

The 450 nm (2.8 eV) cathodoluminescence emission in quartz and its relation to structural defects and Ti contents

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ABSTRACT

The origin of the common blue 450 nm (2.8 eV) cathodoluminescence (CL) emission in natural and synthetic quartz has been investigated using a combination of CL microscopy and spectroscopy, electron paramagnetic resonance (EPR) spectroscopy, and trace-element analysis by electron microprobe analysis as well as inductively coupled plasma-mass spectrometry (ICP-MS). The study shows that the appearance of the ~450 nm emission band can be attributed to two different defects in quartz. First, 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. Second, in Ti-rich quartz from natural samples (e.g., quartz phenocrysts in rhyolites) and synthetic quartz of Ti-diffusion experiments, an additional 450 nm (2.8 eV) emission was detected, which is stable under the electron beam. The intensity of this ~450 nm emission band correlates with the concentration of trace Ti in quartz, and substitutional Ti⁴⁺ at the Si⁴⁺ position was proved by EPR spectroscopy. In quartz crystals with elevated Ti concentrations both intrinsic and extrinsic blue CL emissions at ~450 nm can coexist, hindering a thorough characterization and quantification of the CL signal. A reliable distinction of the two different CL emission bands is possible by fitting the peaks of the CL spectra, and the peak width of the 450 nm emission can be used to differentiate the STE from the Ti⁴⁺ emission. However, the definitive technique is through the observation of CL peak shape change over time at a point by collecting a time series of CL spectra in conjunction with EPR spectroscopy and trace-element analysis of the Ti concentration.

Keywords: Cathodoluminescence (CL), hyperspectral CL, quartz, blue CL emission, electron paramagnetic resonance (EPR), Ti concentration