## **Metal Oxides Series**

Series Editor Ghenadii Korotcenkov

# **Metal Oxide Defects**

Fundamentals, Design, Development and Applications

Edited by Vijay Kumar Sudipta Som Vishal Sharma Hendrik C. Swart



## Contents

List	t of c	ontributors	xi
Ser	ies eo	litor biography	xvii
Pre	face	to the series	xix
1	Tra	insition metal ions in solid electrolytes. Ceramics and glasses	1
	S. 7	Ferny, M.C. Molina and M.A. Frechero	
	1	NASICON-type materials	1
	2	Transition metal oxides in electrical conductor glasses	10
		Acknowledgments	21
		References	21
2	Th	e emergence of analytical techniques for defects in metal oxide	27
	Jay	ashree Swaminathan	
	1	Introduction	27
	2	Transmission electron microscopy (TEM)	29
	3	X-ray diffraction (XRD)	33
	4	X-ray photoelectron spectroscopy (XPS)	36
	5	X-ray absorption spectroscopy	42
	6	Positron lifetime spectroscopy	<b>48</b>
	7	Electron paramagnetic resonance	51
	8	Photoluminescence (PL) spectroscopy	53
	9	UV-visible spectroscopy	54
	10	Scanning tunneling microscopy (STM)	54
	11	Recent advancements for defect characterization	56
	12	Conclusion	57
		References	57
3	Vacancy and defect structures in metal oxides		61
	Hasmat Khan, Atanu Naskar and Susanta Bera		
	1	Introduction	61
	2	Type of defects in metal oxides	62
	3	Effect of factors on defect chemistry	66
	4	Defect engineering in metal oxides	69
	5	Defects in metal oxides and their applications	73
	6	Conclusion	76
		Acknowledgments	77
		References	77

4	<b>Defects disorder of lanthanum cerium oxide</b> <i>Way Foong Lim</i>	83
	1 Introduction	83
	2 Cerium oxide	84
	3 Conclusion	118
	4 Recommendations for future research	118
	References	118
	Further reading	127
	Turiner reading	141
5	Oxidation of metals and formation of defects by theoretical	
	modeling	129
	Yanyan Jiang, Xingfan Zhang, Hui Li, Peiru Zheng, Yingjie Ma and Fan Chen	
	1 Introduction	129
	2 Computational techniques for atomistic simulations	130
	3 Oxidation of bulk metals at the atomic scale	139
	4 Oxidation mechanisms of nanomaterials	147
	5 Concluding remarks	155
	Acknowledgments	156
	References	156
	References	150
6	<b>Role of defects in multiferroic nanoparticles</b> V.G. Shrimali, Keyal Gadani, A.D. Joshi, K. Asokan, P.S. Solanki	161
	and N A Shah	
	1 Introduction	161
	2 Role of defects in multiferroic nanoparticles	172
	2 Role of defects in multicitote nanoparticles	186
	References	100
7	Oxygen defects, morphology, and surface chemistry of metal	
	oxides: a deep insight through a joint experimental and	
	theoretical perspective	191
	Rafael Aparecido Ciola Amoresi, Ubirajara Coleto Junior,	
	Alexandre Zirpoli Simões, Leinig Antonio Perazolli, Elson Longo	
	and Juan Andrés	
	1 Introduction	191
	2 Surfaces	194
	3 Relationship between surfaces and catalytic, photocatalytic,	
	luminescent, and antibacterial/antifungal properties	202
	4 Conclusion and future outlook	207
	References	208
Q	Doint defeats in staightomatric and nonstaightomatric metal	
0	avides for medern microelectronics	217
	Vladimin Kolkovalay and Donald Stiller ar	<b>41</b> /
	viaamir Koikovsky ana Konala Stubner	01 <i>5</i>
	1 mutoduction 2 Constant to sharing their scheme (1,1) 1 (1,1)	217
	2 Growin techniques, their advantages, and disadvantages for the	840
	growth of metal oxides	219

