

Quantitative Imaging Analysis Using the Aberration Corrected Scanning Transmission Electron Microscope (Hitachi HD2700C)

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The first Hitachi aberration corrected scanning transmission electron microscope (HD2700C STEM) was successfully installed at CFN. The instrument has a cold-field-emission electron source with high brightness and small energy spread.¹ The excellent electro-optical design and aberration correction make the instrument ideal for atomically resolved STEM (Z-contrast) imaging and electron energy loss spectroscopy (EELS). In our presentation we will show the capabilities of the new microscope.

Research Achievement

We have utilized the instrument to study various energy related materials ranging from superconducting and thermoelectric materials to core-shell nano-electrocatalysts. Although aberration correction improves spatial resolution of the instrument, it does not make image interpretation easier due to the large convergent angles used to gain beam current. To understand the image contrast, we developed our own computer codes based on the multislice method with frozen phonon approximation to calculate annular-dark-field (ADF) images. Figs.1 compare experiment with calculation of SrTiO₃ in (001) projection, showing very good agreement. Our study demonstrates that the ADF image contrast (or Z-contrast) does not follow the simple $I \sim Z^2$ or $I \sim Z^{1.8}$ power rule as many expect.² Although an ADF image indeed shows Z-dependence contrast, only under very high collection angles (i.e. in a true HAADF mode) it yields strong intensity in high Z atom columns and weak intensity in low Z. The image intensity also strongly depends on sample thickness as well as dynamic and static lattice displacement of the atomic species. To correctly interpret the ADF intensity in STEM images, the effect of atomic thermal vibration (Debye-Waller factor) of the atoms must be taken into account. Even at large collection angles the power law Z-dependence is only valid for very thin specimen.³

Future Work

Our goal is to conduct STEM experiment and retrieve quantitative crystal, chemical and electronic information of the materials under study at atomic resolution. We have been working on single atom imaging and spectroscopy to further test and push the resolution limit of the instrument. We also plan to combine STEM with SEM using second and back-scattered electrons to retrieve surface structural information. The ability to image surface and bulk structure simultaneously at atomic resolution will revolutionize the field of microscopy and better serve the scientific needs of our user community.⁴

References and Publications

- 1 Y. Zhu, and J. Wall, chapter in: *Aberration-corrected electron microscopy, a thematic volume of advances in imaging & electron physics*, ed. Hawkes P W, (Elsevier/Academic Press). pp. 481-523 (2008)
- 2 S.J. Pennycook "Z-contrast transmission electron microscopy – direct atomic imaging of materials". *Annu. Rev. Mater. Sci.* **22**: 171 (1992).
- 3 H. Inada, L. Wu, J. Wall, D. Su, and Y. Zhu, *Journal of Electron Microscopy*, June issue, (2009).
- 4 Work supported by the U.S. DOE, Office of Basic Energy Science, under Contracts No. DE-AC02-98CH10886.

