

## Structural properties of Gadolinium Borate-Tellurate Glasses and Glass Ceramics Inferred from FTIR spectroscopy and DFT Studies

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The structure of tellurate-borate glasses is of great interest due to at least two motives: (i) adding a network modifier oxide breaks the Te-O-Te network bridges (the process is accompanied by the formation of non-bridging oxygen sites) and (ii) the different nature of the oxygen polyhedra surrounding the boron atoms.

The purpose of this paper was to approach the structure of gadolinium borate-tellurate glasses using the infrared spectroscopy investigation and the DFT calculations.

First, we attempt to develop a structural model for the binary  $0.6\text{TeO}_2\cdot 0.4\text{B}_2\text{O}_3$  borate-tellurate glass paying a special attention to the coordination state of tellurium and boron atoms.

As recognized by X-ray diffraction and FTIR analysis, the addition of  $\text{Gd}_2\text{O}_3$  to the  $0.6\text{TeO}_2\cdot 0.4\text{B}_2\text{O}_3$  host glass matrix causes important structural modifications. Thus, up to a content of 25%  $\text{Gd}_2\text{O}_3$  a higher extent of network polymerization occurs. After that, increasing the  $\text{Gd}_2\text{O}_3$  content up to 50 mole% occur the transformation of the  $[\text{BO}_4]$  units into the  $[\text{BO}_3]$  units from boroxol rings and into  $[\text{BO}_3]$  units with varied types of borate groups and also, the coordination of the tellurium atom should be changed progressively from 4 though 3+1 to 3.

Heat treated samples were also investigated. The FTIR data show that these samples consist mainly of  $[\text{TeO}_3]$ ,  $[\text{TeO}_4]$ ,  $[\text{BO}_4]$  and  $[\text{BO}_3]$  structural units. The DFT calculations show that the increase in the number of non-bridging oxygen atoms would decrease the connectivity of the glass network and would necessitate quite a radical rearrangement of the network formed by the  $[\text{TeO}_6]$  octahedron.