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Gadolinium doping of vanadate-tellurate glasses and glass ceramics

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Abstract In order to further elucidate the local structure of ternary $x\mathrm{Gd_2O_3}(100-x)[0.7\mathrm{TeO_2}\cdot 0.3\mathrm{V_2O_5}]$ glasses with $x = 0, 5, 10, 15, 20$ mol%, FTIR spectroscopy, XRD diffraction and density measurement were performed. FTIR and density data show that by increasing the gadolinium ions content of the samples the excess of oxygen may be accommodated by the inter-conversion of some [VO_4] into [VO_5] structural units and of [TeO_3] into [TeO_4] units. The composition of the heat-treated glasses was found to consist mainly of the $Te_2V_2O_9$ crystalline phase. Varying x between 15 and 20 mol% Gd_2O_3 produces structural modification having as result an increase of the glass network polymerization degree. Accordingly, the gadolinium ions play a particular role related to the improvement of the homogeneity of the glasses and in accommodating the glass network with the excess of oxygen.

Introduction

Tellurate glasses are of technical interest because of their low melting points and absence of the hygroscopic properties which limit application of phosphate and borate glasses. Previous works showed that vanadium tellurate glasses are semiconducting and that they switch when a high electrical field is applied [1, 2].

Tellurium dioxide, like vanadium pentoxide, is a conditional glass former [3]. It is very difficult to form pure vitreous TeO_2 and it has been suggested [4] that this is due to the lone pair of electrons in one of the equatorial positions of the [TeO_4] polyhedron. Tellurate glasses are high optical index glasses possessing high levels of infrared transmission and having potential applications as acoustic and optical materials used in laser technology or as photochromic glasses [5]. The repulsive forces in this zone hinder the free movement of the [TeO_4] polyhedra in space during the cooling of the melt. In a binary tellurate composition, the effect of the free electron pair is limited by the introduction of the new structural units which must be compatible with the [TeO_4] polyhedra.

For clarifying the structure of the binary tellurate glasses some works are done in analyzing the basic structural units whereby [TeO_4] trigonal bipyramid and [TeO_3] trigonal pyramids are found in crystals [6, 7] and in glasses [8].

Although the existence of binary and ternary vanadate glasses is well established and the structure of vanadate glasses remains a subject of interest because there is no clear picture of the exact nature of the oxygen polyhedra surrounding the vanadium atoms or of the role played by the other glass components [9]. Moreover, the structure of the vanadate glasses can be related to the nature of the network formers as well as of the network modifiers [10].

Since a certain amount of a secondary glass former/modifier is necessary to stabilize the TeO_2 glass, a content of 30 mol% V_2O_5 was chosen for present study. Four glass compositions, namely 5, 10, 15, and 20% Gd_2O_3, were prepared to investigate the structural modification produced by the addition of Gd_2O_3. The study was performed by using the FTIR spectroscopy, XRD diffraction, and

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density measurement. Some vanadate-tellurate glass ceramics containing Gd_2O_3, obtained after an appropriate heat treatment, were investigated in order to establish the crystallization behavior and structural changes induced by the addition of gadolinium ions into the host glass matrix.

Experimental

Glasses with the $x\mathrm{Gd_2O_3}(100-x)[0.7\mathrm{TeO_2}\cdot 0.3\mathrm{V_2O_5}]$ composition where $x = 0, 5, 10, 15, 20$ mol% were prepared by mixing appropriate amounts of tellurium dioxide, vanadium pentoxide and gadolinium trioxide. After melting at 850 °C for about 10 min in an electric furnace, the melts were rapidly quenched at room temperature by pouring on a stainless steel block. Then, the glassy samples were subject of a heat treatment performed at 400 °C for 48 h.

The samples were analyzed by means of X-ray diffraction using a XRD-6000 Shimadzu diffractometer, with a monochromator of graphite, for the Cu-Kα radiation ($\lambda = 1.54$ Å), at room temperature. The X-ray diffraction patterns did not reveal any crystalline phase in the prepared glass samples up to 20 mol% Gd_2O_3. The position and intensity of diffraction peaks obtains for the heat treated $x\mathrm{Gd_2O_3}(100-x)[0.7\mathrm{TeO_2}\cdot 0.3\mathrm{V_2O_5}]$ samples, consistent with that of the powder diffraction file (PDF), indicate an appreciable crystallization.

