

**X- ray photoelectron spectroscopy
(XPS) studies of Sr-vanadate
glasses**

G.D. Khattak and N. Tabet
Department of Physics, KFUPM,
Dhahran, Saudi Arabia

Introduction

- **General Desirability for XPS Studies**
- **Experimental Procedure**
- **Results / Discussion**
- **Conclusion**

General Desirability for XPS Studies

- **TM oxide glasses Applications : Memory switching, Electrical threshold and optical switching devices, ...**
- **Structural and electronic properties of these glasses depend on the relative proportion of different valence states of the TM ions.**

- **In order to account for the effect of these valence states it is important to control and measure the ratios of the ion concentration in the different valence states of these TM ions.**
- **Mixed clusters appear in glasses containing mixed transition-metal (TM) oxides which also affect the properties of these glasses.**

- **XPS has proven to be an important and powerful technique in assessing the local glass structure of solids as it can distinguish between BO and NBO Oxygen atoms**
- **and also for the identification of different valence states (ratio of different valence states)**

Glass Preparation

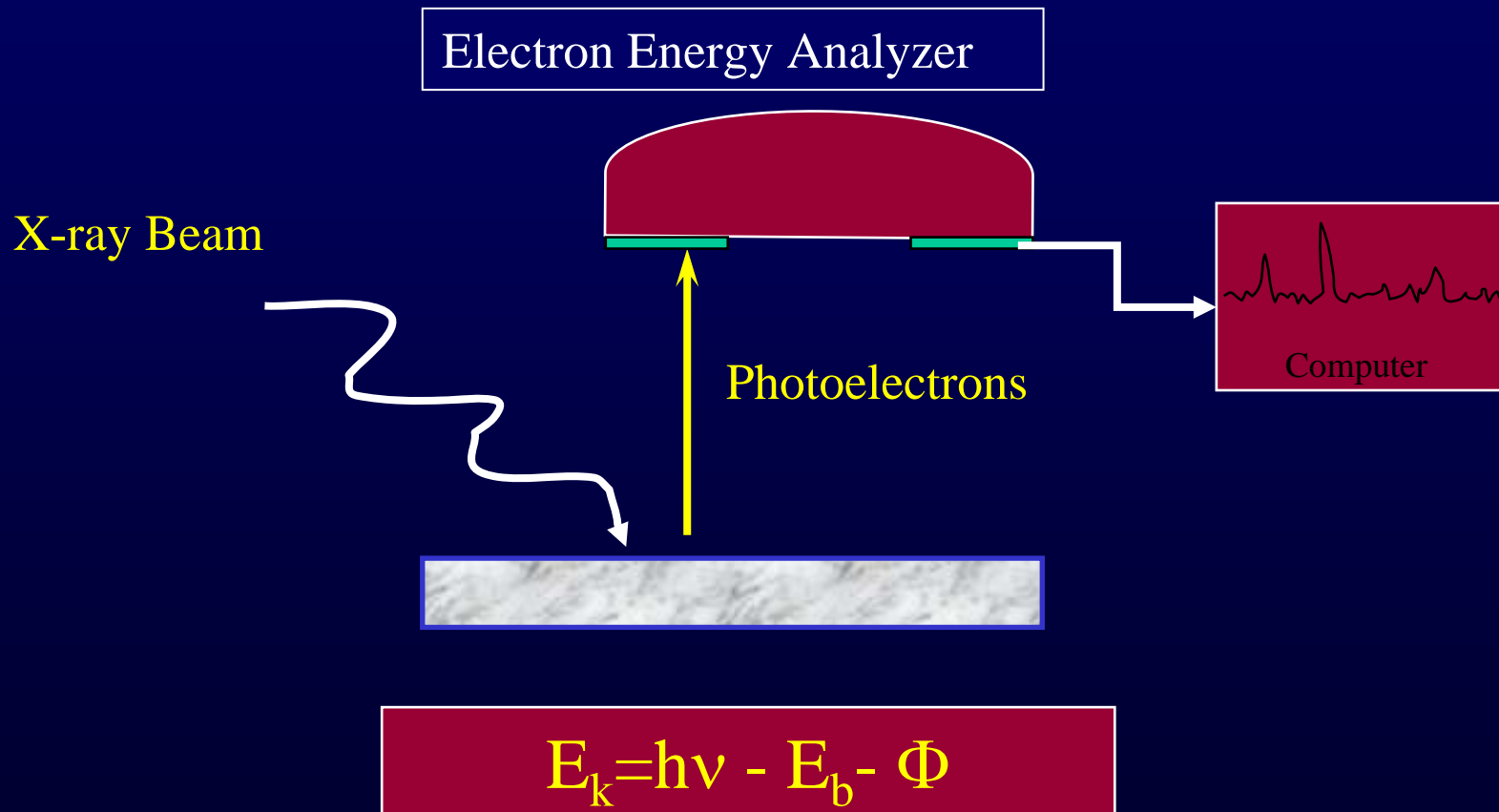
- Batch composition $[(\text{SrO})_x(\text{V}_2\text{O}_5)_{1-x}]$ where $x = 0.2, 0.3, 0.4$ and 0.5 .
 - oxidation and reduction reactions in a glass melt depend
 - i. on the size of the melt,
 - ii. on the sample geometry,
 - iii. on whether the melt is static or stirred,
 - iv. on thermal history and on quenching rate.
- all glass samples were prepared under similar conditions to minimize these factors.

