

Vibrational Spectroscopic and DFT Studies of Gadolinium Vanado-Tellurite Glasses and Glass Ceramics

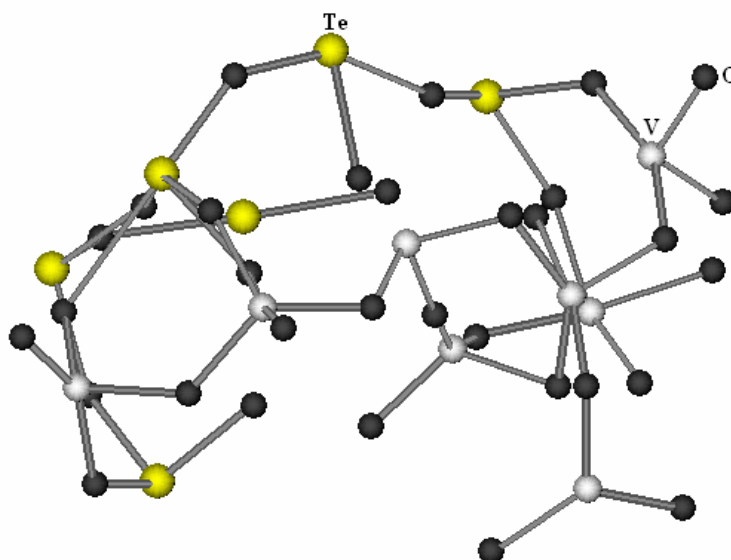
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The structure of $\text{TeO}_2\text{-V}_2\text{O}_5$ glasses is still subject to discussion from two motives: (i) adding to the network modifier oxides occur the broken Te-O-Te network bridges accompanied by the formation of non-bridging oxygen sites, and (ii) the structure of vanadate glasses remains a subject of interest because there is no clear picture as to the exact nature of the oxygen polyhedra surrounding the vanadium atoms or of the role played by the other glass components. Moreover, the structure of the vanadate glasses can be related to the nature of the network formers as well as on the network modifiers.

The purpose of this paper was to approach the structure of gadolinium vanado-tellurite glasses using the infrared spectroscopy and DFT calculations. We attempt to develop such a model for binary vanado-tellurite glasses. Special attention was paid to the coordination state of tellurium and vanadium atoms.



Structural changes, as recognized by analyzing band shapes of X-ray diffraction and FTIR spectra, revealed that Gd_2O_3 causes a higher extent of network polymerization as far as 40 mol%, after that between 40 and 50 mol% reveal a drastic structural modification which lead to the forming of the GdVO_4 crystalline phase.

Then, the present study provides interesting information concerning devitrification behavior of the gadolinium vanado-tellurite vitreous system which occur $\text{Te}_2\text{V}_2\text{O}_9$ and GdVO_4 crystalline phases. Surface of the heat-treated glasses was found to consist mainly of rings containing $[\text{TeO}_3]$, $[\text{TeO}_4]$, $[\text{VO}_4]$ and some $[\text{VO}_5]$ structural units.

The DFT calculations show that the $[\text{VO}_4]$ tetrahedrons are easy distorted whereas the $[\text{VO}_5]$ square pyramids are considerably distorted around vanadium center.