical variations with specific spectral features and Raman shifts.

Clinopyroxene inclusions show variations of chemical content in the wide ranges: SiO₂ 54.1-55.9 wt.%, Al₂O₃ 0.31-4.11 wt.%, Cr₂O₃ 0.32-5.73 wt.%, FeO 1.81-3.49 wt.%, MgO 13.4-18.3 wt.%, CaO 16.1-22.9 wt.%, Na₂O 0.28-3.82 wt.% for peridotitic type inclusions and SiO₂ 52.4-56.8 wt.%, Al₂O₃ 4.46-17.8 wt.%, Cr₂O₃ <0.29 wt.% for eclogitic type inclusions. One of the factors controlling the shifts of position frequencies of n₁₁-mode is composition.

Generally, the inclusions yield Raman spectra with four high-intense modes (v₃, v₁₁, v₁₄, v₁₇). Observed relative intensity of most of these modes (except v₁₁) depend on changing of crystal orientation. The v₁₁-mode belongs to the Si-O stretching vibrations of bridging oxygen atoms (Si-Oₚ). The recorded position of this mode varies in the ranges 665.6-675.1 cm⁻¹ for peridotitic type inclusions and 673.7-688.2 cm⁻¹ for eclogitic type inclusions. One of the factors controlling the shifts of position frequencies of n₁₁-mode is composition.

Peridotitic clinopyroxenes display strong linear correlations between the shifts of position of the v₁₁-mode and contents of Al₂O₃ (correlation coefficient r = 0.94), FeO (correlation coefficient r = 0.68), MgO (correlation coefficient r = -0.52), CaO (correlation coefficient r = -0.69), Na₂O (correlation coefficient r = 0.92). Eclogitic clinopyroxenes show linear correlations between the shifts of position of the n₁₁-mode and contents of Al₂O₃ (correlation coefficient r = 0.95), FeO (correlation coefficient r = -0.64), MgO (correlation coefficient r = -0.85), CaO (correlation coefficient...
r = -0.59), Na₂O (correlation coefficient r = 0.84). The most expressed correlations can be used for estimation of composition of inclusions in diamonds only by Raman spectroscopy data without destruction of diamond-host and for identification of clinopyroxenes from potentially diamondiferous mantle rocks.

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