- **30g of chemicals mixed**
- **Heated at 1000-1100 °C**
- **Homogenized melt, then cast onto a stainless steel plate mold to form glass rods of 5-mm diameter for XPS measurements.**
- **Specimens annealed at 200 °C for 10 hours**

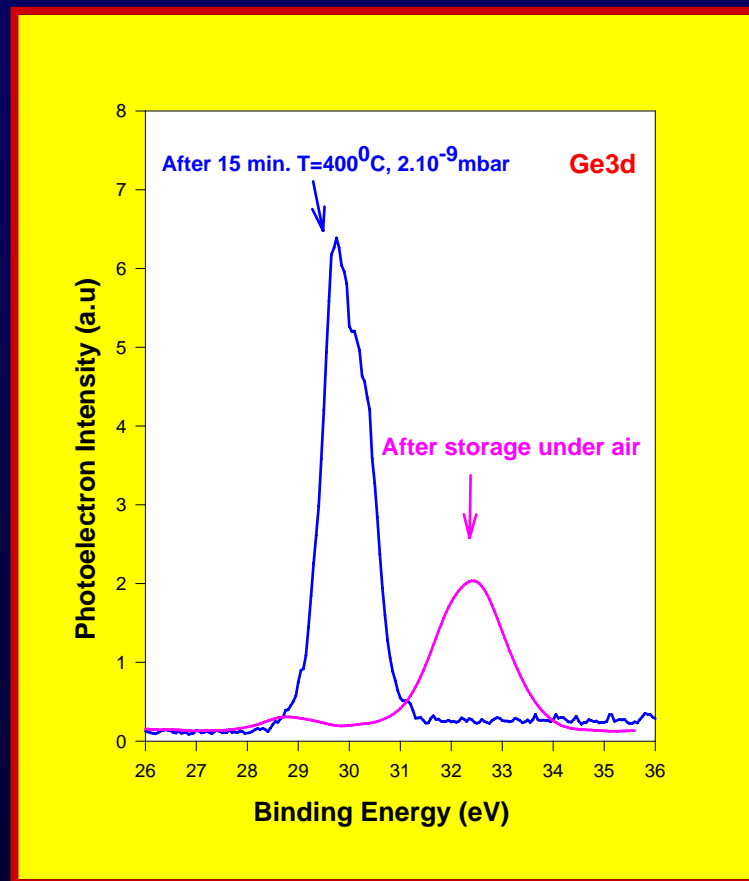
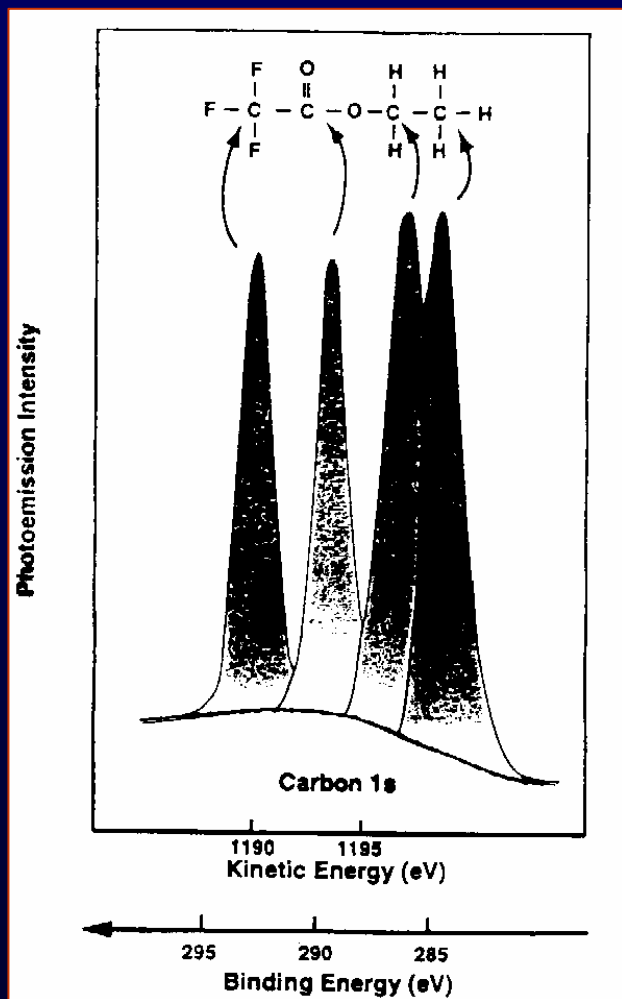
Samples Composition

Batch				Actual (from ICP)	
Glass	x	V ₂ O ₅	SrO	V ₂ O ₅	SrO
G1	0.2	0.80	0.20	0.792	0.208
G7	0.3	0.70	0.30	0.692	0.308
G8	0.4	0.60	0.40	0.591	0.409
G9	0.5	0.50	0.50	0.488	0.511

X-Ray Photoelectron Spectroscopy (XPS)

