Statistical modeling of scanning transmission electron microscopy images of crystal interfaces with atomic resolution

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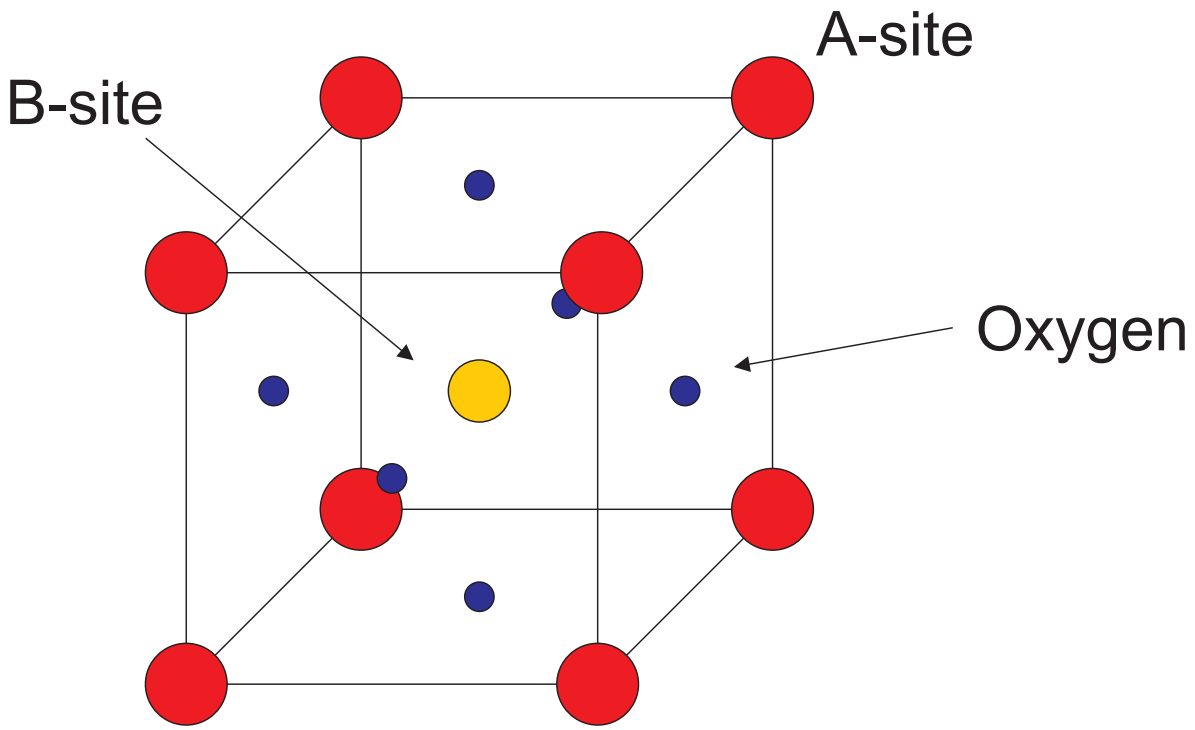
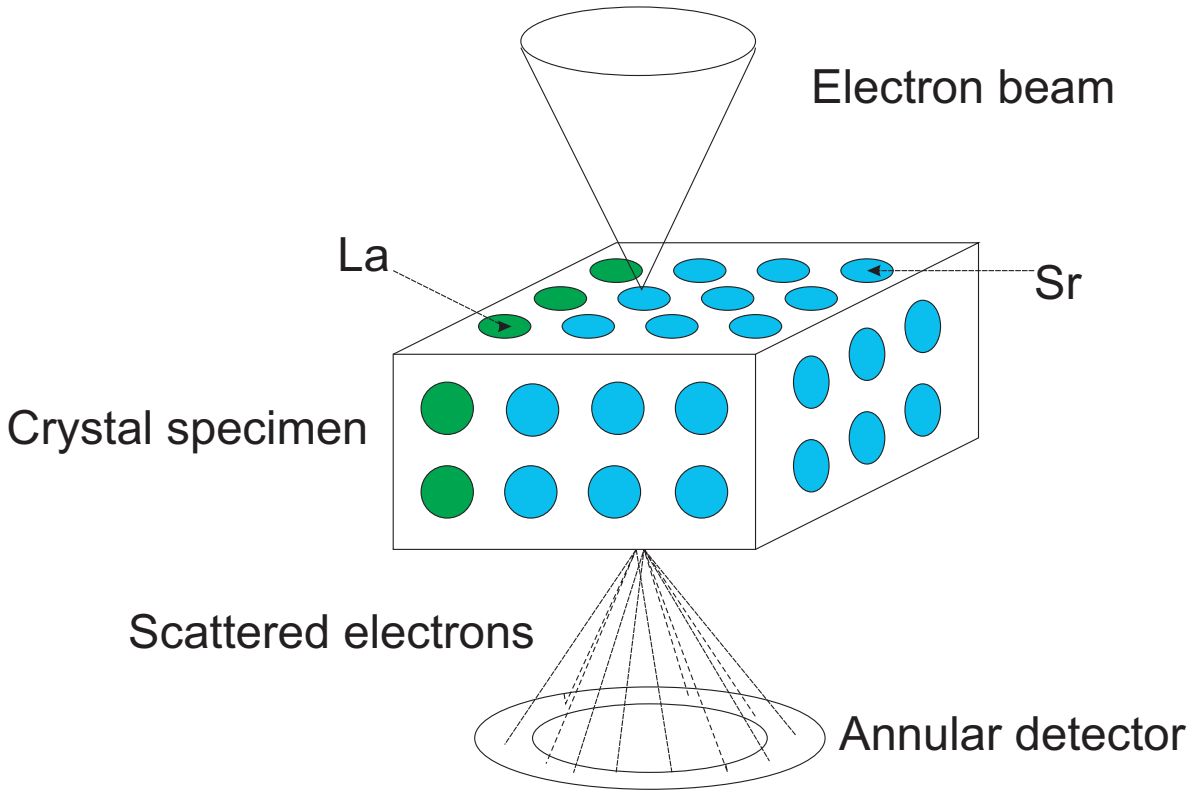
Crystal structure



