Influence of the Fe content on the 417 cm^{-1} and 577 cm^{-1} Raman bands of sapphire

Diep, P.*, Häger, T., Hofmeister, W.

Institute of Geomaterial and Gemstone Research,
Johannes Gutenberg University Mainz, Germany
**e-mail: thphan@students.uni-mainz.de*

Introduction

Raman spectroscopy of corundum Al_2O_3 was studied by Hibben (1932), Deutschbein (1932), Mani (1942), Bhagavantam and Venkatarayudu (1939), Krishnan (1947), Ashkin et al. (1968), Aminzadeh and Sarikhani-fard (1999), and Kadleikova et al. (2001). However correlation between trace elements in sapphire and its Raman spectrum has not been studied thus far. In the present study, sapphire samples from 17 deposits, including Dac Nong, Dac Lac, Nghe An, an unknown source (all Vietnam), Bo Ploi, Khao Ploi (Thailand), Ban HuaySai (Laos), Australia, Shangdon (China), Nosibe, Andapa, Antsirabe (Madagascar), Ballapana (Sri Lanka), Brazil, Russia, Columbia and Tanzania were investigated. Raman spectra were excited with the 532 nm emission of a frequency doubled Nd-YAG laser.

Results

Our results indicate clearly that elevated Fe concentrations in sapphire induce notable changes in Raman spectral parameters. Figures 1 and 2 show that the Raman shifts of the 417 cm^{-1} and 577 cm^{-1} bands decrease with increasing Fe_2O_3 content. The decrease of the Raman shift of the 417 cm^{-1} band is associated with an increase of the FWHM (full width at half band-maximum) of this band (Fig. 3). Due to the correspondence in ion radii with Al^{3+} ions, metal ions such as $Fe^{2+/3+}$, Cr^{3+}, Ti^{4+}, V^{3+}, Mg^{2+} and Ga^{3+} may replace for Al^{3+}-ion positions and cause changes in the sapphire lattice. The most prominent trace element in the investigated samples is Fe^{3+}. Due to the larger ionic radius of Fe^{3+} (0.645 Å) in comparison to Al^{3+} (0.535Å) in octahedral sites, the crystal structure is widened. Therefore the Raman bands shift to lower wave numbers; FWHM increases are assigned to local lattice distortion.

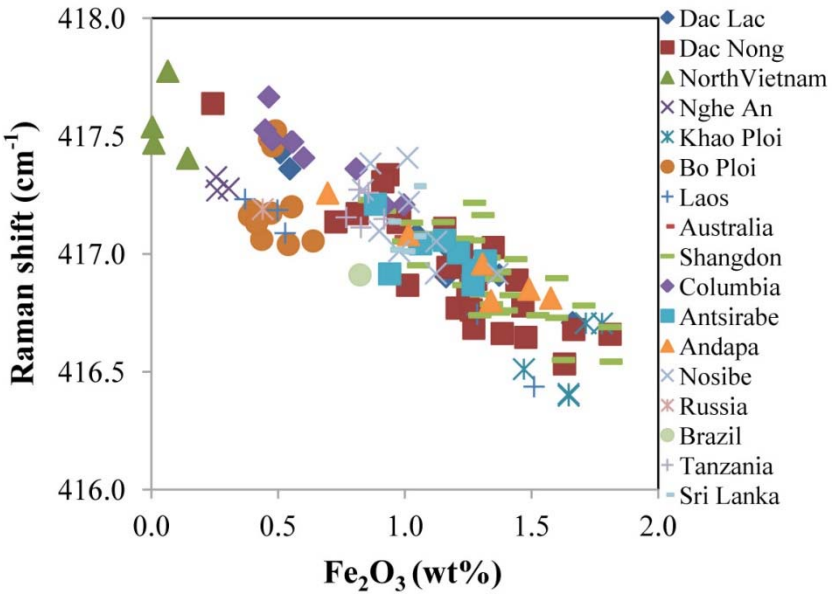

Fig. 1. *The 417 cm^{-1} Raman band of sapphire shifts to lower wavenumbers with increasing Fe_2O_3 content.*

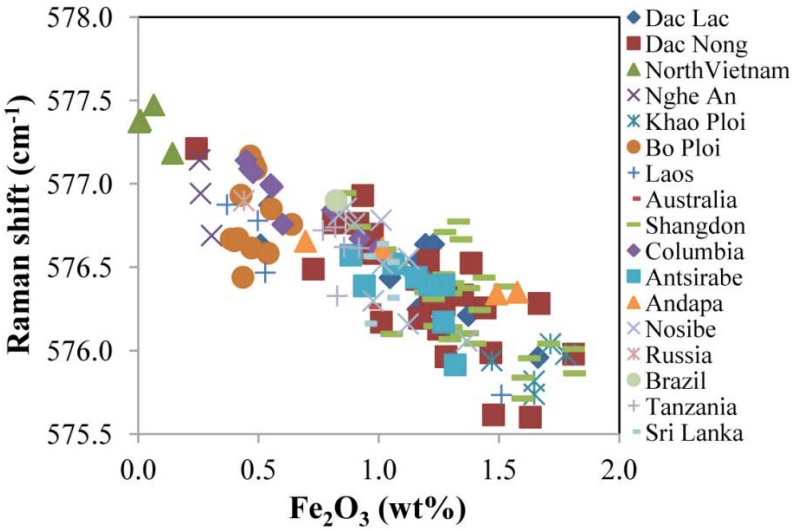

Fig. 2. *The 577 cm^{-1} Raman band shifts to lower wavenumbers with increasing Fe_2O_3 content.*

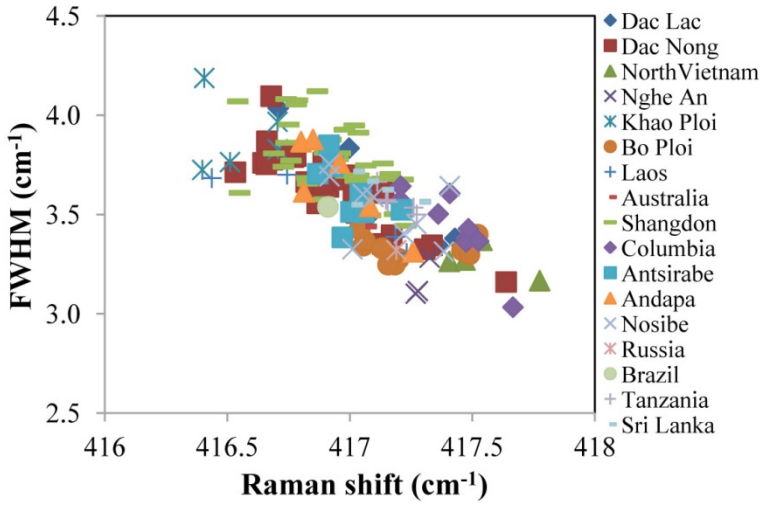

Fig. 3. *Correlation of Raman shift and FWHM of the 417 cm^{-1} Raman band of sapphire.*

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