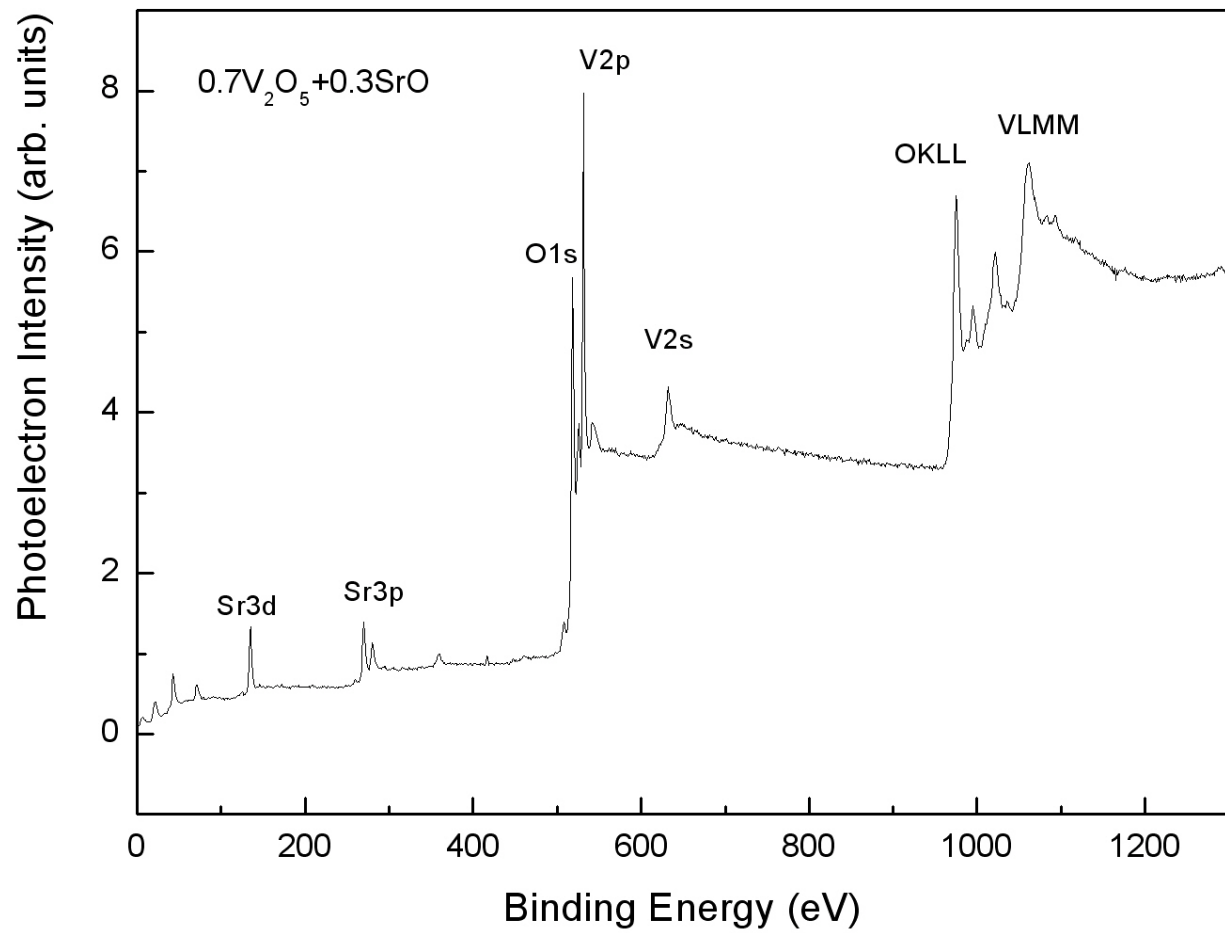


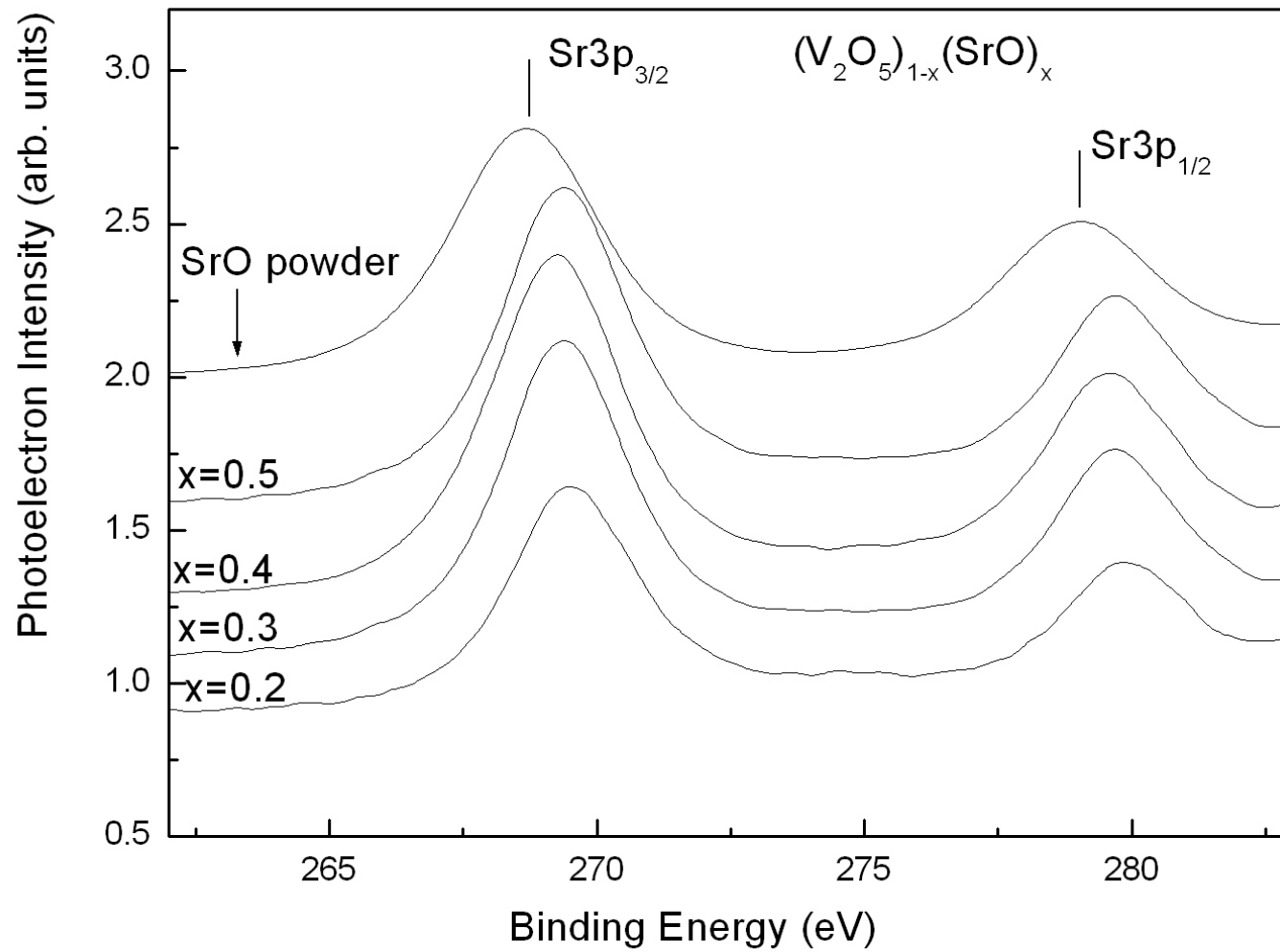
X-ray photoelectron spectroscopy (XPS) showing chemical shift



