

An accurate fitting of the IR-edge tail and the OH-related peaks was needed, to find out whether the IR-edge tail and the absorbance bands in the wavelength range 2700 – 3300 nm were only caused by the absorption of to the glass network bound hydrogen and/or hydroxyl ions, and how far the absorbance of Fe^{2+} ions extended (Chap. 5.).

The OH-bands are caused by OH^- and H^+ ions bound to the glass network. The peaks at 2200 nm (at wavenumber 4480 cm^{-1}), 2600 nm (at 3920 cm^{-1}), 2800 nm (at 3500 cm^{-1}) and at 3500 nm (at 2800 cm^{-1}) are caused by hydroxyl groups. Hydroxyl groups are either singly bonded (also called “free”, i.e. not hydrogen-bonded) to Si-ions (2200 nm, 2600 nm and 2730 - 2800 nm), or form a hydrogen-bond to a neighbouring non-bridging oxygen (3500 - 3600 nm) or to mobile SiO_4 -groups (4300 - 4500 nm)(Geotti-Bianchini, 1995; Adams, 1961; Adams et al 1959; Varshneya, 1994, p. 487 – 488; Zarzycki, 1991, p. 115 - 116; Gaber, 1995 and Navarra et al, 2005). The peaks at 2200 nm and 2600 nm arise from free OH-groups and SiO_4 combination frequencies (Varashneya, 1994, p. 488; Scholze, 1991, p. 240) and their heights are in proportion to the height of the peak at 3500 nm.

The IR-edge tail is assumed to arise from the strong IR absorption peaks at $4,25 \mu\text{m}$, $4,94 \mu\text{m}$ and $5,79 \mu\text{m}$ (O-H bending vibration) (Adams, 1961).

Correction of absorbance data for these peaks and the tail is systematically neglected by most of the earlier researchers (e.g. by Bingham, 2002, who studied Fe-doped silicate glasses).

3.6.2. Fitting of OH-band and IR-edge

A detailed analysis and a set of fitting parameters for summed Gaussian peaks to the OH band at wavenumbers $2500 - 3700 \text{ cm}^{-1}$ (i.e. at 2700 – 4000 nm) was presented recently by Navarra et al (2005). Gaber (1995) discussed the same peaks earlier, both referring to the original literature, where the peak locations and assignments had been identified. Navarra’s fitting data was used as the starting point for fitting of the OH-band above 2700 nm (below 3700 cm^{-1} in this work. The glass compositions studied by Navarra et al (2005) differ slightly from our test glasses, so the positions and heights of the peaks of the OH-band are in this work slightly adjusted for the studied glasses.

The fitted peak parameters, very slightly modified from Navarra’s data, are given in Table 3.6.1 and a graph of all fitted peaks for the OH-band and IR-edge, summed together are shown in Fig. 3.6.4. New fitting parameters were developed by a manual iteration process for the two new peaks at shorter wavelengths that were not included in Navarra’s set of data, i.e. at 2200 nm (4480 cm^{-1}) and 2600 nm (3920 cm^{-1}) (Table 3.6.1 and Fig. 3.6.4). The heights of these peaks scale with the height of the summed OH-band at wavelengths above 2700 nm, and therefore