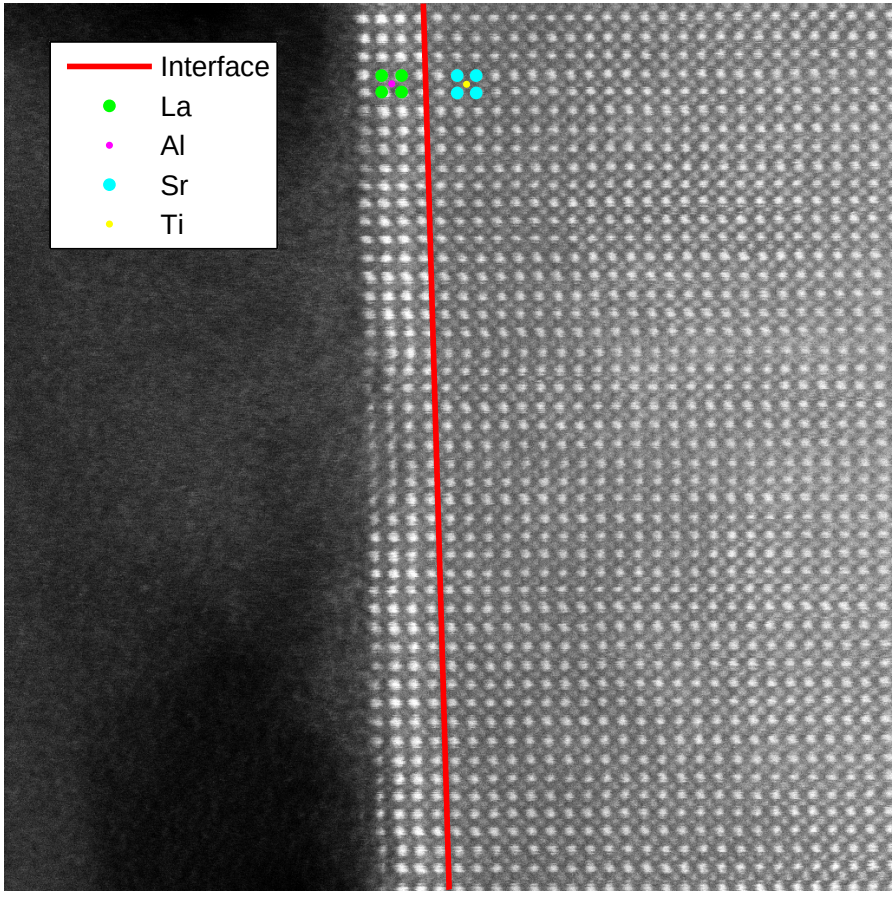
Unit cell

High-Angle Annular Dark Field Scanning Transmission Electron Microscopy



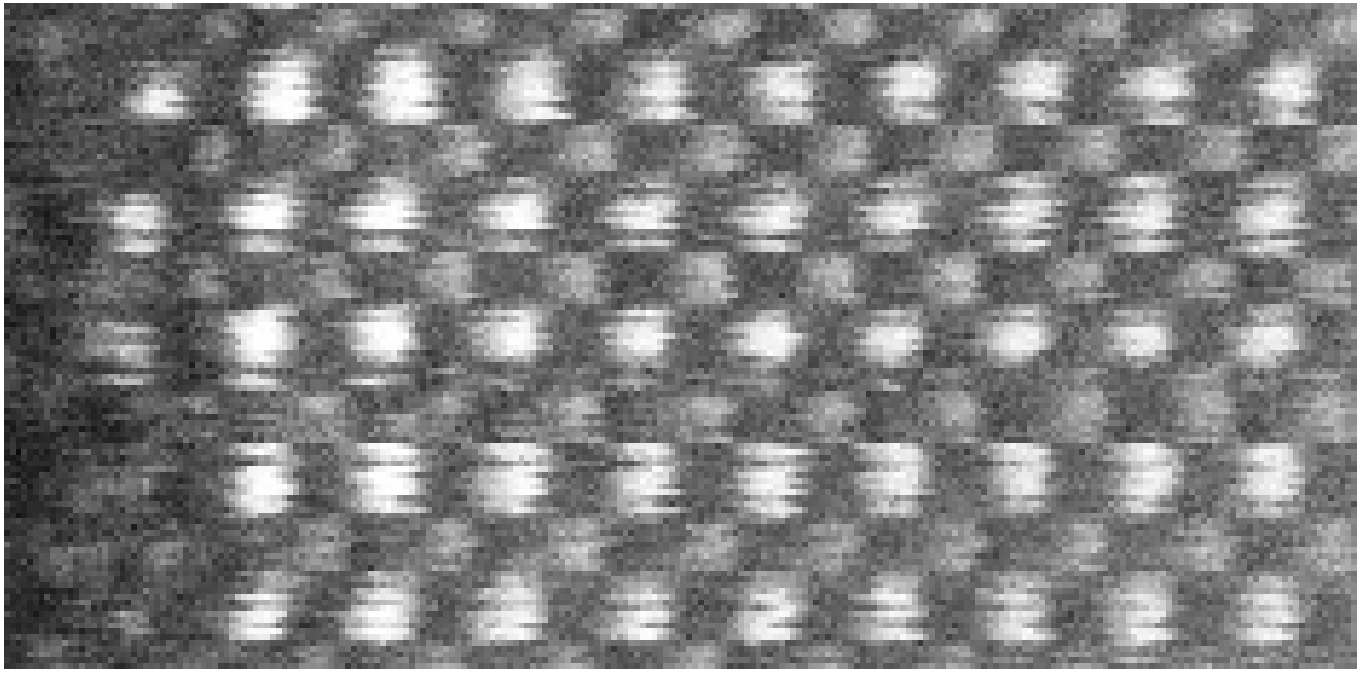
Intensity proportional to atomic number (and number of atoms in a column).

