Use of XRD and PDF Analysis to Define the Roles of Defects in Electrochemical Charge Storage

Scott T. Misture, Robert J. Koch, Madeleine Flint, Peng Gao and Peter Metz
Kazuo Inamori School of Engineering, Alfred University, Alfred, NY 14802
Contact Author's E-mail Address: misture@alfred.edu

Overall charge storage and cyclic stability are key issues in electrochemical energy storage materials. This work relies on ex-situ and *operando* measurement of x-ray pair-distribution function (PDF) data from microgram quantities of electrochemically active MnO_2 nanosheets to elucidate the effects of intentional Mn 3+ defects on their performance. Our earlier work showed that intentional Mn 3+ defects increase the charge storage by a factor of three and dramatically decrease the charge transfer resistance. Operando studies using the PDF method reveal that the Mn-O coordination environment shows slightly contracting bond lengths with increasing charge state, while electrode charging leads to a decrease in surface Mn 3+ Frenkel defect concentration. Discharging reverses this process, creating more defects. The talk will also highlight the practical aspects of designing the new *operando* cell used for this measurement and challenges in successful execution of *operando* studies on such small sample quantities.