The structure of the glasses and glass ceramics was investigated by FTIR spectroscopy using the KBr pellet technique in the 400–1100 cm^{-1} range and a JASCO FTIR 6200 spectrometer.

The density measurements were performed using the picnometric method with water as the reference immersion liquid.

Results and discussion

FTIR spectroscopy

The FTIR features bands for the investigated ternary gadolinium tellurate-vanadate glasses, $x\mathrm{Gd_2O_3}(100-x)[0.7\mathrm{TeO_2}\cdot 0.3\mathrm{V_2O_5}]$, are assigned to the Te–O linkage vibration in $[TeO_4]$ and $[TeO_3]$ structural units and the V–O linkage vibration in $[VO_4]$ and $[VO_5]$ units. In Fig. 1, the bands located in the range of 460–490 cm^{-1}, 610–680 cm^{-1}, and 720–780 cm^{-1} were assigned to the bending mode of Te–O–Te or O–Te–O linkages, the stretching mode $[TeO_4]$ trigonal pyramidal with bridging oxygen and the stretching mode of $[TeO_3]$ trigonal pyramidal with non-bridging oxygen, respectively [11–14].

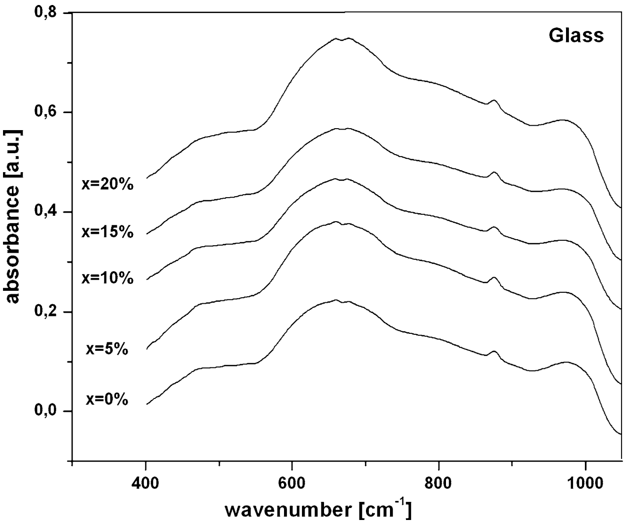

Fig. 1 FTIR spectra of the $x\mathrm{Gd_2O_3}(100-x)[0.7\mathrm{TeO_2}\cdot 0.3\mathrm{V_2O_5}]$ glasses for $x = 0$–20 mol% Gd_2O_3

In the case of pure V_2O_5 glass, it has been reported [14] that V^{5+} ions exhibit both four and fivefold coordination states, depending on the sample preparation conditions. The IR spectrum of the pure crystalline and amorphous V_2O_5 is characterized by the intense band located about 1000–1020 cm^{-1}, related to the vibration of isolated V=O vanadyl groups in $[VO_5]$ trigonal bipyramids [15–17]. The band from 950–970 cm^{-1} was attributed to $[VO_4]$ units [18–21].

A simple inspection of the spectral features presented in Fig. 1 shows that they are those characteristic of the base glass matrix, $0.7\mathrm{TeO_2}\cdot 0.3\mathrm{V_2O_5}$ and no dramatic changes occur with increasing the Gd_2O_3 content in the glasses. Because the majority of the bands are very broad and asymmetric, presenting also some shoulders, a deconvolution of the experimental spectra was necessary.

The deconvoluted IR spectra for the $x\mathrm{Gd_2O_3}(100-x)[0.7\mathrm{TeO_2}\cdot 0.3\mathrm{V_2O_5}]$ sample with $x = 0$ and 20 mol% Gd_2O_3 are shown in Fig. 2a and b and the peak assignments are given in Table 1. The deconvolution procedure allowed us a better identification of all bands that appear in the FTIR spectra in order to realize their correct assignment. The deconvolution was made by using the Spectra Manager program [22] and a Gaussian-type function. The proportion of the particular structures corresponding to different vibration modes was calculated from the areas of the fitted Gaussian bands divided to the total areas of these bands. We assumed that each component band is related to specific vibrations from the structural groups. The concentration of the structural group was considered to be proportional to the relative area of their characteristic band [23, 24]. The deconvolution parameters, the band centers, C, and the relative area, A, as well as the bands assignment for the studied glass are given in Table 1.

