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LETTER

FTIR spectroscopy with a focal plane array detector: A novel tool to monitor the spatial OH-defect distribution in single crystals applied to synthetic enstatite

FELIX PRECHTEL* AND ROLAND STALDER

Institute of Mineralogy and Petrography, University of Innsbruck, Innrain 52 f, A-6020 Innsbruck, Austria

ABSTRACT

Single crystals of pure enstatite ($Mg_2Si_2O_6$) were synthesized under water-saturated conditions at 6 GPa and 1250 °C and variable silica activity. Run products were investigated using a novel technology: a FTIR spectrometer equipped with a focal plane array detector enabling IR-imaging with a spatial pixel resolution of 2.7 µm. IR spectra within the OH-absorption region show strong pleochroic behavior: absorption bands at 3687 and 3592 cm^{-1} show strongest absorptions for $E||n_\beta$, whereas absorption bands at 3362 and 3067 cm^{-1} show strongest absorptions for $E||n_\gamma$. Furthermore, absorption bands are sensitive to the silica activity—the ratio of the integral absorbance of the absorption bands at 3687 and 3592 cm^{-1} to the absorption bands at 3362 and 3067 cm^{-1} increases with increasing Mg/Si-ratio of the bulk charge. The most probable interpretation is an assignment of the high-energy absorption bands to tetrahedral (T-site) defects caused by a lower availability of Si and the low-energy absorption bands to octahedral (M-site) defects caused by a lower availability of Mg. All crystals show an internal zonation pattern with an increasing T-site to M-site defect ratio from core to rim, which is interpreted to be caused by changing silica-activity and *T* during the experiments. The defect ratio and the zonation pattern are applied as a monitor of crystal growth conditions.

Keywords: Enstatite, hydrogen incorporation, IR imaging, high pressure