	3	Native defects in metal oxides: theory and experiment	225
	4	Hydrogen-related defects in metal oxides	239
	5	Conclusion remarks	244
		References	245
9	Int An De	<b>fluence of defects upon mechanical properties of oxide materials</b> <i>nin Hamed Mashhadzadeh, Azam Salmankhani, Maryam Zarghami</i> <i>hghani, Christos Spitas and Mohammad Reza Saeb</i>	253
	1	Introduction	253
	2	Metal-oxide materials of different dimensionalities	255
	3	Structural defects	261
	4	A summary of previous works on oxide nanomaterials	266
	5	Concluding remarks and future perspective	272
		References	272
10	Defect evolution in ZnO nanocrystal films at doping by group IIIA		• • • •
	elements		281
	Te	tyana V. Torchynska, Brahim El Filali and Georgiy Polupan	201
	1	Introduction	281
	2	Samples preparation by USP and experimental setups	282
	3 4	Y row diffraction study	204
	4	A-ray diffraction study	200
	5	Photoluminescence study and its temperature dependences	207
	7	High resolution X-ray photoelectron spectra	297
	8	The discussion of defect evolution versus donor doning levels	300
	9	Conclusions	305
		Acknowledgments	306
		References	306
11	Th	e role of dopant on the defect chemistry of metal oxides	313
	Victor Buratto Tinti, Ahsanul Kabir, Daniel Zanetti de Florio		
	an	d Vincenzo Esposito	
	1	Introduction	313
	2	Intrinsic defects	314
	3	Extrinsic defects	316
	4	Ionic conductivity	317
	5	Electronic conductivity	322
	6	Electromechanical properties	327
	7	Summary	342
		Acknowledgments	344
		References	344

12	Viable defect engineering with templates into metal oxides	355	
	Irfan Ayoub, Rishabh Sehgal, Hendrik C. Swart, Rakesh Sehgal, Vishal Sharma and Vijay Kumar		
	2 Different methods for creating defects	357	
	3 Various defects in metal oxides	361	
	4 Defect engineering and electrode materials	368	
	5 Defect engineering for rechargeable batteries	370	
	6 Conclusions	374	
	References	375	
13	Role of defects on the transparent conducting properties of binary		
	metal oxide thin film electrodes	387	
	R. Ramarajan, D. Paul Joseph, K. Thangaraju and M. Kovendhan		
	1 Introduction to defects in transparent conducting oxides	387	
	2 Defects engineering in transparent conducting oxides	389	
	3 Defects mechanism of transparent conducting oxides	391	
	4 Defect dimensions in transparent conducting oxide materials	392	
	5 Theoretical description of defects in transparent conducting oxides	393	
	6 Factors influencing defects formation in transparent conducting		
	oxides	397	
	7 Influence of defects on the properties of a TCO system	402	
	8 Conclusions	413	
	Acknowledgments	414	
	References	414	
14	Intrinsic defect engineering of metal oxides for lighting applications	421	
	Mohan Lal Meena, Sudipta Som, Chung-Hsin Lu, Rajneesh Chaurasiya,		
	Somrita Dutta, Rajan Kumar Singh and Shawn D. Lin	401	
	1 Introduction	421	
	2 Metal oxides, their properties, and corresponding application	422	
	5 Defects in metal oxides	420	
	4 Theoretical aspects of defects in metal oxides	429	
	5 Various inetal oxides and their synthesis 6 Defect dependent properties of metal oxide metaricle	433	
	<ul> <li>Defect-dependent properties of metal oxide materials</li> <li>Characterization methods to identify defects</li> </ul>	430	
	Conclusions	445	
	o Conclusions Poforences	440	
	Keleiclices	440	
15	Oxygen defects in metal oxides and their impact on the	452	
	electrochemical oxidation of short-chain alcohols		
	Isaac velazquez-Hernandez, Lorena Alvarez-Contreras,		
	1 Overview of ovvgen defects in electrosetelysis	152	
	<ol> <li>Overview of oxygen defects in electrocatalysis</li> <li>Dhysicabornistry of oxygen vacancies and defects</li> </ol>	433 151	
	2 rhystochemistry of oxygen vacancies and defects	434	

