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Cs Corrected Images and What You Don't See: Data Mining to the Physical Limits

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The ultimate goal of electron microscopy is not to obtain nice images but to advance materials science. This means that EM has to evolve from describing to understanding materials properties. Understanding means matching observations with ab-initio calculations. And since all the structure-property relations are encoded in the positions of the atoms, they form the ultimate language between theory and experiment. The future EM is then to be considered as a communication channel between object and observer and the images as data planes from which the 3D atom positions can be extracted quantitatively. With the newest generation of Cs corrected EM's the resolution is sufficient to resolve the individual atoms and to refine their position with picometer precision. If the ideal object would be a phase object and the perfect electron microscope would have no aberrations, the HREM image intensity would show no contrast at all. Hence electron microscopic aberrations such as defocus are necessary to create contrast in the images. But on the other hand they scramble the information about the object. The best way to extract this information is by first undoing (deconvolving) the transfer functions of the electron microscope and the recording device. The first step is thus to retrieve the phase of the image wave. This can be done by off-axis electron holography or by focal series reconstruction, which is a kind of in-line holography. The next step is data mining the exit wave so as to retrieve the 3D positions of the object atoms. Since the exit wave is the result of the interaction of the electron wave with the object we need a physical model for this interaction that can be used for fitting. In general a 2D projection does not have sufficient information to retrieve 3D information so that one needs tomographic methods. But in case of crystalline objects viewed along a zone axis, which all the atoms of a column are aligned in the beam direction the interaction is very strong and nonlinear so that classical tomographic schemes are not applicable. And inverting a kind of multi-slice calculation can be ambiguous.. Fortunately in a zone axis condition the electrons are trapped in the positive potential of the atoms of the column and the propagation (channeling) of the electrons is not influenced by the propagation in neighboring columns up to thicknesses of tens on nm which are typical for HREM. This applies as well for perfect crystalline objects as for defective crystals with a column structure. Thus the exit wave of a crystalline object in a zone axis orientation represents the assembly of the exit waves of the constituting columns. Furthermore the atoms of a column act as weak lenses which focus the electron wave periodically with depth so that the exit wave of a column is a very sensitive peaked fingerprint of the type of column. The theory of channeling is simple [1] and provides a way to interpret the exit wave which can be visualized by plotting the complex values of the pixels in complex 2D space (Argand plot) [2].From the exit wave of a column we can deduce the following information [3].

- Center of the peak: position of the column
- Shape of the peak: defocus distance (with sub-Angstrom precision) and residual aberrations
- Complex value at the peak center: total mass of the column.

By combining this information we can then reconstruct the object in 3D including profile of top and bottom surface. This is demonstrated experimentally below for the case of a Ge foil viewed along (110) and MgO viewed along (100).

