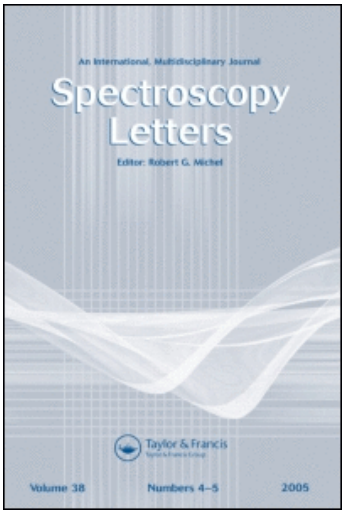

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Coordination of the Titanium in Borosilicate Glasses by XRF, XPS and Raman Spectroscopy

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COORDINATION OF THE TITANIUM IN BOROSILICATE GLASSES BY XRF, XPS AND RAMAN SPECTROSCOPY

Keywords: Coordination, Titanium, Borosilicate glasses, XRF, XPS, Raman.

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ABSTRACT

The coordination of Ti in borosilicate glasses have been studied by XRF, XPS and Raman spectroscopy. The results show that most of the Ti atoms are four-fold coordination in borosilicate glasses.

INTRODUCTION

The Ti atom is known to be four-, five-, and six-fold coordination by oxygen atoms in various crystal structures. A number of spectroscopic and diffraction investigations have been made elucidate the coordination and structural

role of Ti in Ti-containing glasses[1-4]. The present paper reports the results of the Ti coordination in borosilicate glasses.

EXPERIMENTAL

Compounds

Crystalline Ba_2TiO_4 was prepared from certified grade anatase-type TiO_2 and $BaCO_3$ at 1300 C for 20 h. Its formation was confirmed by the x-ray diffraction technique. The Ti atoms in Ba_2TiO_4 and anatase-type TiO_2 are four-fold coordination and six-fold coordination, respectively.

Certified reagent grade SiO_2, $BaCO_3$, H_3BO_3 and anatase-type TiO_2 were used as the starting materials to obtain the glsses with the compositions given in Table 1. The starting materials were weighed, mixed in a roller-mill for several hours and put in a platinum crucible at 1300-1400°Cfor 1 h. The melt were quenched on steal plate. The plates of the glasses obtained were annealed at 550°C for some times and cooled to room temperature.

TABLE 1

Chemical Compositions of Borosilicate Glasses

Glass No.	Composition (wt%)			
	BaO	TiO_2	B_2O_3	SiO_2
G-1	30	10	20	40
G-2	30	10	30	30
G-3	30	20	10	40
G-4	30	20	40	10
G-5	30	30	10	30
G-6	30	30	30	10
G-7	30	40	10	20
G-8	30	40	30	0

TABLE 2

Variance of TiKα from XRF Spectra

Compound	Variance (sq. deg.)	Compound	Variance (sq. deg.)
Ba_2TiO_4	0.12955	G-4	0.12986
TiO_2*	0.13298	G-5	0.12967
G-1	0.12975	G-6	0.12941
G-2	0.12958	G-7	0.12951
G-3	0.12962	G-8	0.12989

* anatase-type

Instrumental

XRF spectra were obtained with a RIGAKU x-ray fluorescence spectrometer employing Cr target, TAP crystal and proportional counter. XPS spectra were obtained with a KRATOS x-ray photoelectron spectrometer employing Al x-radiation. Raman spectra were obtained with a SPEX RAMALOG laser Raman spectrometer employing Ar^+ laser device.

RESULTS AND DISCUSSION

The results obtained from XRF spectra are given in Table 2.

It is seen from Table 2 that the variance of the TiKα of Ba_2TiO_4 and anatase-type TiO_2 are 0.12955 sq. deg. and 0.13298 sq. deg., respectively. The variances of the TiKα of all Ti-containing glasses are in the vicinity of 0.12955 sq. deg.. It suggests that most of the Ti atoms in the borosilicate glasses are four-fold coordination.

TABLE 3

Eb and Ek of $Ti2p^{3/2}$ from XPS Spectra

Compound	Eb (eV)	Ek (eV)	Half-width of Ek (eV)
Ba_2TiO_4	457.9	1018.2	2.1
TiO_2	459.3	1020.9	1.75
G-2	458.3	1017.7	2.0
G-4	458.5	1018.3	2.1
G-6	458.4	1019.1	2.1
G-8	458.1	1020.0	2.15

* anatase-type

The results obtained from XPS spectra are given in Table 3.

It is seen from Table 3 that Eb = 457.9 eV, Ek = 1018.2 eV and the half-width of Ek is 2.1 eV when Ti atom is four-fold coordination, whereas Eb = 459.3 eV, Ek = 1020.9 eV and the half-width of Ek is 1.75 eV when Ti atom is six-fold coordination. The Eb, Ek and the half-width of the $Ti2p^{3/2}$ of the borosilicate glasses are more close to 457.9 eV, 1018.2 eV and 2.1 eV, respectively. So most of the Ti atoms in the borosilicate glasses are four-fold coordination.

The results obtained from Raman spectra are given in Table 4.

It is seen from Table 4 that the Ti-O bonds of the borosilicate glasses are in the vicinity of 754 cm^{-1}, the Ti-O bond of Ba_2TiO_4. It suggests that most of the Ti atoms in the borosilicate glasses are four-fold

TABLE 4

Raman Spectra of the Crystalline and Glassy Compounds

Compound	Raman spectra (cm^{-1})				
Ba_2TiO_4		546m		754vs	1058w
TiO_2*	394s	514m	638vs		
G-1				844s	1016w
G-2				850m	1108w
G-3				860m	1032w
G-4				856m	
G-5				840m	
G-6				838m	
G-7				824m	982w
G-8				832m	

* anatase-type

coordination.

In a word, we may conclude that most of the Ti atoms in borosilicate glasses are four-fold coordination.

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