Journal of Energy Chemistry xxx (2018) xxx–xxx

Contents lists available at ScienceDirect

Journal of Energy Chemistry

journal homepage: www.elsevier.com/locate/jechem

http://www.journals.elsevier.com/journal-of-energy-chemistry/

Review

The application of synchrotron X-ray techniques to the study of rechargeable batteries

Q2 Zhengliang Gong[a], Yong Yang[a,b,*]

[a] College of Energy, Xiamen University, Xiamen 361005, Fujian, China
[b] State Key Laboratory for Physical Chemistry of Solid Surface, Department of Chemistry, College of Chemistry and Chemical Engineering, Xiamen University, Xiamen 361005, Fujian, China

ARTICLE INFO

Article history:
Received 29 December 2017
Revised 20 March 2018
Accepted 29 March 2018
Available online xxx

Keywords:
Rechargeable battery
Synchrotron X-ray techniques
X-ray diffraction
X-ray absorption spectroscopy
Pair Distribution Function
X-ray photoelectron spectroscopy

ABSTRACT

The increased use of rechargeable batteries in portable electronic devices and the continuous development of novel applications (e.g. transportation and large scale energy storage), have raised a strong demand for high performance batteries with increased energy density, cycle and calendar life, safety and lower costs. This triggers significant efforts to reveal the fundamental mechanism determining battery performance with the use of advanced analytical techniques. However, the inherently complex characteristics of battery systems make the mechanism analysis sophisticated and difficult. Synchrotron radiation is an advanced collimated light source with high intensity and tunable energies. It has particular advantages in electronic structure and geometric structure (both the short-range and long-range structure) analysis of materials on different length and time scales. In the past decades, synchrotron X-ray techniques have been widely used to understand the fundamental mechanism and guide the technological optimization of batteries. In particular, in situ and operando techniques with high spatial and temporal resolution, enable the nondestructive, real time dynamic investigation of the electrochemical reaction, and lead to significant deep insights into the battery operation mechanism.

This review gives a brief introduction of the application of synchrotron X-ray techniques to the investigation of battery systems. The five widely implicated techniques, including X-ray diffraction (XRD), Pair Distribution Function (PDF), Hard and Soft X-ray absorption spectroscopy (XAS) and X-ray photoelectron spectroscopy (XPS) will be reviewed, with the emphasis on their in situ studies of battery systems during cycling.

Zhengliang Gong received his Ph.D. in physical chemistry from Xiamen University in 2007. After a post-doctoral fellowship at National University of Singapore, in 2010, he has been working at Xiamen University. Currently he is an associate professor at Xiamen University. His main research interests are materials for rechargeable batteries and the electrochemical processes in these systems.

Yong Yang obtained his Ph.D. in Physical Chemistry from Xiamen University in1992. Except for a one-year (1997,1998) academic visit at Oxford University, he has been working in the State Key lab for Physical Chemistry of Solid Surface at Xiamen University since 1992. Now he is a distinguished professor in Chemistry and Director of Research Institute of Electrochemistry and Electrochemical Engineering over there. His main research interests are new electrode/electrolyte materials for Li/Na-ion batteries, in-situ spectroscopic techniques, and interfacial reaction mechanism study in electrochemical energy storage and conversion system. He has published over 200 papers in many international journals such as Nature Energy, Energy & Environmental Science, Advanced Materials and Chem. Mater., etc with citation > 6000 (H-index = 41). He is also one of the Editors for Journal of Power Sources (IF = 6.3). He has obtained several national/international research awards, e.g. Contribution award given by Chinese Electrochemical Society in 2017, Technology Award given by IBA (International Battery Materials Association) in 2014.

Q3 * Corresponding author at: College of Energy, Xiamen University, Xiamen 361005, Fujian, China.
E-mail address: yyang@xmu.edu.cn (Y. Yang).

https://doi.org/10.1016/j.jechem.2018.03.020
2095-4956/© 2018 Published by Elsevier B.V. and Science Press.

1. Introduction

The use of rechargeable batteries (mainly lithium and sodium based rechargeable batteries) to electrical vehicles and grid energy storage in recent years calls for high energy density, greater battery cycle life and safety characteristics [1–3]. To meet the above requirements, significant efforts are being focused on materials modification, developing promising new materials and new chemistry for the next generation of rechargeable batteries. The performance (energy density, cycle/calendar life and safety) and cost of rechargeable batteries is directly linked to electrode materials (composition, structure and morphology, etc.) and their structural evolution during cycling. It is very important to better understanding various composition-structure-performance relationships and the electrochemical reaction mechanisms for battery systems in order to improve their performance and guide the development and application of high-performance new materials [4,5]. However, the battery systems are inherently complex and difficult to understand. This requires systematical and deep investigations from atomic level to macro level in electron structures, crystal structures, microstructures and morphologies, chemical compositions and physical properties of battery materials and their evolution during the charge–discharge processes. Advanced ex situ and in situ characterization techniques have been used widely to clarify scientific and technological problems in rechargeable batteries.

