Pressure-induced phase transitions in Ilvaite: a Mid/Far Micro-FTIR spectroscopic study

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The mineral ilvaite is a mixed-valence iron sorosilicate with the ideal formular $CaFe_2^{2+}Fe^{3+}[Si_2O_7/O/(OH)]$. In the past it has been the subject of intense research in respect to its physical and chemical properties as it can be treated as analogue material for magnetite (Ghose et al. 1989). It shows a variety of temperature-induced electronic, structural and magnetic phase transitions (see overview in Ghose 1988). More recently a pressure-induced phase transition from monoclinic to orthorhombic has been observed at 2.25 GPa (Ghazi-Bayat et al. 1993).

In this study we collected Mid- and Far-infrared spectra of a natural ilvaite in-situ in a diamond-anvil cell (DAC) as a function of pressure. The composition of the natural material is $<Ca_{0.94}>(Fe^{2+}_{0.61}Mn^{2+}_{0.40})(Fe^{3+}_{1.01}\ Fe^{2+}_{0.96}\ Al^{3+}_{0.02}Mg^{2+}_{0.01})[Si_{2.03}\ O_7/O/(OH)]$ as determined by electron microprobe. Two series of DAC experiments were performed at GFZ in the mid-infrared using Argon as pressure medium and a Globar as light source. Four pressure series were performed at Bessy II in the Far-infrared region using petroleum jelly as pressure medium and synchrotron light. We used a custom-made vacuum FIR-microscope (see Mrosko et al. 2011). Pressure-induced changes in the Mid- and Far-IR spectra were analysed via the autocorrelation function (Salje et al. 2000) for all six pressure series.
All six series confirm the phase transition at about 2.3 GPa. For the first time at much higher pressure (between 10 and 11 GPa) a second pressure-induced phase transition could be observed. It is clearly visible through out the whole spectral ranges: in the OH-stretching region, Mid-IR region from 1400 to 400 cm^{-1} and the far-IR region down to 50 cm^{-1}. What this phase transition causes is not yet clear. Above 11 GPa and up to 20 GPa no further discontinuities could be detected.

References:
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