High Contrast Annular STEM Imaging for Light Elements by a Segmented Detector

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Direct imaging of light element atoms in energy storage materials such as lithium-baring materials is becoming very important for understanding the carrier ion dynamics during the cell reactions. For this purpose, annular bright field (ABF) imaging technique in the scanning transmission electron microscopy (STEM) is now widely used[1]. ABF STEM can robustly visualize light element atoms (even hydrogen atomic columns[2,3]) by using an annular detector in the bright field disk region, but this method may have a limitation for being applied to beam sensitive materials. Though lower accelerating voltage and lower electron dose conditions are necessary to avoid electron irradiation damages, lower accelerating voltage may worsen the contrast of ABF images[4], and lower dose may lead to lower signal-to-noise ratio. The detector geometry of ABF is typically set for the condition where the detector angle is 0.5a-a (a is the convergence semi-angle of electron beam), but there may be a possibility to improve the contrast of ABF imaging by considering different detector geometries.

In this research, a segmented detector was used to reconsider the detector geometries of ABF for observing atomic columns of ultra-light elements such as lithium. The segmented detector has four annular segments as shown in Figure 1 (detector angles are 0-0.25a, 0.25a-0.5a, 0.5a-0.75a, 0.75a-a and called as Layer1-4 respectively), and we can obtain four atomic-resolution images simultaneously with each annular detector geometry[5]. Firstly, to investigate the imaging properties of each annular detector geometry, phase contrast transfer functions (PCTFs) under weak phase object approximation (WPOA) were calculated. However, the electron propagation in specimens should be taken into account because the depth of field is comparable or shorter than a typical thickness of specimens under the condition of an aberration-corrected STEM. In this study, we employed a new type of PCTF (integrated PCTF: iPCTF), which is calculated by the summation of PCTF for each atomic slice to include the effect of finite specimen thickness. Then, we conducted multi-slice simulations and STEM observations for Li_2MnO_3 [001] zone-axis in an accelerating voltage of 120 kV in comparison with the results of iPCTF.

Through the calculation of iPCTF, it was suggested that the Layer4 (detector angle is 0.75a-a) image gives higher contrast than the ordinal ABF image, and the Layer3 image (detector angle is 0.5a-0.75a) may not properly transfer true atomic structure information. These results were agreed with the multi-slice simulations and the experiments as shown in Figure 2. Details will be discussed in the presentation.

[1] S.D. Findlay *et al.*, *Applied Physics Letters*, 2009, **95**, 5.

[2] S.D. Findlay *et al.*, *Applied Physics Express*, 2010, **3**, 1.

[3] R. Ishikawa *et al.*, *Nature Materials*, 2011, **10**, 278.

[4] S.D. Findlay *et al.*, *Ultramicroscopy*, 2011, **111**, 1144.

[5] N. Shibata *et al.*, *Journal of Electron Microscopy*, 2010, **59**, 473.

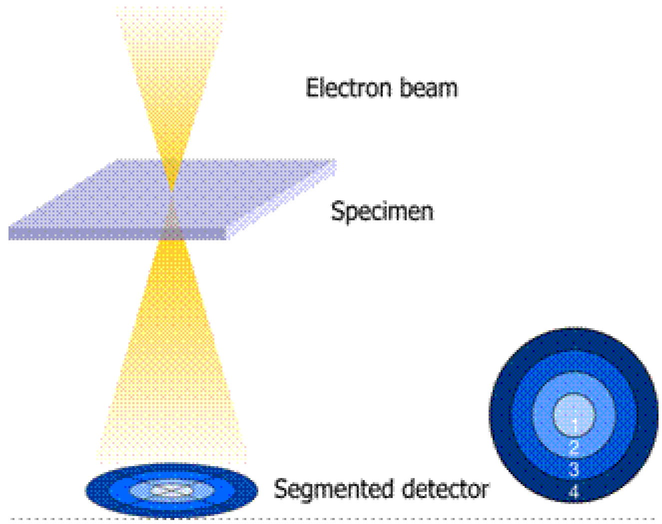

Figure 1: Schematic illustration of STEM optical system with a segmented detector and its annular segments

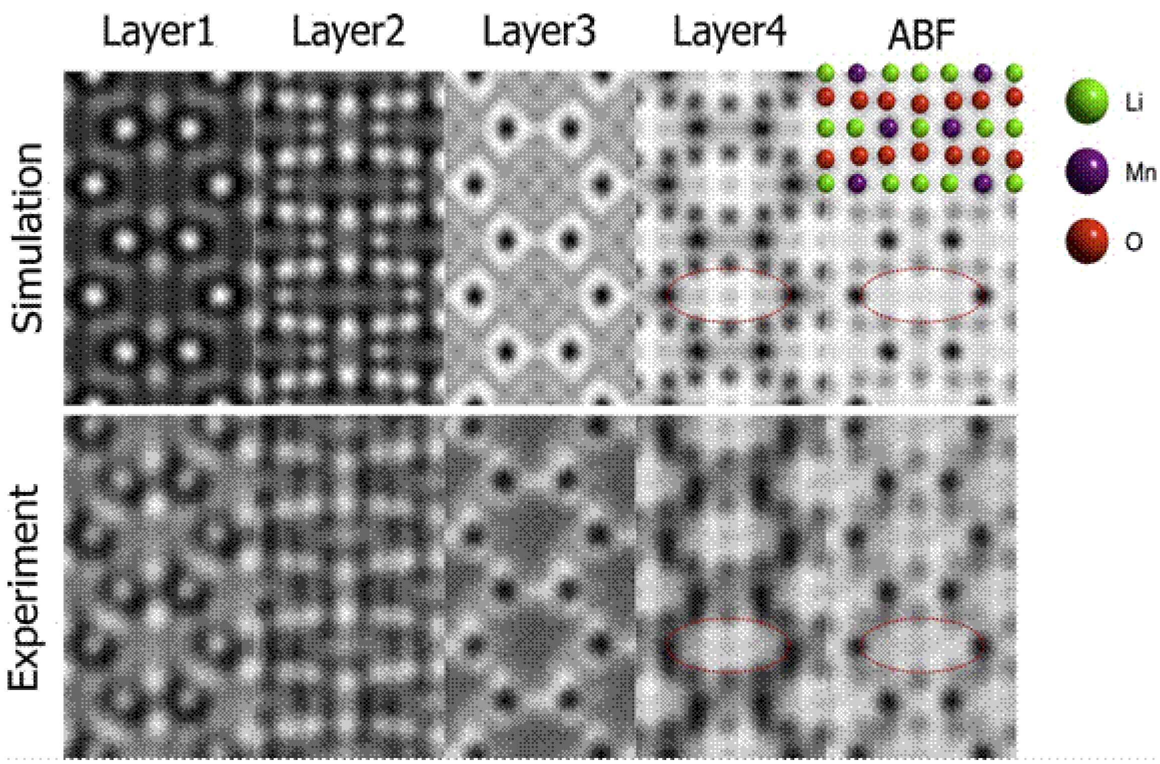

Figure 2: Simulated images of Layer1-4 and ordinal ABF images using multi-slice method, and the corresponding experimental STEM images of Li_2MnO_3 observed from [001] direction. Green, purple and red balls indicate lithium, manganese and oxygen columns, respectively. Ellipses with red dashed lines in the Layer4 and ABF images highlight the area where there are three lithium atomic columns.