Example



$LaAlO_3$ in the film on the substrate $SrTiO_3$

Detail



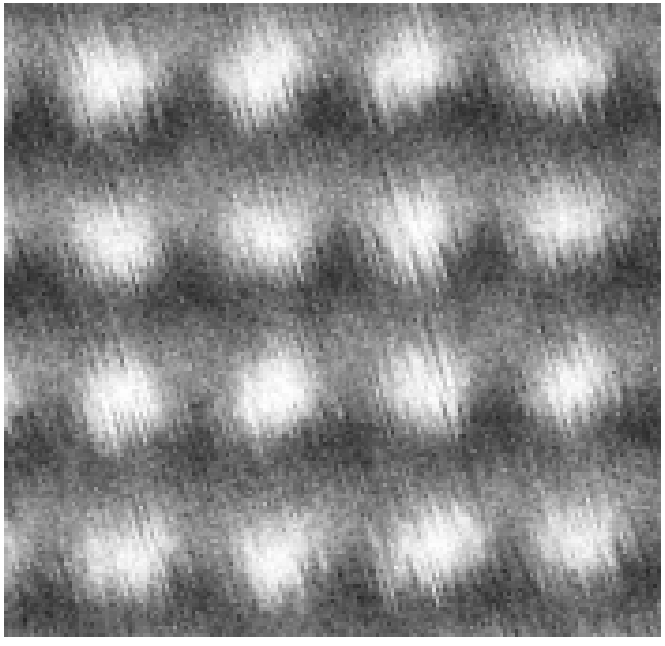
Goals

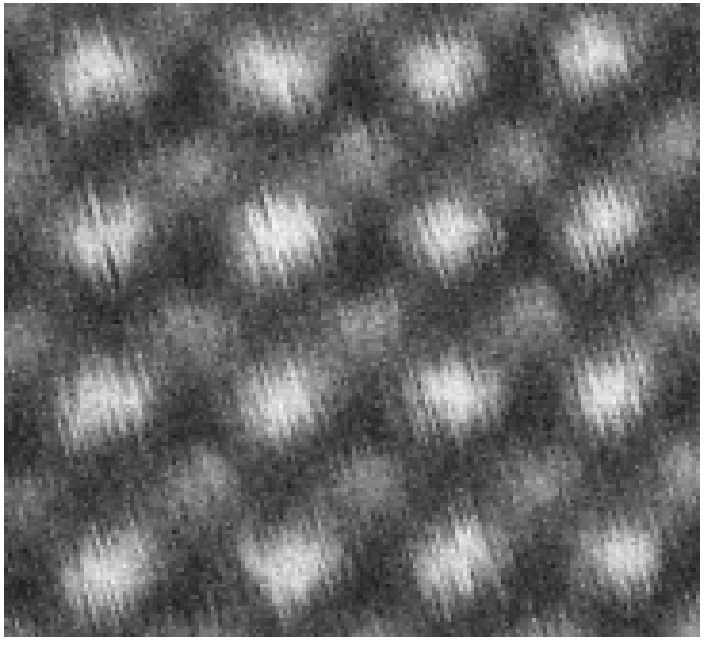
- Characterization of a particular crystal, grown with specific environmental conditions
- The position of the interface and its width, that is the degree of intermixing between atoms across the interface in a narrow region.
- The positions of atoms in the B-sites relative to the atoms in the A-sites. Are they affected in the vicinity of the interface?

Problems

- Physical models are (too) complex
- Imaging. Not constant background. Row-wise dependence.
- A-site atoms have fixed positions in corners of a cube. Not so in images

