Reconstruction of the projected crystal potential using HRTEM – prospects for materials science investigations

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In modern high-resolution electron microscopy various reconstruction methods have proven to be invaluable tools for materials science investigations. They comprise wave function reconstruction methods, which aim to eliminate unwanted imaging artifacts as non-linear contrast modulation and contrast delocalisation owing to the presence of lens aberrations. One of these methods, used also in this work, is the widely known focus-variation method [1, 2].

In the past two decades various forms of potential reconstruction methods have been proposed, which aim to eliminate the problems occuring in the structural interpretation of reconstructed exit wave functions, imposed by the effects of dynamical electron diffraction. These effects give rise to a non-linear relation of scattering power and modulation of the wave function [3], and the local modulation can be further obscured by the presence of crystal tilt.

Materials science investigations using potential reconstruction methods in combination with wave function reconstruction methods require knowledge beyond the idealised conditions for the reconstruction algorithms: in particular object thickness, crystal tilt, residual wave aberrations, and phenomenological absorption are often unknown in experiments. Extensive simulation studies using the channelling model of dynamical electron diffraction [3] and a rapid and stable potential reconstruction algorithm had revealed that the projected crystal potential can be determined for thick objects [4]. A breakthrough for the application in materials science investigations had been achieved by showing that object thickness, residual defocus, and phenomenological absorption can be fitted self-consistently together with the projected potential [5]. The last corner stone, preventing application of the potential reconstruction so far, has been added recently, namely the successful self-consistent fit of crystal tilt [6].

The prospects of potential reconstruction for materials science were explored by investigating the the microstructure of a $Ba_{0.5}Sr_{0.5}Co_{0.8}Fe_{0.2}O_3$ (BSCF) crystal, whose perovskite unit cells can form a variety of polytype structures through rearrangement of oxygen octahedra. A through-focus series of 20 images was recorded from a thin specimen of BSCF with an aberration-corrected TITAN 80-300 operated at 300 kV. Next an exit wave function was reconstructed from the series using the TrueImage package (FEI, Eindhoven), which was then subjected to numerical correction eliminating residual aberrations up to the instrumental information limit of 0.08 nm. Finally the projected crystal potential was reconstructed from the corrected exit wave function using the methods described in [5, 6], and the following parameters were determined through self-consistent fit: 8.4 nm object thickness, 1.6 nm residual defocus, and 7.0 nm^{-1} crystal tilt. The final mismatch of model and experimental exit wave function was S = 4.5%, which is a reasonably small value in view of nearly the same amount of mismatch between model and experimental images during the exit wave reconstruction.

The advantage of potential reconstruction over high-resolution imaging alone can be judged by comparing the structural information accessible through the image intensity (Fig. 1, left), through the phase of the reconstructed exit wave function (Fig. 1, right), or through the reconstructed projected potential map (Fig. 2, left). Although the image was recorded with a pass-band up to the information limit very fine details cannot be seen owing to delocalisation. Investigation of the exit wave reveals such details; they are, however, slightly delocalised and corrupted by the presence of crystal tilt. In the potential map the effects of tilt are strongly reduced, and the non-linear distortion of the atomic contrast modulation owing to dynamical diffraction is eliminated.

Numerical evaluation of the projected potential map allows a quantitative investigation of the projected crystal structure of the BSCF crystal, containing closely-spaced $\Sigma 3$ twin boundaries, in

particular the disorder on the oxygen sublattice. Column-by-column measurement of the maxima of the projected oxygen potential reveals through a histogram of the potential maxima single oxygen atom precision of 2.6 volt per atom (Fig. 2, right). The three maxima of the potential distribution indicate the presence of a high concentration of oxygen vacancies.

