

# Quantitative Image Simulation for Scanning Transmission Electron Microscopy

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Aberration correction of electron microscope optics has led to routine imaging at a resolution of an Ångström, or less. For the scanning transmission electron microscope (STEM), this has led not only to higher resolution, but also greater image contrast. There is however a significant difference between the experimentally measured contrast and that predicted by simulation. Such a discrepancy has been shown to be present for annular dark field (ADF), bright field (BF) and even electron energy loss spectroscopy (EELS) images [1]. This is analogous to the so called Stobbs factor observed in high resolution transmission electron microscopy [2].

The reduced contrast in experimental ADF images has been observed to manifest itself as an additional background, for instance in the case of interfaces, for example  $\text{PbTiO}_3/\text{SrTiO}_3$  [3]. Alternatively, the reduction in contrast can also be modeled by convolving the simulation with a suitable Gaussian, which may describe blurring due to spatial and temporal coherence or environmental instabilities [4]. For truly quantitative comparison of experiment and theory it is essential that both the variation in image intensity and the background are measured on a physically meaningful scale, in other words the true black level of experimental images must be known.

In order to examine the sources of this “Stobbs-like” factor we use a  $\text{LaMnO}_3/\text{SrTiO}_3$  interface and simultaneously acquire ADF and BF images. Both ADF and BF images acquired using ORNL’s aberration corrected VG HB603U STEM are shown in Fig. 1. The black level of each image has been determined and subtracted from the raw experimental data. In the ADF image the La columns are clearly seen as the brightest feature. On the BF image, both the La and Sr columns appear black due to contrast reversal. Line scans (averaged over a width of three pixels) are shown in Fig. 2. For the ADF line profile the  $\text{LaMnO}_3$  has both the greatest contrast and an obviously higher background than the  $\text{SrTiO}_3$  side of the interface. The BF image has strong peaking on the O columns but still has maximum contrast on the  $\text{LaMnO}_3$  side of the interface. The  $\text{SrTiO}_3$  side of the interface however now has the larger background.

Clearly, it is essential that any simulation of the experimental images be able to describe the behavior of both the ADF and BF images across the interface. The formation of contrast in BF images is more complex than that of ADF images (for ADF the atoms are always white), and the determination of specimen thickness and absolute defocus becomes an issue. We will discuss the formation of image contrast in both ADF and BF STEM images and compare different approaches to quantitatively matching experimental results [5].

## References

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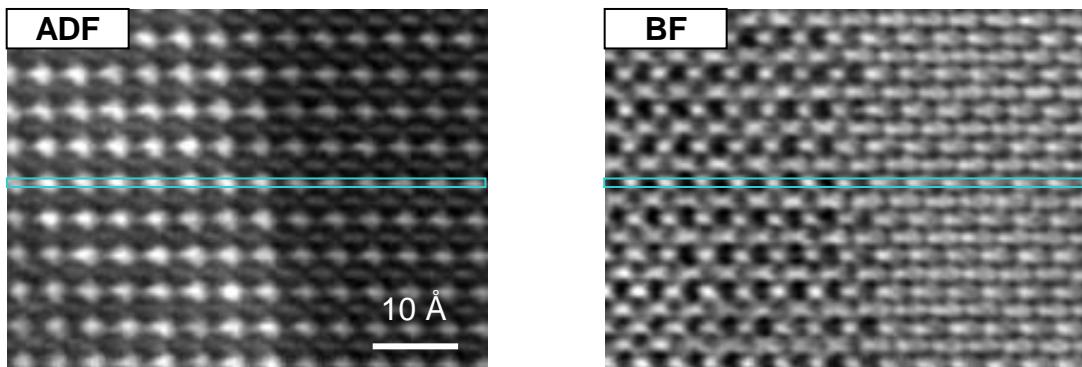


FIG. 1. Simultaneously acquired ADF and BF STEM images of a  $\text{LaMnO}_3/\text{SrTiO}_3$  interface. Images are part of a focal series acquired using ORNL's aberration corrected 300 kV VG HB603U.

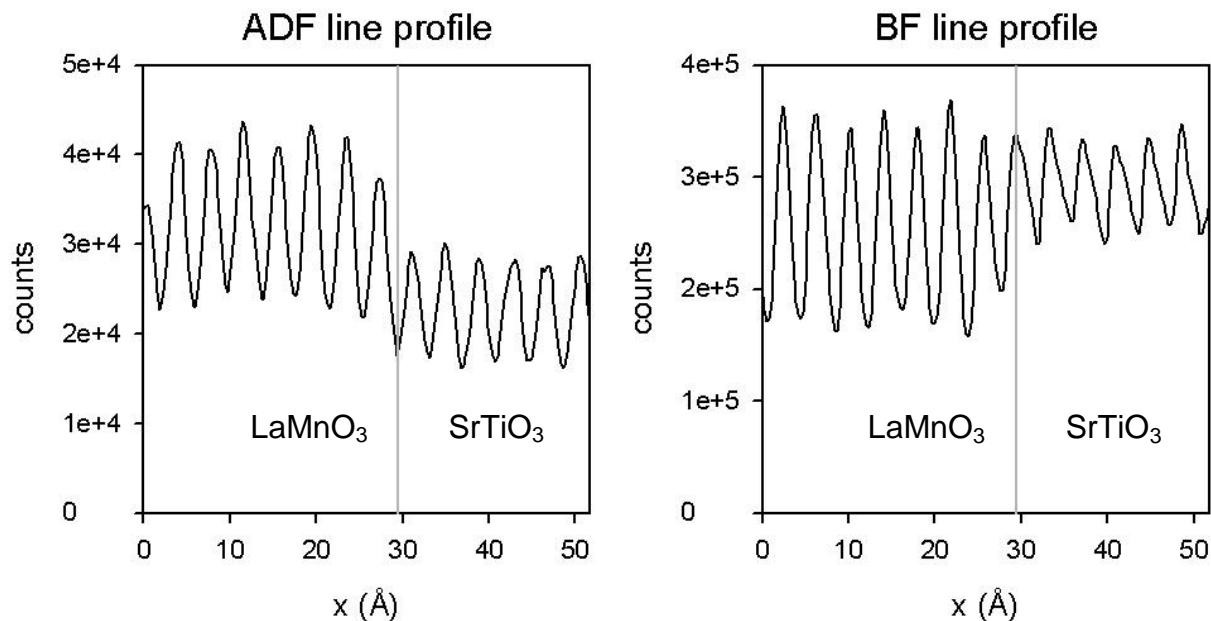


FIG. 2. Line scans across the  $\text{LaMnO}_3/\text{SrTiO}_3$  interface averaged over a width of three pixels as indicated by the blue rectangles in Fig. 1. The vertical grey line is an indication of the position of the interface.