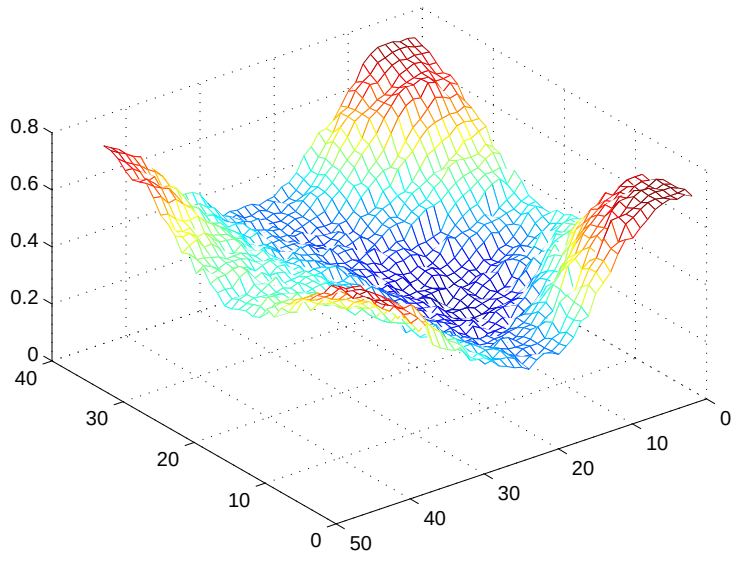
Preliminary analysis

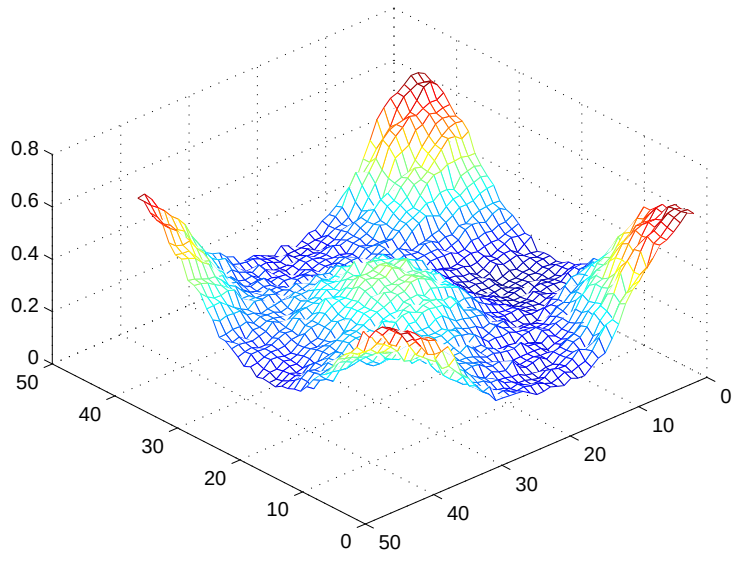




To the left, $LaAlO_3$ in the film, to the right $SrTiO_3$ in the substrate.

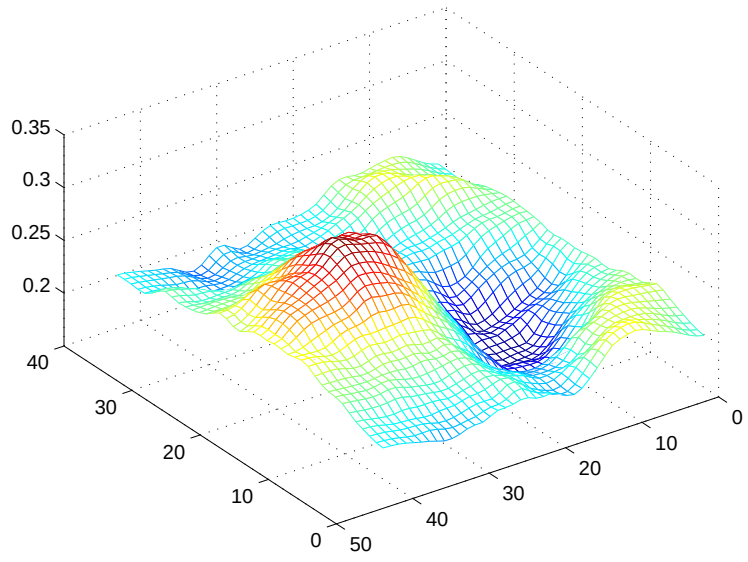
Preliminary analysis

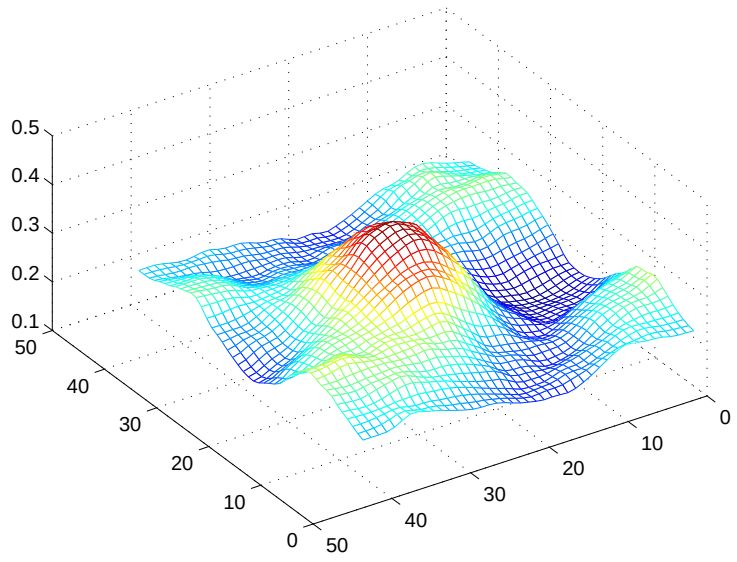




Bilinear transformation of each unit cell giving A-site atoms in corners of square. Average unit cell.