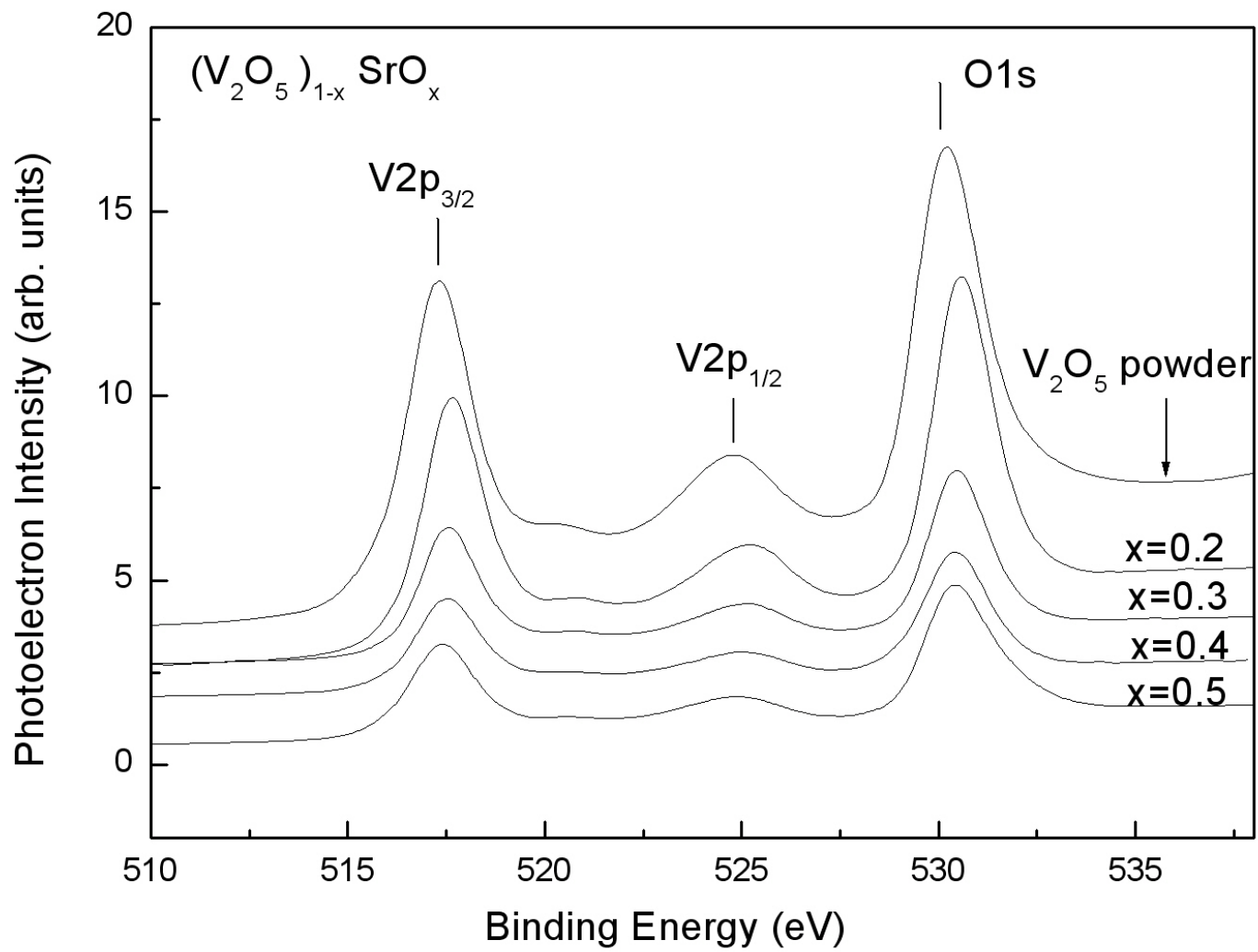
Results

**Wide-scan XPS spectrum
sample with $x = 0.3$**



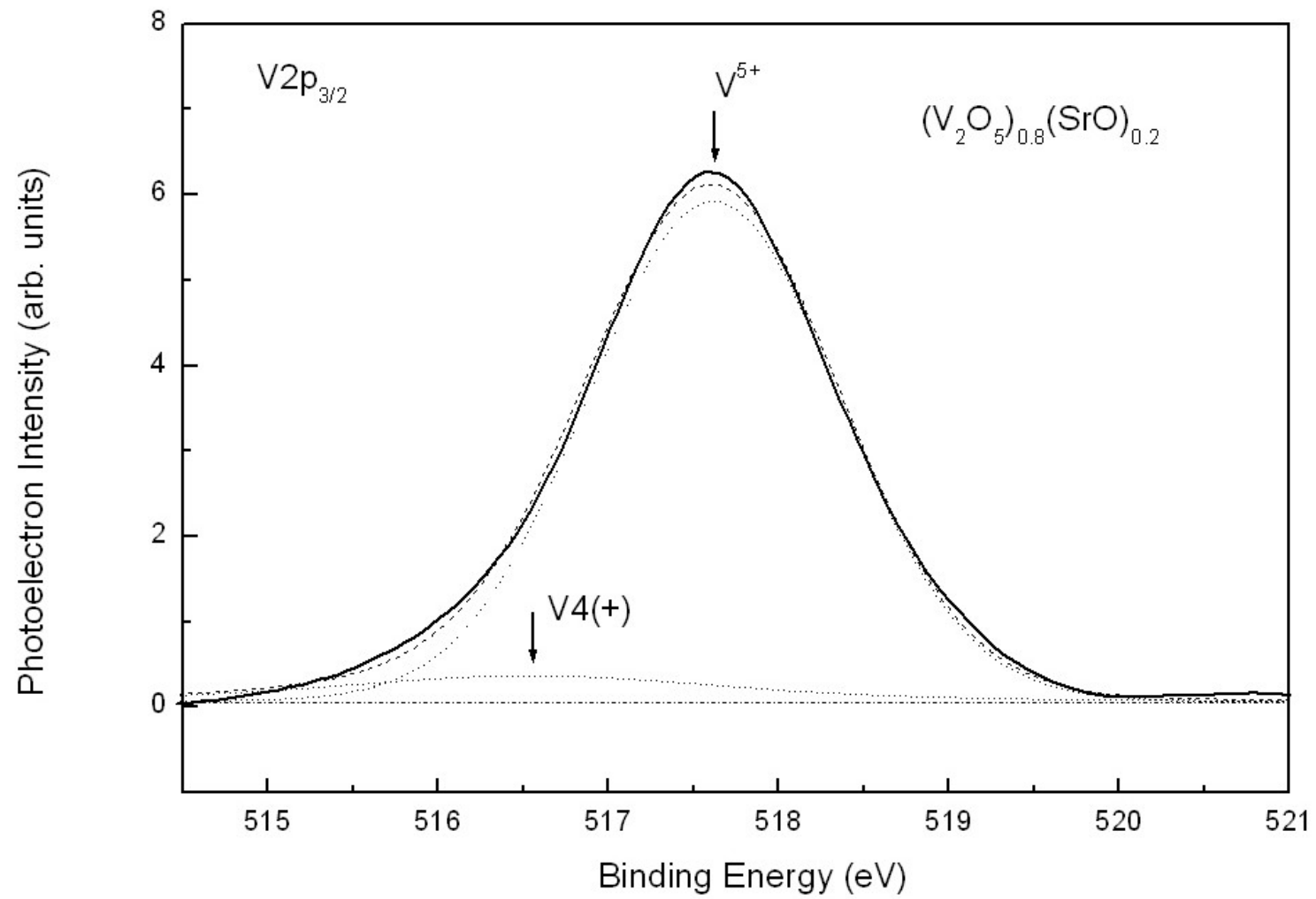


- Sr 3p spectra have the same B.E. for all samples.
- Shifted by 0.5 eV towards higher B.E. in comparison to their values in SrO powder.
- This shift arises from a change in the molecular environment.