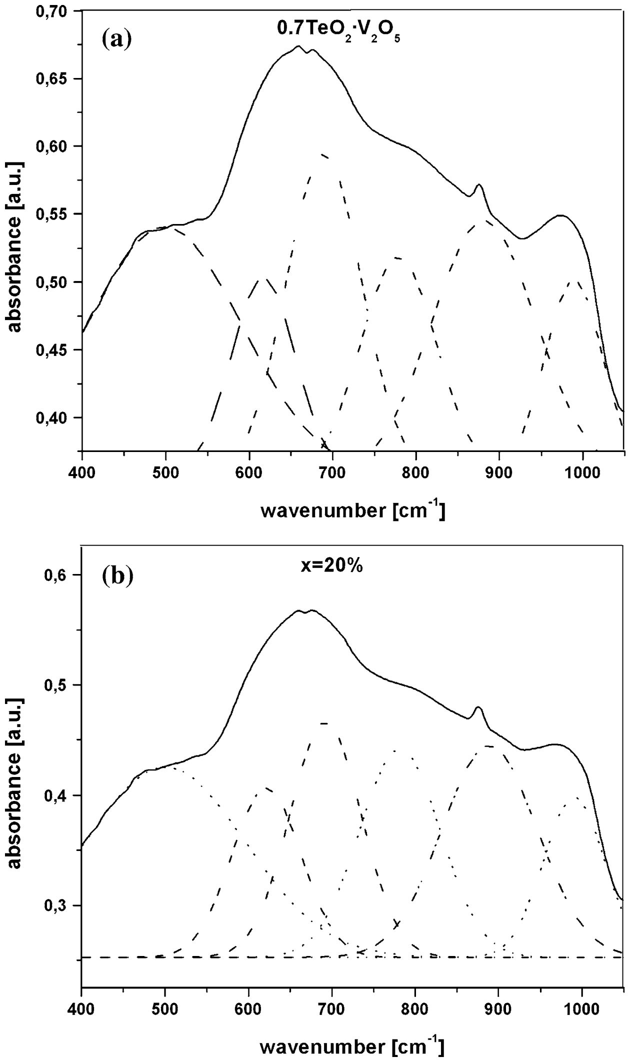

Fig. 2 The experimental and deconvoluted FTIR spectra for the $x\mathrm{Gd_2O_3}(100-x)[0.7\mathrm{TeO_2}\cdot 0.3\mathrm{V_2O_5}]$ system with (**a**) $x = 0$ and (**b**) $x = 20$ mol% Gd_2O_3

The relative area ratio of $[TeO_4]$ and $[TeO_3]$ structural units, hereafter referred as TeO_4/TeO_3, represent the ratio of $[TeO_4]$ and $[TeO_3]$ structural units. In the same way, VO_4/VO_5 represents the ratio of $[VO_4]$ and $[VO_5]$ structural units [24]. The variation of the TeO_4/TeO_3 and VO_4/VO_5 ratios with respect to the Gd_2O_3 content of the samples is illustrated in Table 2.

The ratio TeO_4/TeO_3 increases with the increasing of the gadolinium oxide content up to 5 mol%, while for x between 10 and 15 mol% decreases and after that it increases abruptly. Similar behavior shows the compositional variation of the ratio VO_4/VO_5 up to 15 mol% Gd_2O_3, followed by a decrease with the increase of gadolinium ions content up to 20 mol%.

The evolution of the TeO_4/TeO_3 and VO_4/VO_5 ratios with increasing the Gd_2O_3 content of the $0.7TeO_2 \cdot 0.3V_2O_5$ samples suggests as follows (see Table 2):

1. For $0 \le x \le 5$ mol% and 15 mol% $< x \le 20$ mol% Gd_2O_3, the coordination of the Te atom change progressively from 3 through 3 + 1 to 4 because of a $TeO_3 \rightarrow TeO_4$ conversion process, while for 10 mol% $\le x \le$ 15 mol% the inverse conversion process takes place.
2. For $0 \le x \le 5$ mol% Gd_2O_3 a $VO_5 \rightarrow VO_4$ conversion and for 10 mol% $\le x \le$ 20 mol Gd_2O_3 the $VO_4 \rightarrow VO_5$ conversion process takes place.