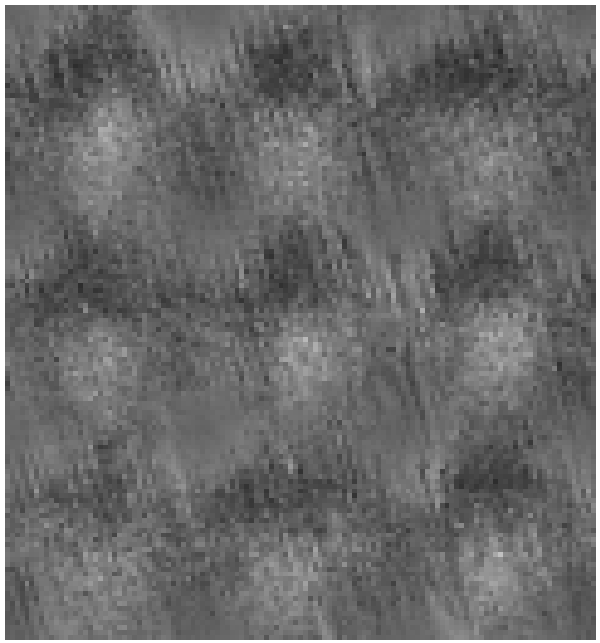
Preliminary analysis

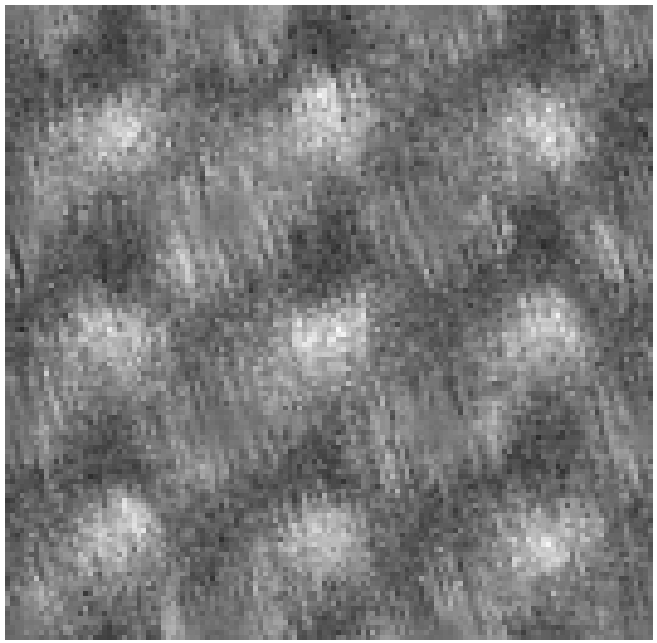




Gaussian function fitted to each A-site atom, then removed.
Smoothed average unit cell.

