

This article was downloaded by:

On: 30 January 2011

Access details: *Access Details: Free Access*

Publisher *Taylor & Francis*

Informa Ltd Registered in England and Wales Registered Number: 1072954 Registered office: Mortimer House, 37-41 Mortimer Street, London W1T 3JH, UK



Spectroscopy Letters

Publication details, including instructions for authors and subscription information:

<http://www.informaworld.com/smpp/title~content=t713597299>

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

Ning Yao^a; Xiaoding Li^a; Xiaonan Song^b

^a Hubei Research Institute of Chemistry Wuhan, China ^b Wuhan University of Industry Wuhan, China

To cite this Article Yao, Ning , Li, Xiaoding and Song, Xiaonan(1990) 'Coordination of the Titanium in Borosilicate Glasses by XRF, XPS and Raman Spectroscopy', *Spectroscopy Letters*, 23: 9, 1153 — 1157

To link to this Article: DOI: 10.1080/00387019008054489

URL: <http://dx.doi.org/10.1080/00387019008054489>

PLEASE SCROLL DOWN FOR ARTICLE

Full terms and conditions of use: <http://www.informaworld.com/terms-and-conditions-of-access.pdf>

This article may be used for research, teaching and private study purposes. Any substantial or systematic reproduction, re-distribution, re-selling, loan or sub-licensing, systematic supply or distribution in any form to anyone is expressly forbidden.

The publisher does not give any warranty express or implied or make any representation that the contents will be complete or accurate or up to date. The accuracy of any instructions, formulae and drug doses should be independently verified with primary sources. The publisher shall not be liable for any loss, actions, claims, proceedings, demand or costs or damages whatsoever or howsoever caused arising directly or indirectly in connection with or arising out of the use of this material.

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

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

Ning Yao, Xiaoding Li

Hubei Research Institute of Chemistry
Wuhan, 430073, China

Xiaonan Song

Wuhan University of Industry
Wuhan, 430070, China

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 glasses 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 °C for 1 h. The melt were quenched on steel 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 $\text{TiK}\alpha$ 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 $\text{TiK}\alpha$ of Ba_2TiO_4 and anatase-type TiO_2 are 0.12955 sq. deg. and 0.13298 sq. deg., respectively. The variances of the $\text{TiK}\alpha$ 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 $Ti_{2p}^{3/2}$ 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 $Ti_{2p}^{3/2}$ 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.

REFERENCES

1. Hanada, T. and Soga, N., J. Non-Cryst. Solid, 38&39, 105 (1980).
2. Sandstrom, D. R., Wong, J. and Schultz, P., ibid, 55, 21 (1983).
3. Emill, M., Fagherazzi, G. and Guglielmi., ibid, 74, 129 (1985).
4. Dumas, T. and Petiau, J., ibid, 81, 201 (1986).

Date Received: 06/04/90
Date Accepted: 07/09/90