Since the early work by Mcbreen et al. around 25 years ago [6], synchrotron X-ray techniques have been widely used to understand the fundamental mechanism and guide the technological optimization of batteries [7–11]. The merits of synchrotron X-rays, such as high brightness (10^5–10^{12} more intense than that from the laboratory sources), highly collimated and energy tunable, align itself perfectly to applications in battery science and technology. The tunability of X-ray energies allows the conduct of experiments which require a scan of the beam energy (e.g. XAS). It also allows the optimization of the experiments to improve the quality of data via optimizing the beam energy (e.g., eliminating fluorescence artifacts during XRD analysis). The highly-collimated and variable focus synchrotron beam allows high spatial resolution spectroscopic mapping (point-by-point measurement) and imaging of electrodes. With increasing sophisticated synchrotron techniques, it also allows the conduct of high temporal resolution (up to milliseconds) studies of the electrochemical/chemical reaction. In particular, the ultrahigh intense and penetration ability of synchrotron X-rays make the in situ and operando investigation of battery systems possible and easier to realize. Compared to ex situ measurements, in situ and operando techniques can provide direct information on the system in a nonequilibrium state, allowing a truer visualization of what is happening during the electrochemical reduction and oxidation processes. Fig. 1 illustrates the applications of common synchrotron X-ray techniques to the study of rechargeable batteries.

This paper reviews the latest developments in the application of synchrotron X-ray techniques, especially their electrochemical in situ techniques to the studies of battery materials and related electrochemical reaction mechanisms. Since a comprehensive review of the field has recently been provided by Lin et al. [10], this paper will focus on the unique advantages and achievements of synchrotron X-ray techniques for effectively providing structural and chemical evolution information about commercially and/or fundamentally important electrode materials and their interfaces, and

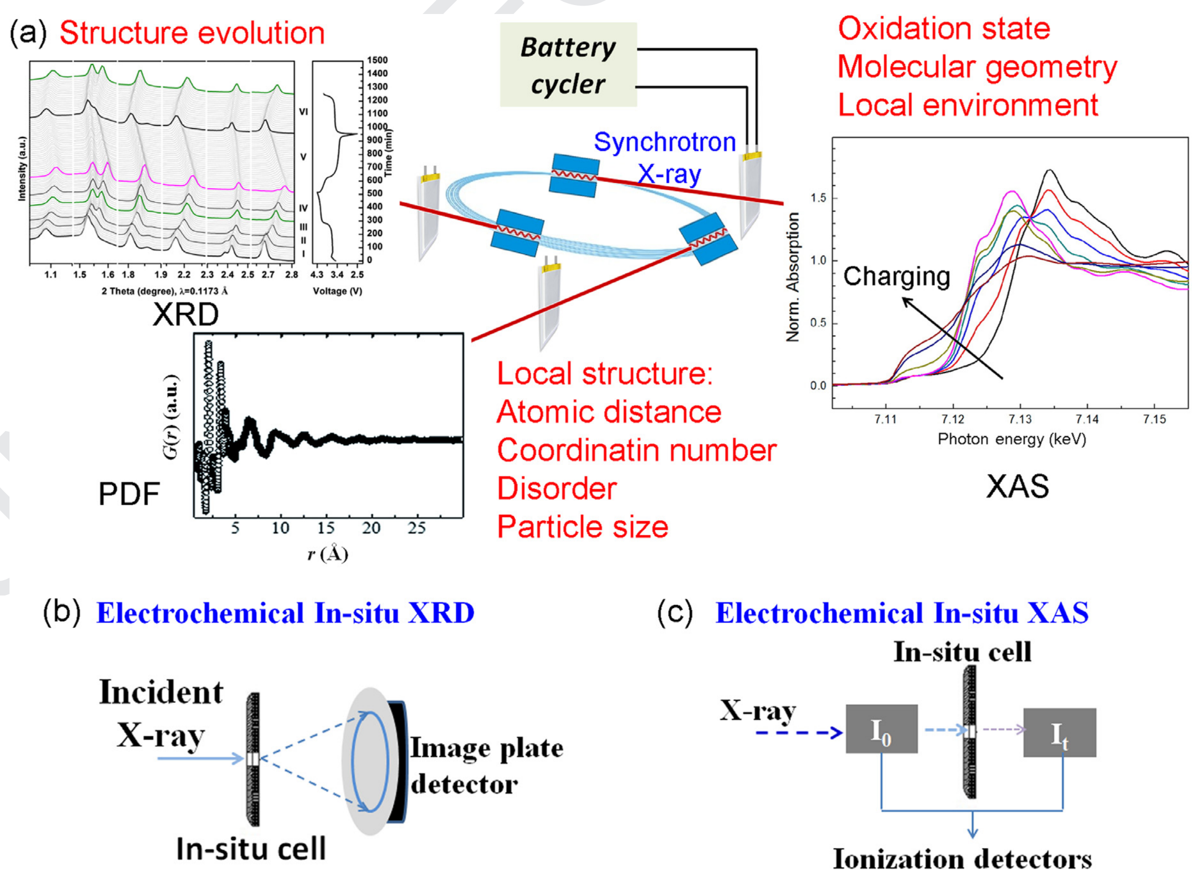

Fig. 1. (a) Common synchrotron X-ray techniques and their applications in battery researches, (b) schematic diagram of the electrochemical in situ XRD, (c) schematic diagram of the electrochemical in situ XAS. Adapted from Ref. [90] and [120] with permission from The Royal Society of Chemistry, and Ref. [153] with permission from American Chemical Society.

Please cite this article as: Z. Gong, Y. Yang, The application of synchrotron X-ray techniques to the study of rechargeable batteries, Journal of Energy Chemistry (2018), https://doi.org/10.1016/j.jechem.2018.03.020