A COMBINED X-RAY DIFFRACTION AND ABSORPTION STUDY OF $Li_2Si_2O_5$ DOPED WITH VANADIUM

W. Paszkowicz [1], A. Wolska [1], M.T. Klepka [1], S. abd el All [1,2], and F.M. Ezz-Eldin [2]

[1] *Institute of Physics PAS, al. Lotników 32/46, Warszawa 02-668, Poland*
[2] *Center of Research and Radiation Technology, Nasr City, Cairo 0002, Egypt*

Keywords: X-ray diffraction, X-ray absorption, XANES, lithium silicate

**) e-mail: paszk@ifpan.edu.pl*

Lithium-based conducting glasses are promising candidates for electrolyte materials of thin-film batteries because they exhibit isotropic ionic conductivity. However, at room temperature most of such conducting glasses exhibit relatively low ionic conductivity values, in the range 10^{-7} to 10^{-8} S/m. In order to increase the conductivity, some specific additives have been used, one of them being vanadium. In a recent work on borate glasses, vanadium dopant at a level of several percent was used for this purpose [1-3]. It has been noticed that annealing of vanadium doped borate glass results in a change of physical properties [1]. This may suggest that vanadium ions occupy specific crystallographic sites.

In this work, a related material, vanadium-doped lithium silicate glass is studied. The glass was prepared by heating a mixture of quartz (SiO_2), lithium carbonate (Li_2CO_3) and vanadium pentoxide (V_2O_5) at a level of up to 5.5 weight percent at 1400 for 3 h and then cooled. As prepared glass was annealed for 4 h at 550°C. The X-ray diffraction experiments were performed at a conventional diffractometer.

The described synthesis procedure gives a virtually pure $Li_2Si_2O_5$ phase of orthorhombic *Ccc*2 space group [4] with vanadium present in the lattice and with traces of impurity phases. We noticed that the observed crystallisation is faster than that reported in literature for phosphate glasses [5]. Rietveld refinements were performed using various models assuming a partial occupation at Li or Si sites. The results indicate that location of vanadium at Si sites is more likely. The lattice parameters are found to vary isotropically with increasing vanadium content.

The X-ray absorption experiment was conducted at the Cemo beamline (Hasylab, Hamburg). XANES spectra at the vanadium K edge were measured at room temperature using fluorescence and transmission detection mode. In all cases, a very pronounced pre-pik was observed. According to Ref. [6], this feature indicates that vanadium atoms are in the +5 ionic state.

References

[1] N.A. El-Alaily, R.M. Mohamed, "Effect of irradiation on differenial thermal properties and crystallization behavior of some lithium borate glasses", *Nucl. Instrum. Meth. Phys. Res. B* **179** (2001) 230-242.

[2] Y.-I. Lee, J.-H. Lee, S.-H. Hong, Y. Park, "Li-ion conductivity in Li_2O–B_2O_3–V_2O_5 glass system", *Solid State Ionics* **175** (2004) 687–690.

[3] S.Y. Marzouk, N.A. Elalaily, F.M. Ezz-Eldin, W.M. Abd-Allah, "Optical absorption of gamma-irradiated lithium-borate glasses doped with different transition metal oxides", *Physica B* **382** (2006) 340–351.

[4] B.H.W.S. de Jong, H.T.J. Supér, A.L. Spek, N. Veldman, G. Nachtegaal, J.C. Fischer, "Mixed alkali systems: Structure and ^{29}Si MASNMR of $Li_2Si_2O_5$ and $K_2Si_2O_5$", *Acta Crystallogr. B* **54** (1998) 568-577.

[5] Y. Iqbal, W.E. Lee, D. Holland, P.F. James, "Crystal nucleation in P_2O_5-doped lithium disilicate glasses", *J. Mater. Sci.* **34** (1999) 4399–4411.

[6] P. Chaurand, J. Rose, V.Briois, M. Salome, O. Proux, V. Nassif, L. Olivi, J. Susini, J.-L. Hazemann, J.-Y. Bottero "New methodological approach for the vanadium K-edge X-ray absorption near-edge structure interpretation: Application to the speciation of vanadium in oxide phases from steel slag", *J. Phys. Chem. B* **111** (2007) 5101-5110.