Sample tilt effects on atom column position determination in ABF–STEM imaging

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A B S T R A C T
The determination of atom positions from atomically resolved transmission electron micrographs is fundamental for the analysis of crystal defects and strain. In recent years annular bright-field (ABF) imaging has become a popular imaging technique owing to its ability to map both light and heavy elements. Contrast formation in ABF is partially governed by the phase of the electron wave, which renders the technique more sensitive to the tilt of the electron beam with respect to the crystal zone axis than high-angle annular dark-field imaging. Here we show this sensitivity experimentally and use image simulations to quantify this effect. This is essential for error estimation in future quantitative ABF studies.

1. Introduction

Annular bright-field (ABF) imaging in scanning transmission electron microscopy (STEM) has intrigued research interest in recent years due to its capability of direct visualization of light elements, such as Li, N, and O [1–6]. Light elements give rise to weak electron scattering to high angles leading to low intensities in high-angle annular dark-field (HAADF) images which are nowadays commonly used for atomic resolution studies. ABF contrast has been shown to be less dependent on atomic number (approximately proportional to Z1/3 in ABF imaging [7] where Z is the atomic number, and Z1.7 in HAADF imaging [8]), enabling it to directly visualize light elements, even in the presence of heavy elements. However, owing to the small scattering angles used in ABF imaging, coherent scattering leads to a non-monotonic intensity relationship with atomic number at all thicknesses. The reduced dependence on atomic number makes distinguishing between two atom columns with close atomic numbers more difficult. Thus it appears that simultaneous acquisition of HAADF and ABF images is a tempting approach to visualize atoms of a large range of atomic numbers. Such an approach is important in the atomic-scale study of a great number of material systems consisting of light and heavy elements. As an example, macroscopic properties of complex oxides can be critically influenced by small changes of the ligand coordination or by the exact arrangement of the oxygen sub-lattice at hetero-interfaces [9]. To extract reliable atom positions directly from the images one has to assume that intensity maxima in HAADF images (bright spots at atom column positions on a dark background), or intensity minima in ABF images (dark spots at atom column positions on a bright background) accurately correspond to the atom positions. Moreover, to extract distances and angles between different atom columns, one has to assume that in the case of deviations between intensity maxima/minima in HAADF/ABF images and real atom positions, the deviations of the compared atom columns from the real positions are the same for the different columns.

Here we investigate the reliability of the atom column position determination in ABF–STEM. We focus on the important issue of how sensitive intensity minimum positions are with regard to small tilts of the electron beam with respect to the crystal zone axis. In (S)TEM experiments, small specimen tilts from the targeted zone axis can easily be present. These can occur by inaccurate tilting by the operator, but can also have intrinsic reasons such as in the case of static tilts of crystal planes or atom columns near crystal defects, such as dislocations or grain boundaries. We perform image simulations of both HAADF and ABF and compare positions of intensity minima and maxima with real atom positions. The effect of specimen tilt on the contrast of ABF STEM imaging has been thoroughly explored in the literature [10,11]. Therefore, we will pay particular attention to the atom position determination in ABF imaging.

To cover both heavy and light elements in this study, we
selected a two-element material system, namely cubic ZrO$_2$ with heavy element Zr columns and light element O columns along the [001] axis. Along this axis Zr and O column separations are quite large (1.8 Å), resulting in a small overlap of their projected atomic potentials. The structure models of ZrO$_2$ are shown in Figs. 1 and 7a along the [001] axis.

We start from the experimental observations of simultaneously acquired HAADF and ABF images with different convergence and collection angles revealing the minima/maxima position sensitivity to specimen tilts. This is followed by image simulation studies.

2. Method

2.1. Experimental

A plan-view specimen of ZrO$_2$–La$_{2/3}$Sr$_{1/3}$MnO$_3$ (LSMO) pillar–matrix structure, as described in reference [12], was investigated. For our current purpose, we use the ZrO$_2$ pillar area, as indicated in Fig. 1 to investigate both the heavy element (Zr) and the light element (O) atom column positions. The electron beam direction is parallel to the [001] axis.

In a previous study [9] we showed that ZrO$_2$ in the pillar region has tetragonal or cubic structure both of which have almost identical $a$ lattice parameters. In our simulations we use the cubic structure as a structural model [13].

Scanning transmission electron microscopy (STEM) experiments were performed using an aberration-corrected JEOL JEM-ARM200F microscope operated at 200 kV acceleration voltage. The microscope is equipped with a DCOR probe corrector (CEOS GmbH, Germany). The experimental convergence semi-angles were 20.4 mrad and 28 mrad. The JEOL HAADF detector was used to collect the HAADF signal and the JEOL BF detector as ABF detector with the central part being blocked by a beam stopper. The corresponding collection angles are 75–310 mrad (HAADF) and 11–23 mrad (ABF) for the 20.4 mrad convergence semi-angle, and 87–361 mrad (HAADF) and 13–27 mrad (ABF) for the 28 mrad convergence semi-angle.

