

Understanding the gas sensing mechanism in vanadium doped tin oxides using X-ray diffraction and X-ray photoelectron spectroscopy

Nirman Chakraborty, Ambarish Sanyal, Sagnik Das, Debdulal Saha, Samar Kumar Medda, and Swastik Mondal

CSIR Central Glass and Ceramic Research Institute, 196 Raja S. C. Mullick Road, Jadavpur, Kolkata-700032

swastik_mondal@cgcri.res.in

Gas sensing is primarily considered as a surface property of materials. The surface structure however depends to a large extent on bulk crystal structure. Knowledge of surface structure in combination with the knowledge of bulk crystal structure is thus helpful in improved understanding of the surface properties of materials [1, 2]. In the present work, vanadium doped tin oxide samples $\text{Sn}_{1-x}\text{V}_x\text{O}_2$ ($x=0, 0.304$ and 0.343) have been synthesized by simple precipitation methods. All samples have exhibited ppm level ammonia sensing property. Doped samples have been found to be more sensitive to ppm level ammonia in air in comparison to pristine SnO_2 . In order to understand the enhancement in ammonia sensing property due to vanadium doping, all samples have been characterized extensively by X-ray diffraction and X-ray photoelectron spectroscopy. Bulk crystal structures of the samples have been established by Rietveld refinements [3] using high quality powder X-ray diffraction data with the aid of the computer program Jana2006 [4]. Surface electronic structures of the samples have been determined by X-ray photoelectron spectroscopy. Analysis of surface electronic states and crystal structures has revealed a direct correlation between surface electron deficiencies and sensing responses. Based on this correlation a model mechanism has been proposed which explains the enhancement in ammonia sensing property of vanadium doped samples in comparison to pure SnO_2 [5].

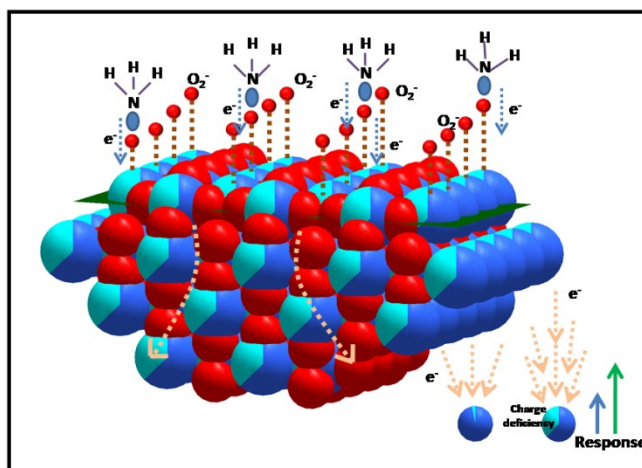


Figure 1. Schematic of the mechanism for enhancement in gas sensing property

[1] Chakraborty, N., Das, S., Saha, D. & Mondal, S. (2021). arXiv:2104.14867 [physics.chem-ph].

[2] Chakraborty, N., Das, S., Srihari, V., Mondal, D. J., Saha, D., Konar, S., Mishra, A. K. & Mondal S. (2021). *Materials Advances* **2**, 3760-3769.

[3] Rietveld, M. H. (1969). *J. Appl. Crystallogr.* **2**, 65–71.

[4] Petricek, V., Dusek, M. & Palatinus, L. Institute of Physics, Czech Academy of Sciences, Prague, Czech Republic, Jana2006.

[5] Chakraborty, N., Sanyal, A., Das, S., Saha, D., Medda, S. K. & Mondal, S. (2020). *ACS Appl. Nano Mater.* **3**, **8**, 7572-7579.

Keywords: Powder X-ray diffraction; X-ray photoelectron spectroscopy; crystal structure; electronic structure; gas sensing mechanism

Nirman Chakraborty would like to thank DST INSPIRE (IF170810) for his research fellowship.