Density and molar volume data

The density of glasses is of special importance in the context of the study of their structure. Thus, such importance arises when the density of a glass shows a non-linear compositional dependence because this behavior suggests structural changes produced by compositional modifications.

Table 2 shows the variation of density as function of the gadolinium oxide content of the studied glasses. The estimated error for the determined density values was less than 0.2 g/cm^3.

Note that the relation between the density and the gadolinium ions content is not linear and shows important variations. The density decreases abruptly when 5 mol% gadolinium oxide was added. This may be related to the

Table 1 Deconvolution parameters (the band centers C and the relative area A) and the bands assignments for the $x\mathrm{Gd_2O_3}(100-x)[0.7\mathrm{TeO_2}\cdot 0.3\mathrm{V_2O_5}]$ glasses

$x = 0$		$x = 5$		$x = 10$		$x = 15$		$x = 20$		Assignments
C	A	C	A	C	A	C	A	C	A	
493	42.6	491	46.7	490	41.5	496	37.7	490	53.4	Bending vibrations of Te–O–Te or O–Te–O linkages
616	14	611	10.7	621	16	620	15	612	11.8	Stretching vibrations $[TeO_4]$
680	26.8	678	90.7	680	23	680	22	680	41.2	Stretching vibrations $[TeO_4]$
780	18.3	779	32.6	781	23	780	22	781	16	Stretching vibrations $[TeO_3]$
882	29.5	890	29.8	889	27	890	23.5	881	41	Stretching vibrations $[VO_5]$
982	12.6	970	15	980	13	981	11.7	981	14	Stretching vibrations $[VO_4]$

Table 2 The composition dependence of the relative area ratio of TeO_4/TO_3 (a) and also VO_4/VO_5 units (b), the density (c) and the molar volume (d) in the xGd$_2$O$_3$(100 − x)[0.7TeO$_2$ · 0.3V$_2$O$_5$] system

Characteristic	$x = 0$	$x = 5$	$x = 10$	$x = 15$	$x = 20$
(a) TeO_4/TeO_3	2.23	3.11	1.69	1.68	3.31
(b) VO_4/VO_5	0.42	0.50	0.48	0.49	0.34
(c) Density (g/cm^3)	4.23	4.10	4.58	4.59	3.95
(d) Molar volume (cm^3/mol)	393.7	388.7	330.7	314.4	347
$TeO_3 \leftrightarrow TeO_4$ inter-conversion	$TeO_3 \rightarrow TeO_4$		$TeO_4 \rightarrow TeO_3$		$TeO_3 \rightarrow TeO_4$
$VO_4 \rightarrow VO_5$ inter-conversion	$VO_5 \rightarrow VO_4$		$VO_4 \rightarrow VO_5$		$VO_4 \rightarrow VO_5$

formation of Gd–O–Te or Gd–O–V linkages, with strong Gd–O ionic bond [25], having as result the weakening of cross-linking with the glass network [26, 27]. When 10–15 mol% gadolinium oxide was added, the density increased from 4.10 to 4.59 g/cm^3. This could be explained by considering that the excess of oxygen may be accommodated by the conversion of some [VO$_4$] into [VO$_5$] units, [TeO$_4$] into [TeO$_3$] units and probably the formation of covalent Gd–O bonds which will lead to an open structure of the glasses.

The increase of the gadolinium ion concentration up to 20 mol% surprisingly causes a drastic decrease of the density, suggesting the conversion of [TeO$_3$] into [TeO$_4$] units and [VO$_4$] into [VO$_5$] structural units, respectively.

The molar volume is of high interest because it is directly related to the spatial distribution of the oxygen in the glass network. Theoretically, the substitution of TeO_2 by Gd_2O_3 in the glass matrix may lead to the increase of the molar volume because the molecular volume of Gd_2O_3 is larger than that of the TeO_2. Actually, the experimental data show that the molar volume is decreased by adding the gadolinium oxide. The observed decrease in the molar volume may be attributed to a decrease in bonds length and/or inter-atomic spacing between atoms and/or considering that gadolinium ions substitute the vanadium ions (the atomic weight of Gd_2O_3 and V_2O_5 are 205.25 and 181.88 g/mole, respectively) [28].

