

The Origin of 2.98eV Cathodoluminescence Emission in Quartz and its Relation to Structural Defects and Ti Content

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The origin of the common bluish-violet ~416 nm (2.98 eV) cathodoluminescence (CL) emission in natural and synthetic quartz has been investigated by a combination of CL microscopy and spectroscopy, electron paramagnetic resonance (EPR) spectroscopy, and trace-element analysis by electron microprobe (EPMA). The study shows that the appearance of the 2.98 eV emission band can be attributed to two different defects in quartz. A transient luminescence can be explained by structural defects in oxygen deficient quartz. The luminescence model implies self-trapped exciton (STE) emission related to oxygen vacancies. This type of CL emission is frequent in high-purity synthetic quartz and natural quartz of hydrothermal origin. In Ti-rich quartz from natural samples (e.g., quartz phenocrysts in rhyolites) and synthetic quartz of Ti-diffusion experiments, an additional 416 nm (2.98 eV) emission was detected that is stable under the electron beam. The Ti content display significant ranges and vary with inferred crystallization temperature and other factors [1-3]. The intensity of this 2.98 eV emission band correlates with the concentration of trace Ti in quartz and is often referred to as a geothermometer for Ti-in-quartz or TitiniQ [4,5]. To improve the accuracy of the peak shape measurements by CL a correction for the spectral response has been made for the various optical components within the collection optics. It has been found that the CCD and associated grating within the spectrometer together with the fibre have a significant non-linear transmission which must be corrected for in each spectrum, Fig 1. When the correction is made to quartz spectra from phenocrysts in rhyolite from Hausdorf (Saxony, Germany) we observe the non-bridging oxygen hole center (NBOHC) moves from 1.95eV (636nm) uncorrected to 1.93eV (642nm) corrected while the peak associated with Ti moves from 2.86eV (433nm) to 2.98eV (416nm) when corrected. The shapes of both the NBOHC and Ti peak show shape changes when corrected for the optical response. However, little to no variation is observed in the R^2 value when point elemental Ti measurements are compared with the fitted Ti peak variation. Further measurements are being made to correct for the optical response of the hemispherical mirror and lenses within the optical assembly of the JEOL EPMA.

Samples were prepared by mounting in either 25mm rounds or as thin sections, polishing down to 1 μ m diamond and finished using vibro-polishing in a colloidal silica media. Samples were coated with a 5-8 nm C film. Maps were collected on a JEOL 8530F in the wavelength range 200 – 990nm at 20kV and 30ms dwell, the stage was scanned with a 2 μ m step [6]. Quantitative microanalysis was performed at 20kV, 100nA with Ti measured using a PET crystal on a high countrate spectrometer resulting in a 1 σ detection limit of 8 ppm. The analysis points on the quartz grain are shown in Figure 2 and the resulting comparison of the fitted Ti peak (2.98eV) versus the measured Ti concentration is given in Figure 2b [7].

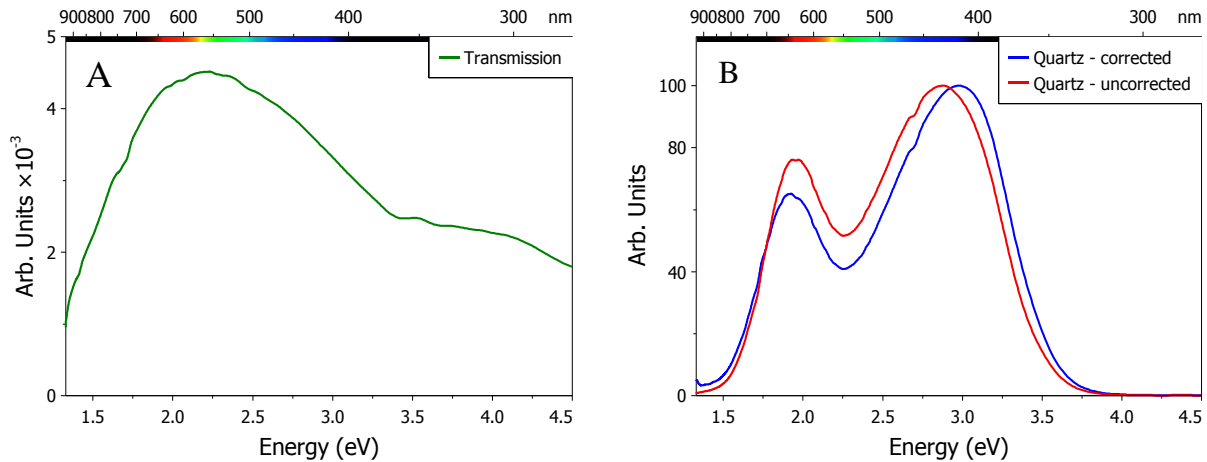


Figure 1. (a) Transmission curve for the spectrometer including the CCD, grating and the optical fiber. (b) Cathodoluminescence spectra from a quartz phenocryst in the rhyolite from Hausdorf (Saxony, Germany) showing the change in peak position and shape after the transmission correction is applied.

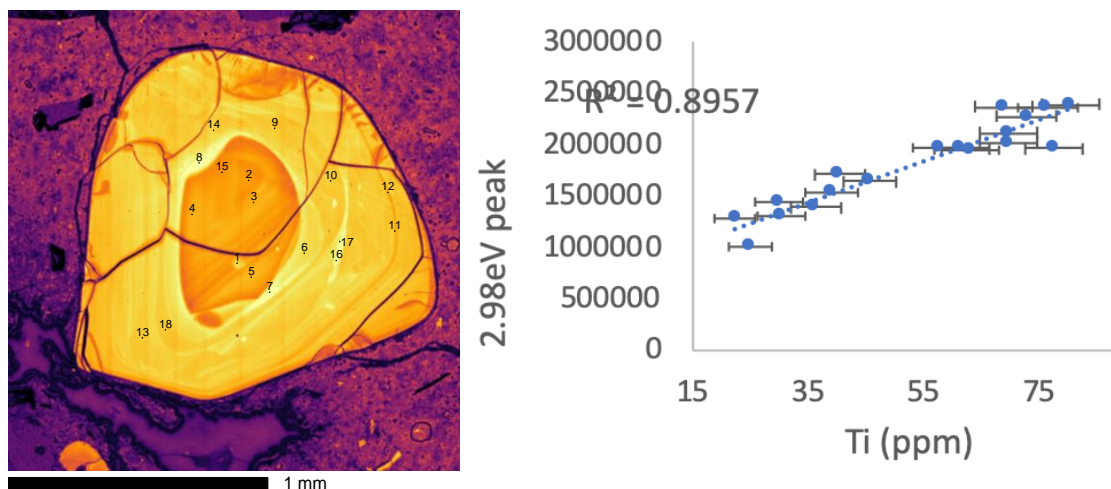


Figure 2. (a) Panchromatic CL image of a quartz phenocrysts in the rhyolite from Hausdorf (Saxony, Germany) with the analytical points for Ti measurements; (b) correlation of the 2.98 eV CL emission intensities and the analyzed Ti contents. The error bars on Ti are 1σ .

References:

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