Effect of VO^{2+} ion on EPR and optical band gap of calcium oxychloro bismuth borate glasses

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Abstract: The present work deals with the compositional dependence of optical absorption and Spin Hamiltonian parameters in calcium oxychloride bismuth borate glasses prepared by melt-quench method [1].

X-ray diffraction studies confirm amorphous nature of doped glasses. The variation in molar volumeand density with increasing $CaCl_2$ concentration indicates strong structural changes that are taking place inside the glass matrix. The optical absorption data (200-800 nm) is analysed by means of Davis-Mott model to evaluate optical band gaps corresponding to indirect allowed transition (r=2)and indirect forbidden transition (r=3) [1]. The optical band gap is lying in the range 2.41–2.60 eV and 2.18–2.35 eV for r=2 and r=3 respectively.

Spin Hamiltonian parameters, dipolar hyperfine coupling parameters, covalency rates are calculated from the EPR spectra of vanadyl ions. EPR spectra confirms the octahedral coordination of V^{4+} ion (exists as VO^{2+}) [2]. The hyperfine coupling parameter (P) and Fermi contact interaction term (K) were calculated by using Kivelson and Lee formulations and obtained values indicated that the term -PK contributes to hyperfine coupling which arises due to interaction of polarized ‘s’ electron with unpaired ‘d’ electron of vanadyl ion

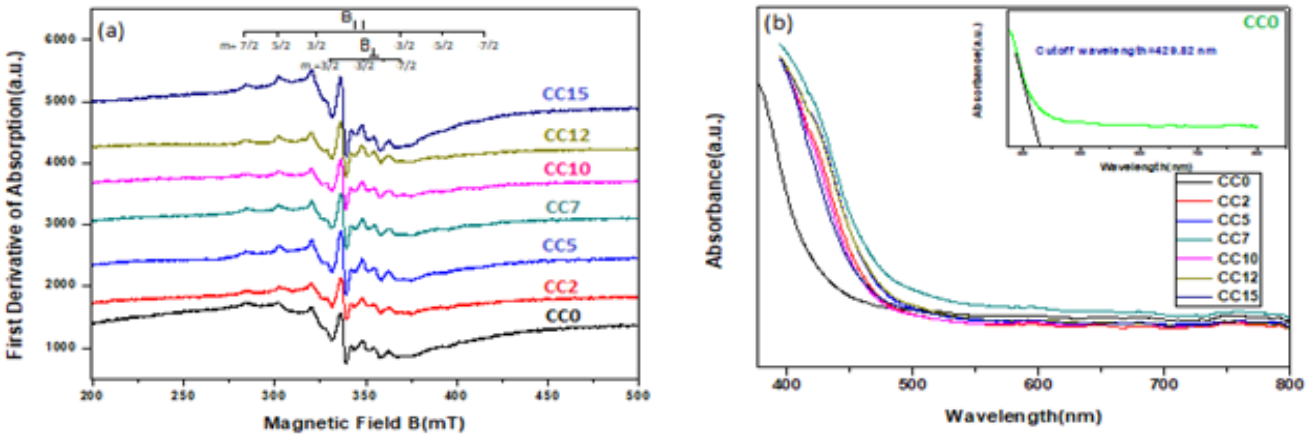

Figure 1: (a). The EPR spectra of VO2+ ions in prepared glass samples. (b) Optical absorption spectra of $x CaCl_2.(30-x)CaO.20Bi_2O_3.50B_2O_3$, where ($x$ = 0, 2, 5, 7, 10, 12, 15) doped with 2 mol% V_2O_5(inset: for x=0).

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