In brief, the gradual increase of gadolinium oxide in the glass up to 15 mol% results in the transformation of some [TeO$_4$] trigonal bipyramids into [TeO$_3$] trigonal pyramids units. This leads to a decrease in the connectivity of the glass network (i.e., a layered structure appears instead of the three-dimensional network) as evidenced by the observed decrease in the relative intensity of IR absorption bands, the decrease of molar volume and the increase of density. Thus, the density data show that the rare earth ions exert a particular influence on the homogeneity and stability of the glass network and in accommodating the vitreous network with the excess of oxygen in the studied glasses. This effect was previously reported for other glasses containing rare earth ions, too [14, 29–32].

In order to better understand these data concerning the vibrations of the massive [TeO$_4$] structural units, the glassy samples were subject to heat treatment.

Glass ceramics

After heat treatment some structural changes were observed for the studied samples. Thus, in the glass samples with up to 20 mol% Gd_2O_3 the $Te_2V_2O_9$ crystalline phase appears (Fig. 3). The intensities of the peaks corresponding to these glass ceramics are reduced by increasing the concentration of gadolinium ions from 5 to 15 mol% Gd_2O_3. This suggests that the addition of rare earth oxide modifier up to 20 mol% causes structural changes, namely the gradual decrease of the crystalline phase and an increase of the glass network polymerization degree. Thus, increasing the gadolinium oxide content leads to a relaxation of the glass network and the increase of the vitreous phase in the studied samples.

The examination of the FTIR spectra of the xGd$_2$O$_3$(100 − x)[0.7TeO$_2$ · 0.3V$_2$O$_5$] glass ceramics with $x =$ 0–20 mol% (Fig. 4) shows that the increase of Gd_2O_3 content modifies the characteristic IR bands as follows:

1. The prominent band centered at about 478 cm^{-1} (Fig. 1) splits into four components located at ~420, 446, 490 and 525 cm^{-1} for x between 0 and 15 mol% Gd_2O_3 (Fig. 4). After that, the intensity of this band increases with the increasing of the content of Gd_2O_3

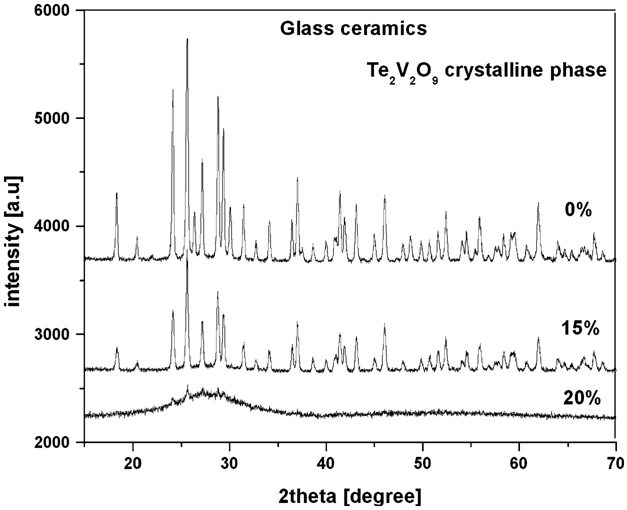

Fig. 3 X-ray diffraction patterns for xGd$_2$O$_3$(100 − x)[0.7TeO$_2$ · 0.3V$_2$O$_5$] glass ceramics with x = 0, 15 and 20 mol%

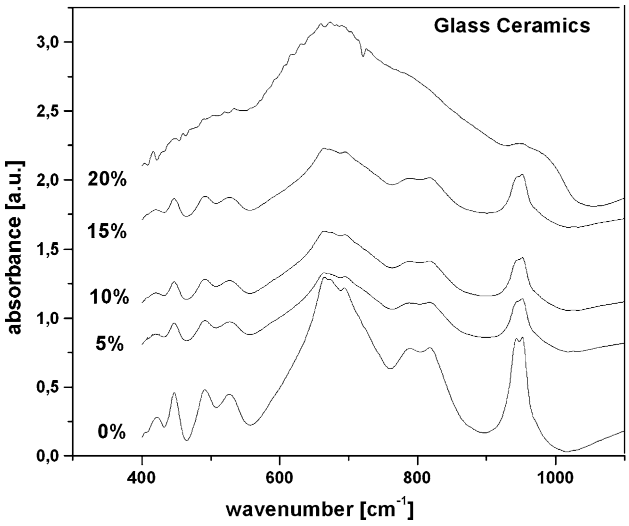

Fig. 4 FTIR spectra of the $xGd_2O_3(100 - x)[0.7TeO_2 \cdot 0.3V_2O_5]$ glass ceramics for $x = 0$–20 mol% Gd_2O_3

up to 20 mol%. All these bands are assigned to the bending mode of Te–O–Te or O–Te–O linkages [33, 34].