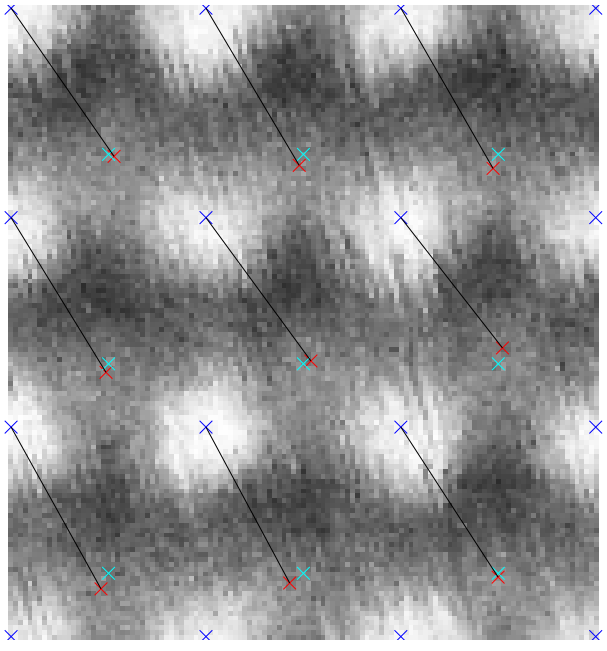
Preliminary analysis

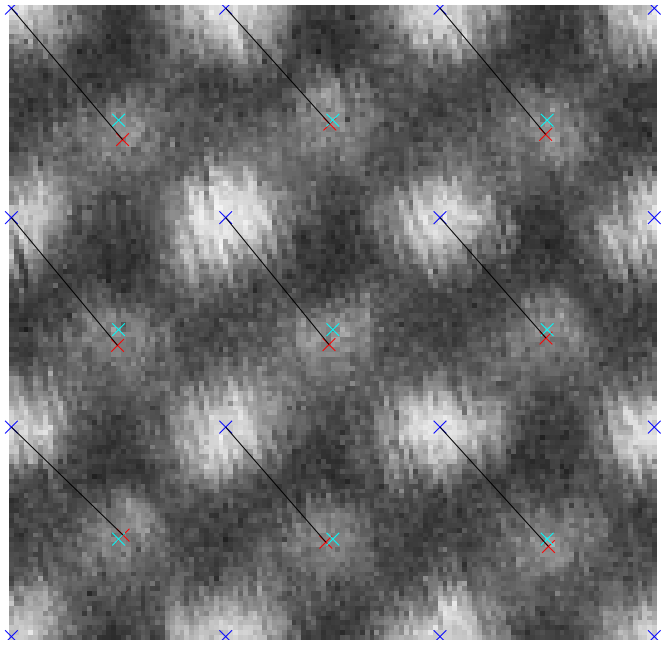




A-site atoms removed.

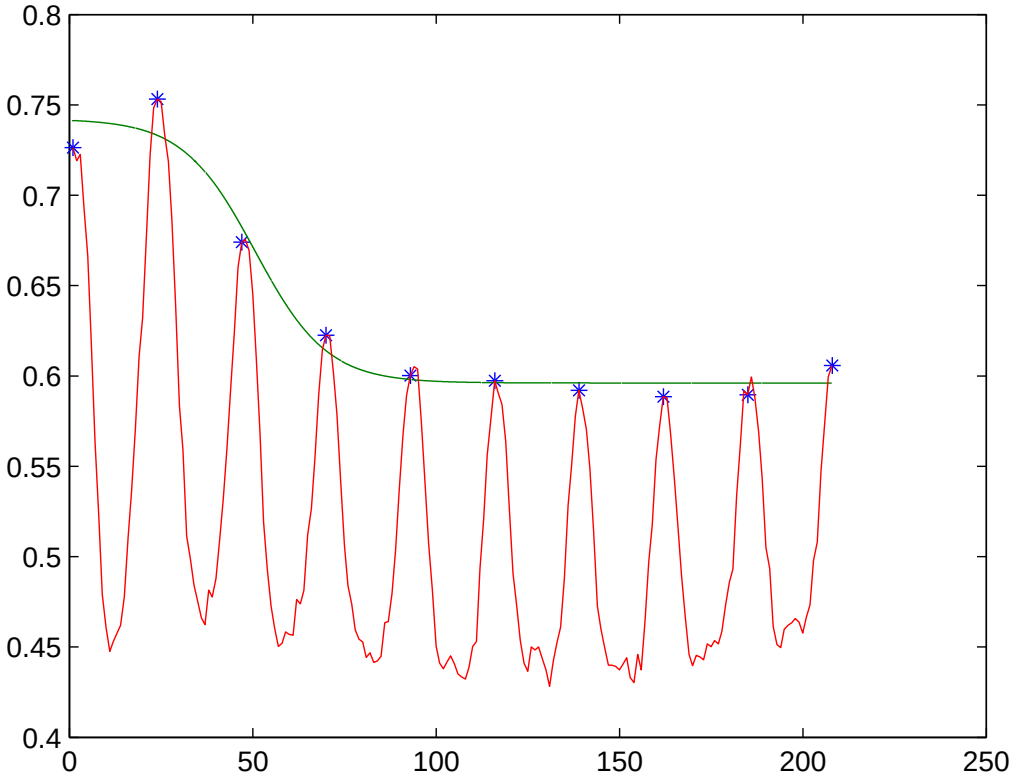
Preliminary analysis





Gaussian function fitted to B-site atoms.

Image



Vertical averaging. Logistic function fit to A-site atoms.

Modeling ideas

1. Image results from a convolution of an object function (atom column as seen by electrons) with a probe intensity profile
2. Probe intensity profile - "known".
3. Object function - possibly Gaussian. (Want to estimate position and height for each atom)
4. Incorporate function describing the interface.
5. Estimate with maximum likelihood.

1-3 already in van Aert et al. (2009)

More future work

- More than one image of each sample with different rotations in x-y plane
- Images with higher resolution. Possible to see oxygen atoms?
- Testing. Is there a significant difference of atom positions for crystals grown at different oxygen pressure?