References

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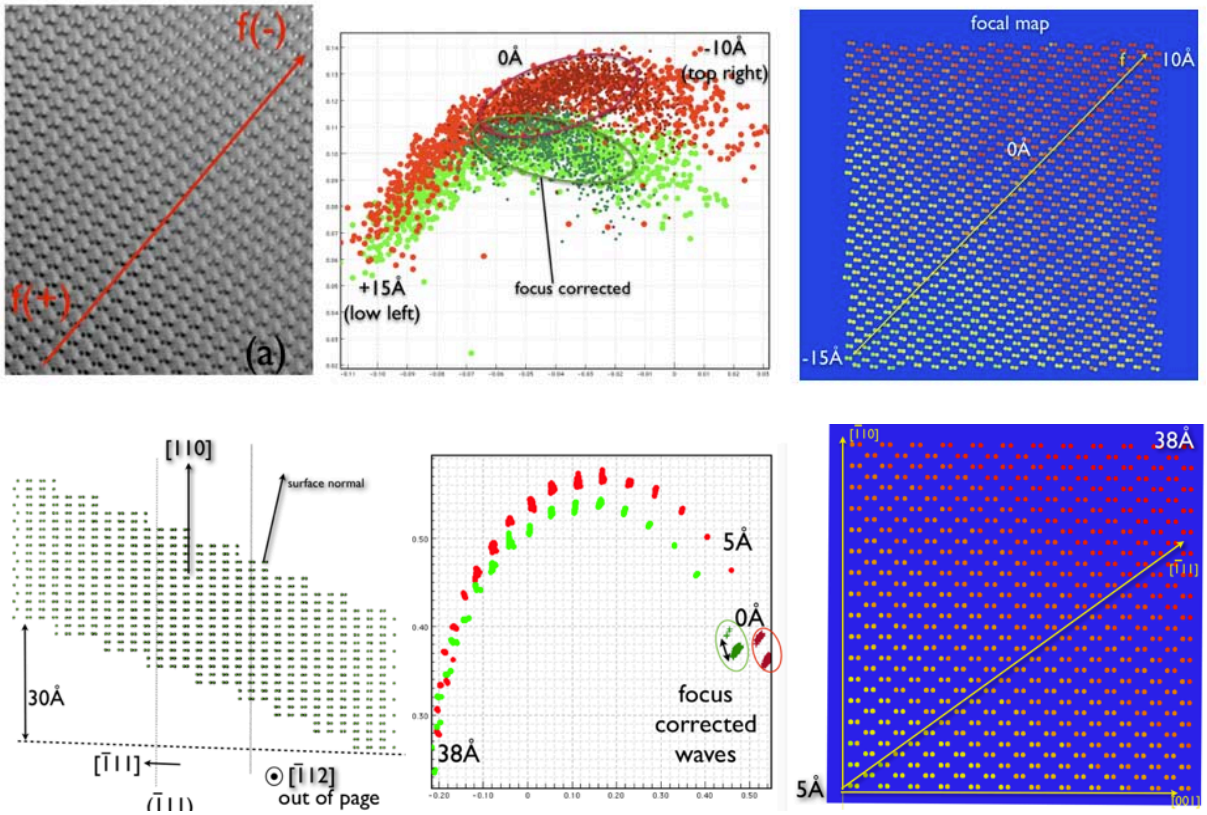

Fig.1: Experimental results for a Ge foil viewed along the (110) zone.
Top: From left to right: 1) phase of exit wave showing the peaks of the columns. 2) Argand plot showing two branches corresponding with the left (red) resp. right (green) columns of the dumbbells. The position along a branch varies with defocus. And the separation between the two branches corresponds with a mass difference of 1 atom. 3) Defocus corrected exit wave
Bottom: from left to right. 1) 3D structure of the ge foil. 2) Simulation of the Argand plot and 3) simulation of the defocus corrected exit wave.

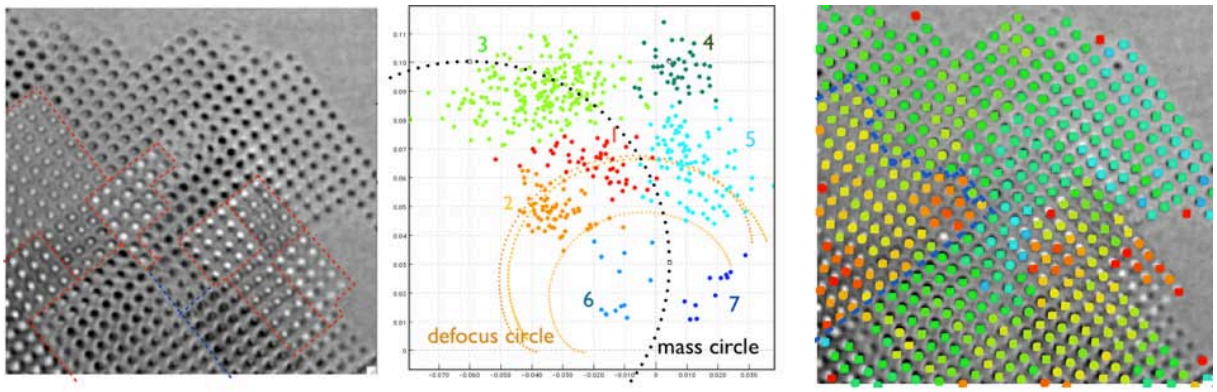

Fig.2: Preliminary experimental results for a MgO foil viewed along the (100) zone.
Top: From left to right: 1) phase of exit wave showing the peaks of the columns. 2) Argand plot with clusters of columns that differ in mass and/or defocus. 3) Color mapping of the different columns showing domains with different surface profile.

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