2.2. Simulation

The simulated results presented here were computed with the absorptive potential multislice algorithm as implemented in the STEMsim-software [14]. In this method, the thermal vibrations of the atoms are included in the calculation by an absorptive potential [15]. The size of the [001]-oriented cubic ZrO$_2$ (Fm-3m, $a=0.507$ nm) supercell was 5 × 5 unit cells in the lateral directions with the $x$-direction parallel to the [100]-axis and the $y$-direction parallel to the [010]-axis, computed on a numerical grid of 50 × 50 pixels per unit cell. All simulations were computed for an accelerating voltage of 200 kV. To get collection-angle-dependent results, we subdivided the calculated angular range (0–100 mrad) into 100 rings of 1 mrad width. The signals from the individual angular ranges were obtained by incoherently adding all signals in the corresponding rings. The sampling in reciprocal space is 0.99 mrad/pixel with an angular range between 0 and 123.75 mrad.

STEM images were simulated with a sampling in real space of 600 × 600 scan-positions per unit cell. This allowed precise determination of maxima/minima positions in simulated HAADF/ABF images. We found that for the aberration-free probe, as expected due to symmetry, there is no shift of maxima/minima positions along the direction perpendicular to the shift direction of the Laue circle center. Therefore, in order to save computing time, we calculated maxima/minima positions only from line scans of the STEM probe along the directions parallel to the shift direction of the Laue circle center.

For the line scan simulations, we used 600 scan-positions per line. As illustrated in Fig. 7a, the line scan extends between two Zr or O atoms along the [100] direction resulting in a sampling of 0.4225 pm/pixel.

There are in general 3 options to model specimen tilt, which are all implemented in the STEMsim package: (i) tilt the whole supercell (Fig. 2b), (ii) tilt the electron beam (Fig. 2c), and (iii) tilt via the propagator [16] (Fig. 2d). Although option (i) resembles the experimental situation, it is not applied due to the increased computing time and complexity caused by varying slice potentials with specimen tilt. For small-angle tilts, there are no differences in the results when tilting the beam or tilting via propagator using an aberration-free probe or a nearly aberration-free probe as in modern aberration-corrected TEMs. In our current study, despite of a small amount of residual aberrations in our experimental probe, we will limit our discussions to an aberration-free probe introducing the tilt via the propagator.

2.3. Data processing

All experimental HAADF and ABF images were filtered using a Wiener filter (in reciprocal space) to reduce image noise [17].

![Fig. 2.](image)

(a) Situation without specimen tilt. Illustrations of the three options to model the tilt between electron beam and specimen in STEMsim, (b) tilt of the whole crystal, (c) tilt of the electron beam and (d) tilt via propagator. (For interpretation of the references to color in this figure, the reader is referred to the web version of this article.)
maxima/minima positions in acquired HAADF/ABF images were extracted by maximum/minimum finding and refined by parabolic fitting using the ImageEval software package developed by Knut Müller-Caspary, who is one of the co-authors. All simulated STEM intensities are presented as fractional intensities, normalized to the incident intensity.

Image maxima/minima of simulations were determined by the same parabolic fitting as for the experimental data. In this paper, we compare maxima positions in HAADF images and minima positions in ABF images and compare them with the true positions. Without tilt (Fig. 2a), both positions correspond to the projection of the atoms parallel to the electron propagation direction. On the other hand, in the tilted case it is not obvious whether real positions correspond, e.g., to the atom positions in the top plane (black dash line in Fig. 2d) or in the central plane (magenta dash line in Fig. 2d). Considering the focal plane and limited depth of focus in aberration-corrected STEM imaging, we use the atom positions of the top plane as “true positions” for all specimen tilt situations.

3. Experimental results

Fig. 3 shows three groups of simultaneously acquired HAADF and ABF images of the ZrO₂ sample area marked in Fig. 1. Three different specimen tilt conditions were used, called “tilt 1” “tilt 2” and “tilt 3” in the following, as revealed by the diffraction patterns shown in Fig. 3a, d and g. Because of the simultaneous acquisition direct comparison of Fig. 3b and c, e and f, and h and i is possible. The position averaged convergent beam electron diffraction (PACBED) patterns were acquired with the CCD camera through incoherent averaging of convergent beam electron diffraction patterns [18,19] while the beam was scanned through the whole area shown in Fig. 1, including both LSMO and ZrO₂ regions. To
improve the visibility the intensities in the diffraction patterns were color-coded.

For each specimen tilt, we acquired the HAADF and ABF images at two different convergence semi-angles ($\alpha$) and corresponding different collection semi-angles ($\beta$) to make the collection semi-angle of ABF imaging approximately half the convergence semi-angle. The angle values can be found in the experimental section and in Fig. 3. For the reasons discussed in Section 5, we only selected the ones shown in the figures.

