MS19-P5 X-ray Scattering Analysis of the Morphology of TiO_2 (B) Nanoparticles

Xiao Hua[1,2], Zheng Liu[3], Peter G. Bruce[4], Clare P. Grey[1]

1. University of Cambridge
2. Adolphe Merkle Institute
3. University of St. Andrews
4. University of Oxford

email: xiaohua716@gmail.com

The morphological characteristics of a nanomaterial, *i.e.*, geometric shape and dimension, and the arrangement of atoms, which both vary depending on specific nanostructures, have a considerable impact on properties such as electronic structure, ionic diffusion, and surface structure. It is, therefore, essential to determine the nanomorphology of the electrode materials so as to link shape with the electrochemical performance.

Conventional microscopy methods used to characterize the morphology of nanomaterials sometimes involve practical challenges arising from the aggregation of nanoscopic structure. In order to determine the morphology of a TiO_2 (B) nanoparticle sample that shows excellent electrochemical performance[1,2], we have performed a comprehensive X-ray scattering analysis of SAXS, PDF and XRPD data. The scattering pattern within a particular angular range encodes distinct structural features of the materials ranging from mesoscale to nanoscale. The combination of small- and wide-angle measurements therefore covers a full angular range that enables us to access a complete set of morphological and structural characteristics including size and shape via SAXS, particle asymmetry and long-range structure via XRPD, and short-range atomic ordering via PDF.

From the analyses, we conclude that the particles are oblate-shaped, contracted along the [010] direction[3]. This particular morphology provides not only a plausible rationale for the excellent electrochemical behavior of these TiO_2 (B) nanoparticles, but also a structural foundation to model the strain-driven distortion induced by lithiation. A more complex displacement model incorporating this lithiation-induced strain was developed making use of the oblate particle model. It clearly shows the importance of determining the morphology of the nanoparticle so as to understand the lithiation mechanism and rationalize the rate performance of nanostructured materials.

Reference:

[1] Ren, Y.; Liu, Z.; Pourpoint, F.; Armstrong, A. R.; Grey, C. P.; Bruce, P. G. Angew. Chem. Int. Ed. 51 (2012) 2164-2167.

[2] Andreev, Y. G.; Panchmatia, P. M.; Liu, Z.; Parker, S. C.; Islam, M. S.; Bruce, P. G. J. Am. Chem. Soc. 136 (2014) 6306-6312.

[3] Hua, X.; Liu, Z.; Bruce, P. G.; Grey, C. P. J. Am. Chem. Soc. 137 (2015) 13612-13623.

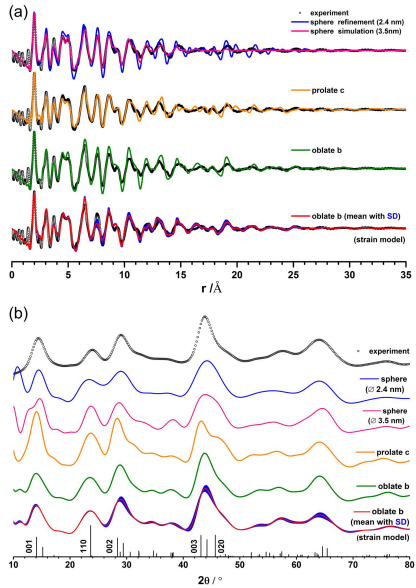

Figure 1. Comparison of (a) PDF and (b) XPRD data for the fully lithiated TiO_2 (B) nanoparticles between experiment and simulations using the PDF refined spherical, prolate c, oblate b, and the oblate b strain model averaged over 20 particles.

Keywords: PDF, SAXS, XRD, nanomaterials, batteries