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Editorial for the JECR Special Issue on Electro-Chemo-Mechanics

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Electro-chemo-mechanics is the relationship between electrical, chemical and mechanical properties and the study of adjusting one property through the control of another. This relationship can result in beneficial properties, for instance mixed ionic and electronic conductivity, in oxides, upon oxygen deficiency or lithium insertion (electro-chemo) and/or changes in ionic and electronic mobility observed in strained systems (electro-mechano). This relationship can also be responsible for detrimentally large stresses from non-stoichiometry induced lattice dilation (chemo-mechano). While significant attention has been given to studying the origins and characteristics of electro-chemical relationships – they form the well-know field of electrochemistry - *much less is known regarding the corresponding electro-mechanical, chemo-mechanical, and electro-chemo-mechanical relationships*. Indeed, the typical subject matter for the Journal of Electroceramics is governed by studies of electrical properties controlled through manipulation of material composition.

In this special issue, we have assembled a group of invited and contributed articles which focus on adding the mechanical coupling term. These papers span a wide range of technological applications, including solid oxide fuel cells, Li-ion batteries, piezoelectrics, and capacitors. We have applied the most stringent quality criteria to make sure that only contribution of the utmost quality would be published. Indeed, of the original 45 submissions, only 13were accepted in the end, an acceptance ratio of less than 30%.

An invited review of recent electro-chemo-mechanical coupling studies of ionically conductive ceramics for energy conversion and storage by Swallow et al. starts the special issue [1]. In this paper, materials processing, *in-situ* characterization and computational modeling and simulations are discussed; for example, one key way in which electro-mechanics can be studied is to take advantage of a clamping force on a film induced by a substrate. Following this article, Burbano et al. show that application of a strain in computational simulations on yttria doped ceria (YDZ) leads to a modest enhancement in ionic conductivity [3]. This electromechanical effect is further highlighted in the YSZ thin film conductivity review by Jiang and Hertz where a range of conductivities, differing by as much as four orders of magnitude have been reported, with discussion of the role of film thickness, interfacial effects, and microstructure as well as highlighting the importance of strain characterization of these films [4]. Furthermore, Kossoy et al. point out in their invited paper that small, stress driven changes in point defect arrangements, may lead to inconsistent relationships between in and out of plane lattice constants of acceptor doped ceria thin films – i.e. the effective Poisson's ratio and elastic modulus of these materials is apparently not constant [5]. As a way to locally probe electrochemomechanical effects of thin film and bulk materials, a new technique under development, known as electrochemical strain microscopy (ESM), is discussed in the invited contribution of by Kalinin and Morozovska [6]. Mathematical relationships describing the time dependent bias induced displacements of the material surface are developed to support the ESM technique.

Following this work, Madsen and White discuss a U.S.A. National Science Foundation initiative in the field of Science, Engineering and Education for Sustainability [2]. This paper describes current funding opportunities available in the US to researchers working in the area of ceramic materials and how the structure and composition, coupled with electrical and mechanical properties, are of great importance. One example is the large defect induced expansion, known as chemical expansion, in battery electrodes upon lithiation/de-lithiation with consequent changes in morphology. Song et al. demonstrates a new microstructural method to overcome chemical expansion by using SiN or SiOxNy nanoscale sheaths to retain battery electrode morphology upon the large changes in volume of Si with lithiation and delithiation [7].

Ahn et al. then focuses on the mechano-chemical coupling, demonstrating through computational studies that the energy for oxygen vacancy formation decreases upon isotropic lattice dilation and vice versa for compressive strain in Gd doped ceria, and find that oxygen vacancies prefer to be located near Gd dopant in nearest neighbor positions [8]. Indeed, in an invited paper, Kawada et al. presents a unique measurement demonstrating that compressive stresses applied to bulk ceria drives oxidation, effectively causing the magnitude of defect formation energy to increase [9].

In papers by X. Li et al., E. Markiewicz et al., and Swain and Kumar, the impact of lattice defects on dielectric properties of oxides in ferroelectric materials are discussed [10-12]. The paper by Yang et. al. addresses high voltage Ta oxide capacitors, and demonstrates that degradation at high voltages is related to mechanical stresses created by multiple chemical mechanisms and electrostriction [13].

The guest editors believe that this multi-disciplinary area, combining electrical, chemical, and mechanical properties in a simultaneous fashion, is of rapidly growing interest with many new discoveries to made with the aid of developing novel in situ and in operando measurement techniques and computational methods. The guest editors are extremely grateful to the authors and the reviewers for their invaluable contributions. We also thankful to Prof. Harry Tuller, who gave us the opportunity to act as guest editors of such an exciting special issue, and to the entire editorial team of the Journal of Electroceramics, Dr. Allan Nebres, Ms. Anne Medina and Mr. Michael Luby in particular.

Sean R. Bishop is an Assistant Professor in the International Institute for Carbon Neutral Energy Research (I2CNER) Kyushu University, Japan. He received his PhD (2009) from the Materials Science Department at the University of Florida, USA, for his work on chemical expansion in materials related to solid oxide fuel cells. He continued his work on chemomechanics as a postdoctoral associate at MIT and is continuing to study electrochemomechanical properties of materials for energy and related applications.

Dario Marrocchelli received his PhD (2010) in Chemistry from the University of Edinburgh, UK. From 2010 to 2013 he was a postdoctoral fellow at MIT, USA and Trinity College Dublin, Ireleand. He has now returned to MIT as a Research Scientist. Dario's current research interests are the use of atomistic simulations to study and understand the properties of energy materials.

Brian W. Sheldon is a Professor of Engineering at Brown University, USA. He holds an ScB in Chemical Engineering and an ScD in Materials Science, both from MIT, USA. His research focuses on the formation and mechanical behavior of advanced ceramic materials, particularly those used for energy applications.

Koji Amezawa is a Professor in the Institute of Multidisciplinary Research for Advanced Materials at Tohoku University, Japan. In his research, he develops novel solid state ionic materials to improve performance and reliability of energy conversion devices.

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