#### University of Wollongong

### **Research Online**

Faculty of Engineering and Information Sciences - Papers: Part A

Faculty of Engineering and Information Sciences

1-1-2014

# In-situ synchrotron diffraction study of the phase evolution of the novel $Na_x(Fe_{1/2}Mn_{1/2})O_2$ cathode for use in sodium-ion batteries

Wei Kong Pang University of Wollongong, wkpang@uow.edu.au

Sujith Kalluri University of Wollongong, sk027@uowmail.edu.au

Vanessa K. Peterson Australian Nuclear Science and Technology Organisation, vep@ansto.gov.au

Neeraj Sharma University of New South Wales, n.sharma@ansto.gov.au

Hua-Kun Liu University of Wollongong, hua@uow.edu.au

See next page for additional authors

Follow this and additional works at: https://ro.uow.edu.au/eispapers

Part of the Engineering Commons, and the Science and Technology Studies Commons

#### **Recommended Citation**

Pang, Wei Kong; Kalluri, Sujith; Peterson, Vanessa K.; Sharma, Neeraj; Liu, Hua-Kun; Dou, Shi Xue; and Guo, Zhenyan, "In-situ synchrotron diffraction study of the phase evolution of the novel Na<sub>x</sub>(Fe<sub>1/2</sub>Mn<sub>1/2</sub>)O<sub>2</sub> cathode for use in sodium-ion batteries" (2014). *Faculty of Engineering and Information Sciences - Papers: Part A*. 6622.

https://ro.uow.edu.au/eispapers/6622

Research Online is the open access institutional repository for the University of Wollongong. For further information contact the UOW Library: research-pubs@uow.edu.au

## In-situ synchrotron diffraction study of the phase evolution of the novel $Na_x(Fe_{1/2}Mn_{1/2})O_2$ cathode for use in sodium-ion batteries

#### Abstract

Abstract of a poster presentation at the 5th Australia-China Conference on Science, Technology and Eduction with the 5th Australia-China Symposium for Materials Science, at the University of Wollongong (UOW), Australia, on 21st - 23rd July 2014.

#### Disciplines

Engineering | Science and Technology Studies

#### **Publication Details**

Pang, W. Kong., Kalluri, S., Peterson, V. K., Sharma, N., Liu, H., Dou, S. X. & Guo, Z. (2014). In-situ synchrotron diffraction study of the phase evolution of the novel  $Na_x(Fe_{1/2}Mn_{1/2})O_2$  cathode for use in sodium-ion batteries. 5th Australia-China Conference on Science, Technology and Education with the 5th Australia-China Symposium for Materials Science (ACSMS) (pp. 72-72). Australia: University of Wollongong.

#### Authors

Wei Kong Pang, Sujith Kalluri, Vanessa K. Peterson, Neeraj Sharma, Hua-Kun Liu, Shi Xue Dou, and Zhenyan Guo

efforts have been put into oil-water separation materials, no effective devices have been fabricated to date, mainly because the materials are easily blocked and then cease to work. Herein, a novel device has been designed, based on the use of a special mesh that can properly deal with the spilled oils. In detail, ultrathin  $Co_3O_4$  nanosheets are grown onto the stainless steel mesh by a hydrothermal method. The obtained  $Co_3O_4$ -coated mesh shows superhydrophilic and underwater superoleophobic properties. When wetted by water, the mesh also exhibits high water permeability and oil impermeability. By installing the wet mesh on a ship model with a certain inclination angle and moving it along the oil-water interface, the water flow can easily pass through the bottom of the mesh, while the oil flow can be blocked and driven upward along the mesh to a rotating temporary storage facility with another separation mesh fixed at the bottom by which can realize rapid purification. Such a novel device can effectively "shovel" the oil layer off the water surface and efficiently purify the oil. It may find wide application in the near future to deal with various oil spills happened in the sea environment.

### PSMS03 Wei Kong Pang "Operando neutron powder diffraction studies of batteries on WOMBAT"

Neutron powder diffraction (NPD) is a non-destructive method increasingly being used in the studies of the structural and phase evolution of electrode materials within batteries during electrochemical cycling. In particular, the sensitivity of NPD to lighter elements Li, O, and Na, in the presence of other heavier atoms, enables the direct measurement of the charge-carrier location and content within electrodes at the same time as redox-active couples are determined by tracking the transition-metal valence via the oxygen to transition-metal distance in the oxide electrodes, i.e. commercial Li(Ni<sub>1/3</sub>Mn<sub>1/3</sub>Co<sub>1/3</sub>)O<sub>2</sub>, high-voltage LiNi<sub>0.5</sub>Mn<sub>1.5</sub>O<sub>4</sub> cathode, and zero-strain Li<sub>4</sub>Ti<sub>5</sub>O<sub>12</sub> anode.NPD allows to probe in real-time the bulk crystallographic changes of electrodes in functioning batteries, opening the way for exciting new in-operando studies. Ultimately, operando NPD can be used to "track" not only the reaction mechanism and lattice parameter evolution, but also the details of the charge-carrier insertion/extraction process in electrode materials. WOMBAT, a high-intensity neutron powder diffractometer at the OPAL research reactor at ANSTO allows rapid collection of data and is used widely for operando studies of Li-ion batteries. We report an overview of the approach and technique taken on WOMBAT to obtain operando NPD data of Li-ion batteries with sufficient information to extract detail of the Li-ion insertion/extraction mechanism.

## PSMS04 Wei Kong Pang "In-situ synchrotron diffraction study of the phase evolution of the novel $Na_x(Fe_{1/2}Mn_{1/2})O_2$ cathode for use in sodium-ion batteries"

Sodium-ion batteries are considered one of the best alternatives to lithium-ion battery technology, due to their similar electrochemistry, potentially non-toxicity, and the greater elemental abundance of sodium leading to low-cost. However, there remains concern regarding the optimization of sodium-based electrode materials for capacity and energy performance, as well as structural and electrochemical stability. This work presents the promising P2-type  $Na_{2/3}(Fe_{1/2}Mn_{1/2})O_2$  cathode material for use as a cathode in sodium-ion batteries. We prepare  $Na_{2/3}(Fe_{1/2}Mn_{1/2})O_2$  via a facile single-step sol-gel method, with the nano-sized powders obtained delivering an initial discharge capacity of ~ 175 mAh.g<sup>-1</sup> with an average working potential of 3 V and a moderate capacity retention of 64.0% over 80 cycles at 0.1 C. We use in-situ synchrotron X-ray diffraction to explore the sodiation/ desodiation mechanism and establish the structure-function relation of the  $Na_{2/3}(Fe_{1/2}Mn_{1/2})O_2$  cathode in a functioning cell. This work reveals that  $Na_{2/3}(Fe_{1/2}Mn_{1/2})O_2$  sodiation/desodiation proceeds through a solid-solution reaction involving a relatively minor (0.27%) volume change where the c lattice parameter increases during charging and decreases during discharging, with the opposite behavior found for the a lattice parameter. Overall, this mechanistic understanding will be useful to rationally improve the related family of sodium-based cathode materials.