2. The intensity of the bands centered at ~653 and 678 cm^{-1} in glasses decreases with increasing of Gd_2O_3 content and shifts to ~663 and 693 cm^{-1} for the glass ceramics. For $0 \leq x \leq 15$ mol% Gd_2O_3, these bands split into some components located at about ~665, 675 and 695 cm^{-1}, while for 20 mol% Gd_2O_3 its intensity increases. These bands are attributed to the stretching vibrations in [TeO_4] units [27].
3. The intensity of the band centered at ~795 cm^{-1} increases slowly with the increasing of the gadolinium ions content up to 20 mol%, while for small contents ($0 \leq x \leq 15$ mol%) the band splits into two components located at ~785 and ~820 cm^{-1}. All these bands are corresponding to the stretching vibrations in [TeO_3] structural units [12].
4. The band centered at about ~970 cm^{-1} splits into two components located at 942 and 953 cm^{-1} at a small content of Gd_2O_3 ($0 \leq x \leq 15$ mol%). After that, this band shifts to higher wavenumbers at ~950 and 983 cm^{-1}. All these bands are due to the V–O stretching vibrations in [VO_4] units [13, 14, 18, 20, 35].

Structural changes in $xGd_2O_3(100 - x)[0.7TeO_2 \cdot 0.3V_2O_5]$ glass ceramics, as recognized by analyzing the X-ray diffraction patterns and the IR spectra, revealed that the gadolinium ions play an essential network modifier role. For x between 15 and 20 mol%, Gd_2O_3 produces structural modifications which lead to an open structure of the glass. This results in a relaxation of the glass network, an accommodation of the network with the excess of oxygen and an increase of the content of vitreous phase by heat treatment. This could be explained by considering that the excess of oxygen may be accommodated by the conversion of some [TeO_3] into [TeO_4] units and [VO_4] into [VO_5] structural units and/or the formation of covalent Gd–O bonds.

Thus, for the heat-treated samples the apparition of the $Te_2V_2O_9$ crystalline phase was observed. The content of the $Te_2V_2O_9$ crystalline phase decreases with increasing the gadolinium oxide content up to 20 mol% Gd_2O_3.

In conclusion, the structural changes observed by increasing the Gd_2O_3 content in $xGd_2O_3(100 - x)$ $[0.7TeO_2 \cdot 0.3V_2O_5]$ glass ceramics and evidenced by the XRD, FTIR investigation and density measurements suggest that the gadolinium ions play an essential network modifier role.

Conclusion

FTIR spectroscopy, X ray diffraction studies and density measurement have been utilized in order to study structural changes produced by the variation of the Gd_2O_3 content in the ternary $xGd_2O_3(100 - x)[0.7TeO_2 \cdot 0.3V_2O_5]$ glasses with $x = 0, 5, 10, 15, 20$ mol%.

Structural changes produced by varying the Gd_2O_3 content of the glass matrix determine variations of the TeO_4/TeO_3 and VO_4/VO_5 ratios of the studied glasses. This compositional evolution of the structure could be explained by considering that the excess of oxygen may be accommodated by the inter-conversion of some [VO_4] into [VO_5] structural units and of [TeO_3] into [TeO_4] units. These results are supported by the density and molar volume data.

The composition of the heat-treated glasses was found to consist mainly of the $Te_2V_2O_9$ crystalline phase. Structural changes in $xGd_2O_3(100 - x)[0.7TeO_2 \cdot 0.3V_2O_5]$ glass ceramics, as recognized by the X-ray diffraction patterns and the IR spectra, revealed that increasing the Gd_2O_3 content up to 20 mol% causes structural modifications and an increase of the polymerization degree of the glass network.

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