**Synthesis, electronic polarizability and optical basicity of a novel zinc phospho-tellurite glass**

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**Highlights**

* A novel zinc phospho-tellurite glass was synthesized for applications in photonic field
* Optical band gap was graphically determined based on optical absorption property
* Metallization criterion in dependency on different physical properties was evaluated
* Electronic polarizability was investigated in correlation with optical basicity

**1. Introduction**

The present work is focused on the investigation of optical properties, electronic polarizability, optical basicity and other physical features of a novel zinc phospho-tellurite glass, as good candidate for photonic devices. Based on the refractive index and optical band gap, molar refractivity and polarizability have been calculated that, in turn, is decisive for optical basicity [1, 2].

**2. Methods**

The vitreous material prepared in this work belongs to the 45ZnO 10Al2O3 40P2O5 5TeO2system (code Te-5, taking into account the amount of TeO2 in mol. %) being characterised by a chemical stable composition. The glass has been prepared by a non-conventional wet route of processing the starting reagents followed by melting-stirring and annealing of the glass [3, 4]. In order to prepare a glass having a high optical homogeneity, the melt batch was mechanically stirred aiming to reduce the gaseous inclusions and grooves embedded in the bulk samples. The density of the glass was experimentally determined by hydrostatic method [1, 2], absorption coefficients was plotted based on experimentally optical transmission spectroscopy [1, 2]. The refractive index was measured at λD = 589 nm (yellow doubled D line of sodium) by means of the Pulfrich refractometer. Mott and Davis relationship was applied to graphically determine the optical band gap, Eg and, subsequently, polarizability, metallization criterion and optical basicity have been calculated [1, 2]. Other physical properties, such as molar volume, oxygen packaging density, reflexion loss and optical transmission have been calculated [1, 2].

**3. Results and discussion**

In the Table 1, Te-5 glass properties are presented: glass density (ρglass), average molecular mass (Mav), molar volume (VM), oxygen packaging density (OPD), refractive index measured at 589 nm (nD), refractive index measured from dispersion graph (nDD), molar refractivity (Rm), electronic polarizability (αm), reflection loss (RL), optical transmission (T) (see Fig.1, absorption coefficient). Table 2 presents: refractive index-based non-bridging oxygen atoms polarizability ($α\_{O\_{2}^{-}}\left(n\right)), $band gap-based non-bridging oxygen atoms polarizability ($α\_{O\_{2}^{-}}\left(nE\_{g}\right)), $optical band gap (Eg) (Fig.2), refractive index-bazed metallization criterion (M(n)), band gap-based metallization criterion (M(Eg)), Duffy optical basicity (ΛD), refractive index based-polarizability-based optical basicity (Λ($α\_{O\_{2}^{-}}\left(n\right)$), band gap based-polarizability-based optical basicity (Λ($α\_{O\_{2}^{-}}\left(E\_{g}\right))$ and Pauling optical basicity (ΛP).

Table 1. Te-5 glass properties: ρglas, VM, OPD, Mav, nD, nDD, Rm, αm, RL, T

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| ρglassg/cm3 | VMcm3/mol | OPDO atom/lglass | Mavg/mol | nD | nDD | Rmcm3/mol | αmcm3/mol | RL | T |
| 2,936 | 37,95 | 75 | 111,45 | 1,54616 | 1,54 | 12,02 | 4.75‧10-24 | 0,046 | 0,912 |

Table 2. Te-5 glass properties:$ α\_{O\_{2}^{-}}\left(n\right)$, $α\_{O\_{2}^{-}}\left(n\right), $ M (n), M (Eg), ΛD, Λ($α\_{O\_{2}^{-}}\left(n\right), $Λ($α\_{O\_{2}^{-}}\left(E\_{g}\right), $ΛP

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| $α\_{O\_{2}^{-}}\left(n\right) $cm3/mol | $$α\_{O\_{2}^{-}}\left(E\_{g}\right)$$ | M(n) | M(Eg) | ΛD | Λ($α\_{O\_{2}^{-}}\left(n\right)$ | Λ($α\_{O\_{2}^{-}}\left(E\_{g}\right)$ | ΛP |
| 1.59 | 1.59 | 0,6832 | 0,6832 | 0,702 | 0,62 | 0,62 | 0,4617 |

|  |  |  |
| --- | --- | --- |
|  Fig.1. Optical absorption of Te-5 glass versus wavelength |  Fig. 2. Graphical determination of Eg for Te-5 glass |  Fig.3. Refractive index dependence on wavelength for Te-5 glass |

**4. Conclusions**

(i) Refractive index measured by Pulfrich refractometer is in a good accordance with the refractive index value determined from dispersion graph; (ii) the metallization criterion reveals an intermediate electrical conductivity vitreous material; (iii) Duffy optical basicity is relative close to refractive index-based polarizability- based optical basicity and to band gap-based polarizability- based optical basicity, respectively, but higher than Pauling optical basicity; (iv) based on optical basicity values it is worth to conclude that Te-5 oxide composition exhibits a relative high tendency to form a vitreous network structure.

**References**

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