

Studying the Atomic Structures by Aberration-Corrected and Conventional Electron Microscopy

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Image resolution is mainly limited by the spherical aberration (Cs) of the objective lens. There are two effective approaches to correct the Cs. One is the hardware aberration correction, so-called Cs-corrector [1]. The other is software method including electron crystallographic image processing [2-4] and exit wave reconstruction [5,6]. With a Cs-corrector, the image resolution can be extended to sub-angstrom level such that oxygen atoms can be relatively easily detected by the negative Cs imaging technique [7] and lithium atoms identified by annular-bright-field (ABF) image [8]. By software method, the light atoms such as lithium [9], were directly resolved from HRTEM images by the exit wave reconstruction. Using two-stage electron crystallographic image processing [4]—image deconvolution and phase extension the light atoms as oxygen and boron atoms [10] have been resolved from a single image.

In the present paper, we will show the results in atomic-scale structure investigations using the software and hardware aberration correction, respectively. For software correction, we take advantage of the two-stage image processing technique, using the iron-based superconductor $\text{SmFeAsO}_{0.85}\text{F}_{0.15}$ as an example, to improve the image resolution. Compared with other method in HRTEM, the approach used here only need one image collected at arbitrary defocus value rather than a series of through focus images. Image deconvolution as a special kind of image processing in HRTEM is used to restore the image distortion due to the lens aberrations. More accurately, it aims at transforming an image not representing the crystal structure intuitively into the structure projection, the resolution of which is limited by the information limit of the microscope. Electron diffraction unrestricted by lens aberrations could overcome this resolution limit. The reachable image resolution is better than 1Å using a combination of the electron diffraction and the image deconvolution. By this approach, the atomic columns of O and considerably heavier Sm at a very close distance (1.17Å) in $\text{SmFeAsO}_{0.85}\text{F}_{0.15}$ are simultaneously revealed from a single image taken with a conventional 200 kV electron microscope [11]. It is for the first time that the O atoms adjacent to the heavier atoms at a so close distance are imaged by this approach. In addition, we will report three different types of interlocked ferroelectric-antiphase DWs and two abnormal topological four-state vortex-like domain patterns at the atomic level in multiferroic manganite YMnO_3 by using the hardware correction method, i.e. the CS-corrected high angle annular dark field scanning transmission electron microscope (HAADF-STEM) imaging techniques. Recently, Cs-corrected electron microscopy, especially the STEM technique has been widely used to provide high-resolution structural information. Unlike that of conventional HRTEM images, the contrast of HAADF-STEM images is roughly proportional to $Z^{1.7}$, where Z is the atomic number. And it is rarely affected by a small variation of the specimen thickness. Using this imaging technique, three different types of ferroelectric-antiphase DWs with a translation vector (i.e., $1/6[210]$ or $-1/6[210]$) are observed at atomic level. Then the configurations of the two abnormal topological four-state vortex-like domains with different DWs are directly determined at the

first time, which are different from the traditional four-state vortex domain caused by edge dislocations[12]. [13]

References:

- [1] M. Haider, G. Braunshausen and E. Schwan, *Optik* **99** (1995), p.167.
- [2] F.H. Li, *Phys Status Solidi A* **207** (2010) p.2639.
- [3] L. De Caro *et al*, *Nat. Nano.* **5** (2010), p. 36.
- [4] W. Wan, S. Hovmöller and X.D. Zou, *Ultramicroscopy* **115** (2012), p.60.
- [5] M. OpdeBeeck, D. VanDyck, *Ultramicroscopy* **64** (1996), p.153.
- [6] J.H. Chen, H.W. Zandbergen and D. VanDyck, *Ultramicroscopy* **98** (2004), p.81.
- [7] C.L. Jia, M. Lentzen and K. Urban, *Science* **299** (2003), p.870.
- [8] Y. Sun *et al*, *Nat. Commun.* **4** (2013), p.1870.
- [9] Y. Shao-Horn *et al*, *Nat. Mater.* **2** (2003), p.464.
- [10] H.B. Wang *et al*, *Acta Cryst. A* **58** (2002), p.494.
- [11] Y.M. Wang, B. H. Ge and G. Che, *Micron* **71** (2015), p.32.
- [12] L. Tian *et al*, *APL* **106** (2015), p.112903.
- [13] The author acknowledge funding from the National Natural Science Foundation of China (Grant No. 11474329).

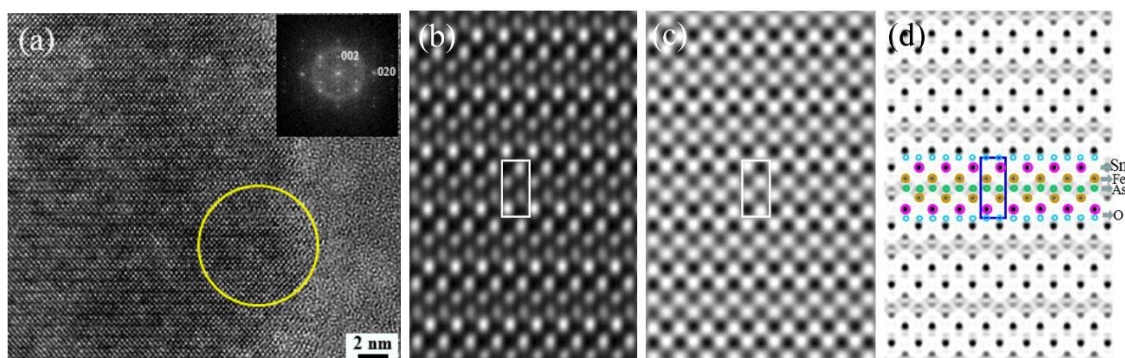


Figure 1. (a)[100] zone-axis HRTEM image, (b) and (c) Fourier filtering image and deconvoluted image, (d)

structure projection after phase extension in combination with the diffraction intensity correction.

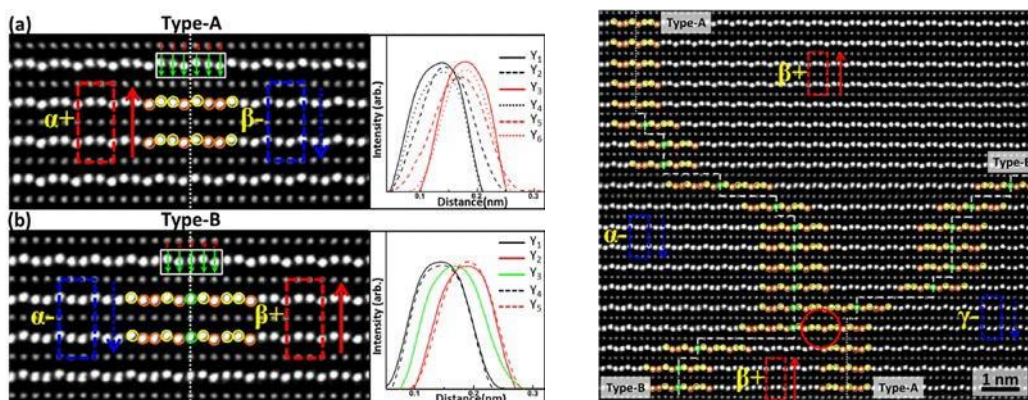


Figure 2. HADDF-STEM images for (a) Type-A, (b) Type-B interlocked ferroelectric DWs along [010] direction, and (c) for the four-state vortex-like domain.