References

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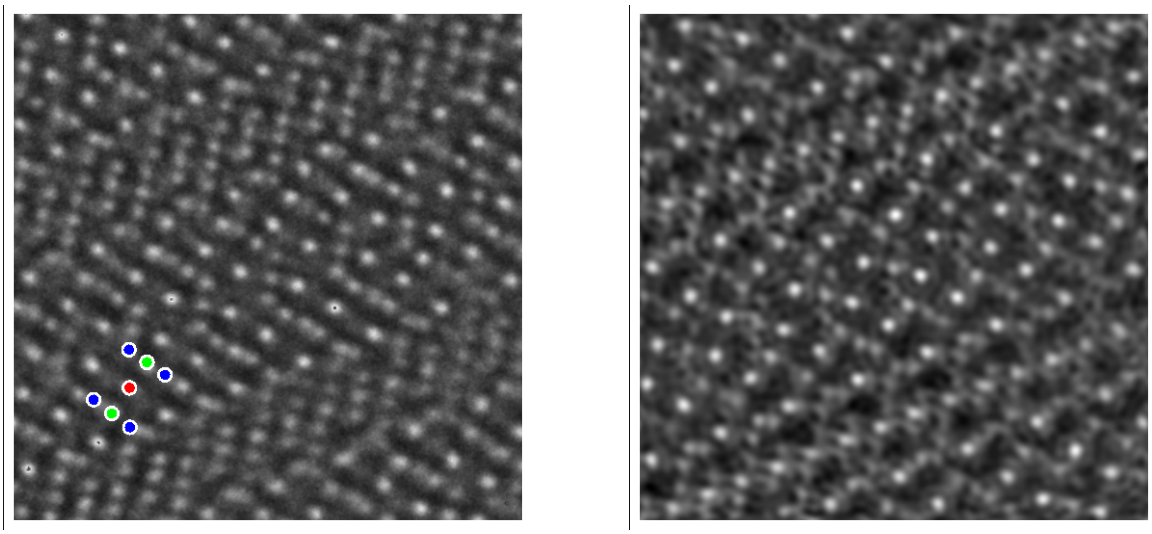

Figure 1. *(left) High-resolution image of BSCF at bright-atom pass-band conditions, red: Ba/Sr, green: Co/Fe, blue: O. (right) Phase of reconstructed exit wave function of BSCF. Frames are 3.4 nm × 3.4 nm.*

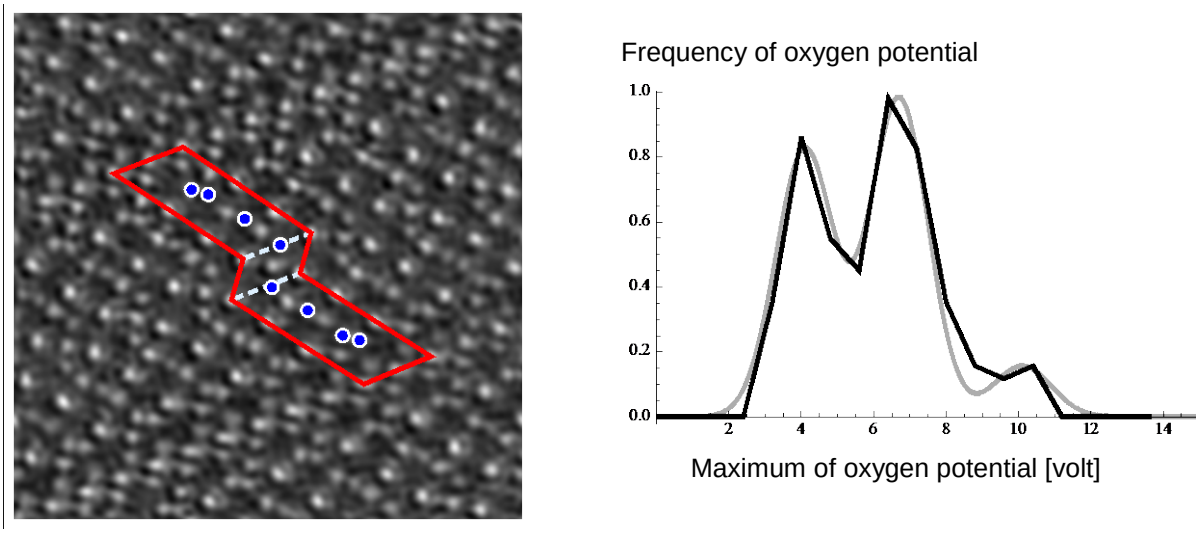

Figure 2. *(left) Reconstructed projected potential of BSCF, frame 3.4 nm by 3.4 nm, red: projected unit cell, blue: oxygen columns used for histogram analysis, dashed: Σ3 twin boundaries. (right) black: frequency of oxygen potential maxima, grey: fit of the distribution with three gaussians.*