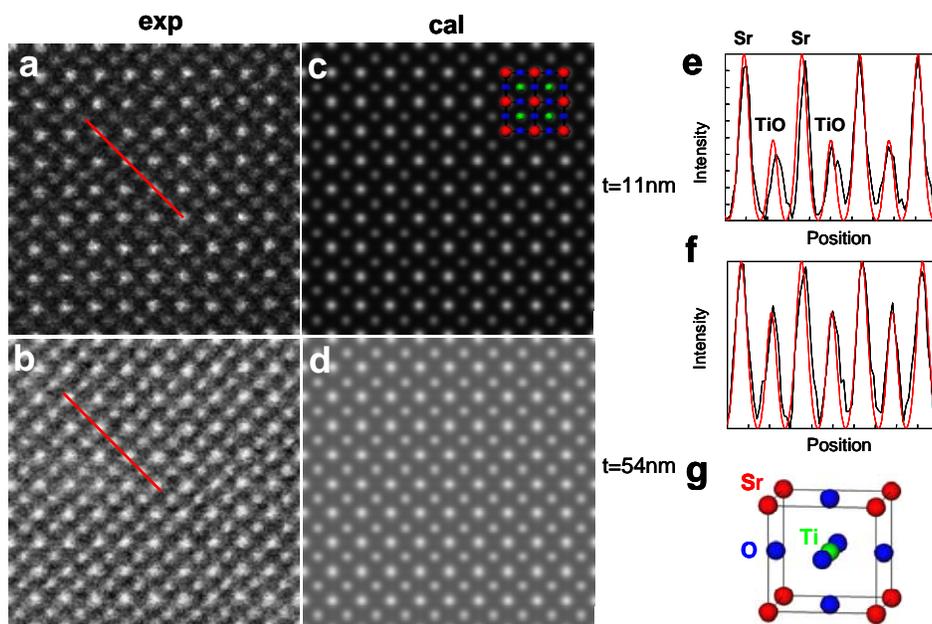


Fig.1 (a-b) Experimental images with convergent angle $\alpha=27$ mrad and collection angle $\beta=64$ -341 mrad (a) in thin area, and (b) in thick area. (c-d) Simulated images with (a) thickness=11 nm, and (d) thickness=54 nm, in the image condition of $\alpha=27$ mrad and $\beta=64$ -341 mrad. The simulated images are convoluted with a Gaussian point spread function (HMF_W=0.09nm). (e-f) Intensity profiles from (a)-(d) with black lines from experiments and red lines from calculations. (g) The crystal model of SrTiO₃ where blue dots represent Sr, green dots represent Ti and yellow dots represent O.

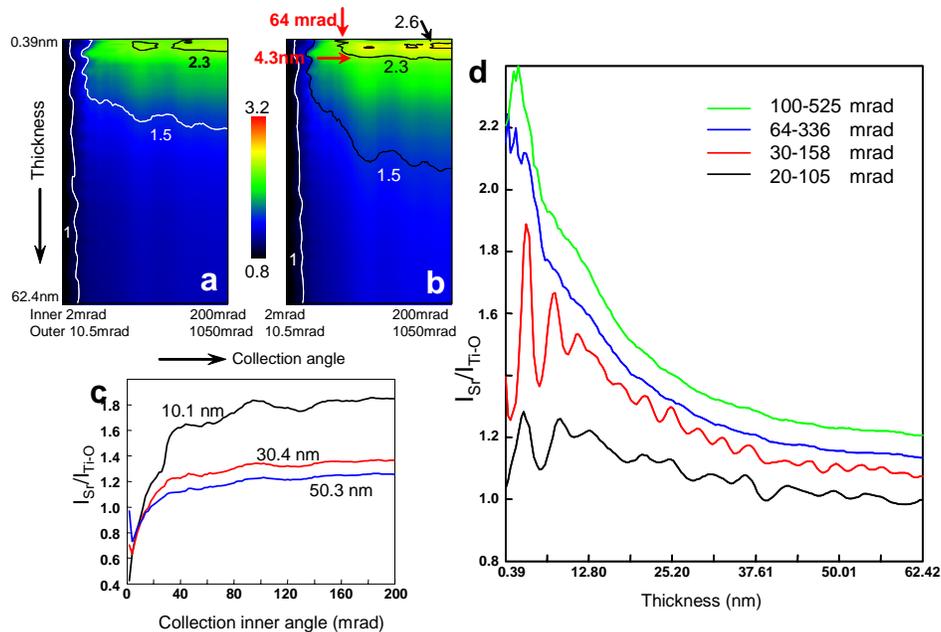


Fig. 2 (a) Intensity ratio I_{Sr}/I_{TiO} with the collection angle increasing from left to right and thickness from top to bottom (Debye-Waller factors $B_{Sr}=0.6214$, $B_{Ti}=0.4398$ and $B_{O}=0.7323$). (b) Intensity ratio I_{Sr}/I_{TiO} with $B_{Sr}=B_{Ti}=B_{O}=0.5$. The area with collection angle ≥ 64 mrad and thickness ≤ 4.3 nm is considered to comply with a power law Z-dependence (Z^n) with n ranging from 1.77 to 2, as outlined by the intensity contour (>2.6). (c) Intensity ratio profiles of collection angle with thickness being 10.1, 30.4 and 50.3 nm. (d) Intensity ratio profiles of thickness with inner collection angle being 20, 30, 64 and 100 mrad (for details, see ref 3).