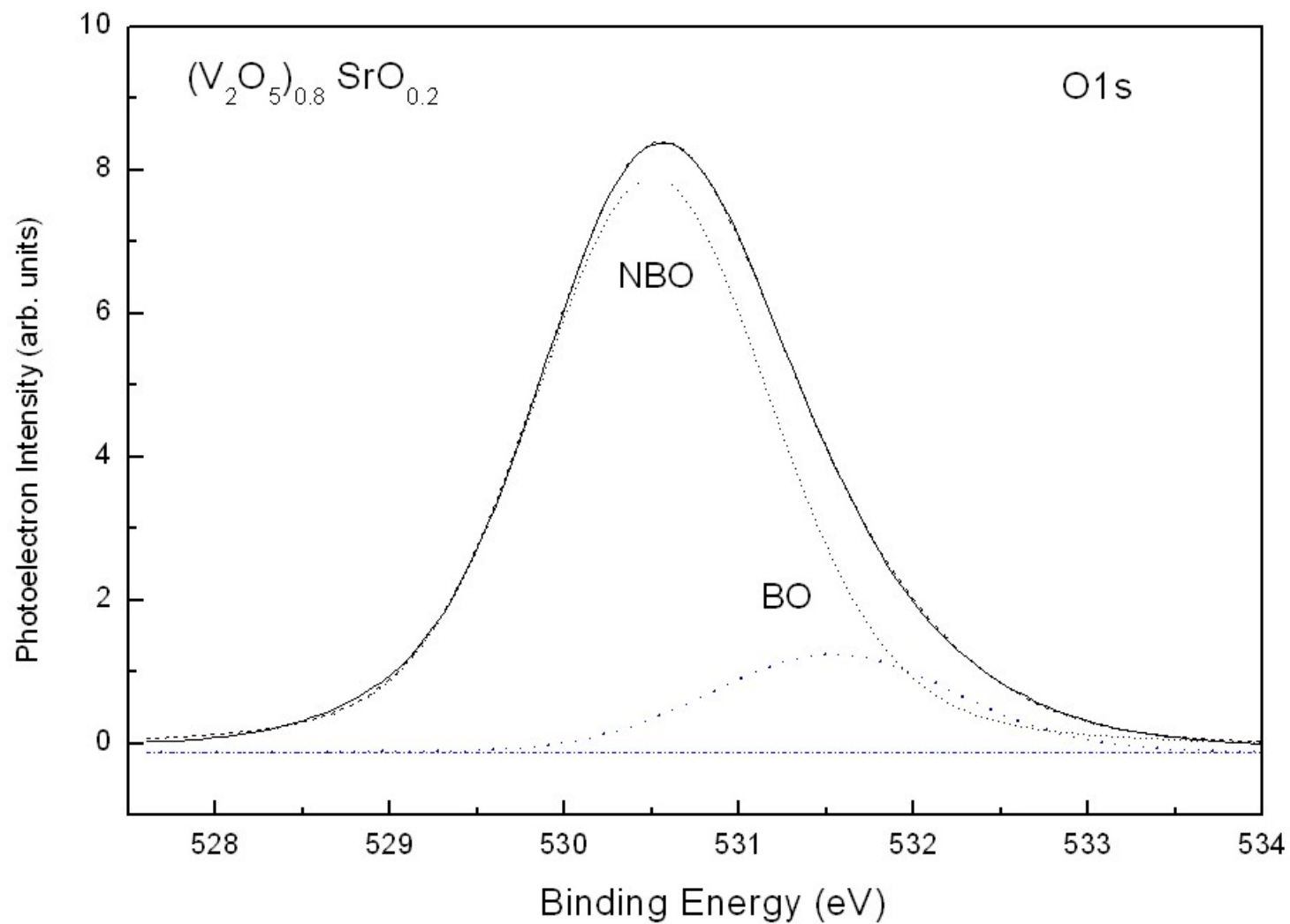
V 2p spectra

- . the V $2p_{3/2}$ spectra for the glass samples are sufficiently broaden such that two peaks are fitted to the data.
- These peaks are associated with the presence of V^{5+} and V^{4+} and the relative area under each peak reflects the relative amount of each ion.
- More than 90% of the V is found to be in the V^{5+} state in these glass samples.



O 1s spectra

- V-O-V bridging oxygen (BO)
- V-O-Sr, Sr-O-Sr, V = O non-bridging oxygen
- $\text{NBO/TO} = (4-3x)/(5-4x)$
- Good agreement between calculated and measured.
- NBO/TO 87-100%



Conclusions

- The binding energies of Sr 3p are found to increase by 0.5 eV in comparison to those for pure SrO powder
- the binding energy of V 2p for glasses increases by 0.2 eV in comparison to those pure V_2O_5 powder.
- These shifts are explained in terms of changes in their electron densities as a result of differences in the next-nearest neighbor environment between the local structures in these glasses and powders.

Conclusion (Cont')

- **NBO/TO ranges between 85-87% for $x = 0.2$ & 0.3 .**
- **NBO/TO is 100% for $x = 0.4$ & 0.5 .**
- **More than 90 % of V ions are in the V^{5+} state.**