	3	The role of oxygen defects on oxygen reactions	458
	4	The role of oxygen defects on water splitting	466
	5	The role of oxygen defects on alcohols electrooxidation	469
	6	Molybdenum oxides as cocatalysts during the ethylene glycol electrooxidation reaction	470
	7	Iron oxides as cocatalysts during the ethanol electrooxidation reaction	474
	8	Manganese oxides as cocatalysts during the glycerol	477
	9	Conclusions and remarks References	479 481
16	De	efects engineering in metal oxides for gas sensing and	101
	ele	ectromagnetic wave absorption	491
	We	enjing Du, Xue Zhang, Lili Wu, Zhou Wang, Wei Liu,	
	Jiu	rong Liu and Fenglong Wang	
	1	Introduction	491
	2	Synthetic strategies and characterization methodologies	
		of defected metal oxides	495
	3	Defects engineering in metal oxide for gas sensors	497
	4	Defects engineering in metal oxide for EM wave absorption	513
	5	Conclusions and prospect	521
		References	522
17	O	dered vacancy compounds: the case of the Mangéli phases	
	of	TiO <sub>2</sub>	533
	An Gu	tonio Claudio Michejevs Padilha, Alexandre Reily Rocha and Istavo Martini Dalpian	
	1	Introduction	533
	2	Structural and electronic properties of the Magnéli phases of TiO <sub>2</sub>	536
	3	Band offset	546
	4	Application of Magnéli phases as memristors	551
	5	Calculations details	557
	6	Conclusions	559
		Acknowledgments	560
		References	560
18	Io	n beam-induced defects in ZnO: A radiation hard metal oxide	567
	S.	Pal, A. Mondal, A. Sarkar, S. Chattopadhyay and D. Jana	
	1	Introduction	567
	2	Ion beam-induced processes in solids	568
	3	Irradiation and implantation-induced defects creation and	
		stabilization in ZnO	569
	4	Tuning resistive property via ion bombardment	574
	5	Optical signatures of ion beam-induced defects	579
	6	Irradiation-induced ferromagnetism in ZnO	591

	7	Concluding remarks	594
		Acknowledgments	594
		References	595
19	<b>Role of point defects in gas sensing effects of metal oxides</b> <i>Vinayak Kamble</i>		611
	1	Introduction	611
	2	The chemical stoichiometry and point defects	618
	3	Oxide sensors and their defect studies	622
	4	Summary	630
		Acknowledgments	631
		References	631
		Further reading	634
20	<b>Role of grain boundary defects in nanostructured manganites</b> <i>Keval Gadani, V.G. Shrimali, A.D. Joshi, K. Asokan, N.A. Shah and</i> <i>P.S. Solanki</i>		637
	1	Mixed valent manganites—an overview	637
	2	Role of grain boundary defects in nanostructured manganites	646
	3	Applications of nanostructured manganites	656
	4	Summary and perspectives	659
		References	659
21	De	efects chemistry and catalysis of Indium oxide	665
	Mı	uthu Kumaran Gnanamani and Jothi Ramalingam Rajabathar	
	1	Introduction	665
	2	Structure of indium oxides	667
	3	Methods of defects generation in indium oxide	670
	4	Defects characterization in indium oxide	673
	5	Catalysis of indium oxide	674
	6	Concluding remarks	686
		Acknowledgments	687
		References	687
22	Ef	fect of swift heavy ion irradiation on the electrical characteristics	60.4
	of oxide-based heterojunction		691
	<i>P</i> .	Mallick and P.K. Das	(0.1
	1	Introduction	691
	2	Swift heavy ion irradiation as a unique tool for materials	
	2	engineering	692
	3	Effect of SHI irradiation on the electrical characteristics of	100
	4	oxide-based heterojunction	693
	4	Summary	707
		References	708

### Metal Oxides Series

## **Metal Oxide Defects**

#### Fundamentals, Design, Development and Applications

Metal Oxide Defects: Fundamentals, Design, Development and Applications provides a broad perspective on the development of advanced experimental techniques to study defects and their chemical activity and catalytic reactivity in various metal oxides. This book highlights advances in characterization and analytical techniques to achieve better understanding of a wide range of defects, most importantly, state-of-the-art methodologies for controlling defects. The book provides readers with pathways to apply basic principles and interpret the behavior of metal oxides.

After reviewing characterization and analytical techniques, the book focuses on the relationship of defects to the properties and performance of metal oxides. Finally, there is a review of the methods to control defects and the applications of defect engineering for the design of metal oxides for applications in optoelectronics, energy, sensing, and more. This book is a key reference for materials scientists and engineers, chemists, and physicists.

#### **Key Features**

- Reviews advances in characterization and analytical techniques to understand the behavior of defects in metal oxide materials
- Introduces defect engineering applied to the design of metal oxide materials with desirable properties
- Discusses applications of defect engineering to enhance the performance of materials for a wide range of applications, with an emphasis on optoelectronics

#### About the Editors

Vijay Kumar, Assistant Professor, Department of Physics, National Institute of Technology Srinagar, Jammu and Kashmir, India

Sudipta Som, Postdoctoral Researcher, Department of Chemical Engineering, National Taiwan University, Taiwan

Vishal Sharma, Assistant Professor, Institute of Forensic Science and Criminology, Panjab University, Chandigarh, India

Hendrik C. Swart, Senior Professor, Department of Physics, University of the Free State, Bloemfontein, South Africa



elsevier.com/books-and-journals