The high symmetry of the diffraction pattern intensity of “tilt 1” (Fig. 3a) indicates that the specimen is in or at least very close to the [001] zone axis. The asymmetry of the diffraction pattern intensity of “tilt 2” (Fig. 3d) indicates a specimen tilt away from [001] axis, represented by a shift vector of the Laue circle center ($[k_x, k_y]$) with $|k_x| < |k_y|$. The diffraction pattern of “tilt 3” (Fig. 3g) indicates a specimen tilt away from the [001] axis represented by a shift vector of the Laue circle center ($[-k_x, -k_y]$) with $|k_x| > |k_y|$. In the HAADF images, maxima positions correspond to Zr atom column positions, while O atom column positions are invisible due to the low scattering cross-section. In the ABF images, the minima positions with larger radius correspond to Zr atom column positions and the less dark minima positions with smaller diameter to O atom column positions. To show the relationship of maxima and minima positions of the same element, Zr, from simultaneously acquired HAADF and ABF images, we display both the fitted maxima positions corresponding to the Zr atom columns in HAADF images, labeled by red circles, and the fitted minima positions corresponding to the Zr atom columns in ABF images, labeled by green crosses.

The numerical data of the relative shift of maxima positions in HAADF images to the minima positions in ABF images for Zr are shown in Table 1. They show complexity but also with some apparent trends. For example, for “tilt 1”, considered as “in zone axis orientation” from the diffraction pattern, non-negligible deviations are found. Thus, it seems that even very small specimen tilts, not visible from the diffraction pattern, lead to a detectable shift of minima/maxima in ABF and HAADF images. For “tilt 2”, a parallel but opposite direction relationship can be found between the deviation direction and the shift direction of the Laue circle center, i.e. $|\Delta x| < |\Delta y|$ and $|k_x| < |k_y|$. For “tilt 3” it can be seen that the observed deviation direction directly correlates with the shift direction of the Laue circle center, i.e. $|\Delta x| > |\Delta y|$ and $|k_x| > |k_y|$.

Moreover, in ABF images differences exist in the relative position of minima corresponding to O and minima corresponding to Zr. The fitted minima positions are displayed on the ABF images by green (Zr) and yellow (O) crosses. Taking the O positions in “tilt 1” as a reference, we obtain the relative shift of O minima positions, as shown in Table 2. However, we find a good match of the O minima position shift direction and the shift direction of the Laue circle center for both “tilt 2” and “tilt 3” between ABF and HAADF images and. Details about how we get these data are as follows. To numerically show the shift of the minima positions corresponding to O, we firstly set the coordinates of the minima positions corresponding to the top left Zr atom columns to zero in Fig. 3c, f, i. By doing this, we manually set the minima positions corresponding to Zr atom columns to be the same in all ABF images and assume them to be the rigid reference system, whose validity, however, needs verification by simulations. In a second step, the minima positions corresponding to O atom columns in Fig. 3c are taken as a reference which is more close to the zone axis as revealed by the PACBED pattern intensity symmetry. Thus the relative shifts of the minima positions (O) of the other images compared to Fig. 3c can be obtained by deducting their coordinates from those in Fig. 3c, as shown in Table 2. Images with an apparent sample drift are excluded from the analysis.

To understand these observed complexities, STEM simulations are essential. The detailed contrast and shape of the minima positions in ABF images vary with both the specimen tilt and experimental imaging conditions. However, these analyses are beyond the scope of this paper.

4. Simulation results

4.1. Preliminary remarks

When interpreting the experimental results we assume taking the maxima positions shown in HAADF images as reference with all shift measurements made with respect to their positions. These positions are assumed to be well defined due to the incoherent nature of STEM imaging. To verify these assumptions, however, image simulations are indispensable.

Before correlating the maxima/minima position shift observed in HAADF/ABF images with specimen tilt, the non-tilted situation at different convergence and collection semi-angles was calculated. The quantitative results show no shift of maxima/minima positions along either the [100]- or [010]-direction in the HAADF/ABF images. These results demonstrate that these images are free from image delocalization which is very common in bright-field images.

Results simulated with a specimen tilt of 5 mrad with a shift of the Laue circle center along the [100]-direction showed no atom position shift along the [010]-direction (the direction perpendicular to the tilting direction) whereas maxima/minima position shift along the [100]-direction are present both in HAADF and ABF images for both Zr and O with different shift length and thickness variation characteristics (e.g. Fig. 4a and b). The details will be explained in Section 4.2. The position shift along and opposite to the shift direction of the Laue circle center matches with the experimental data in tilt 2 (opposite to the shift direction) and tilt 3 (along the shift direction) situations. These results also confirm that a small specimen tilt in the “tilt 1”-condition must have been present although invisible from the diffraction pattern.

By now, we can see that, for an aberration-free electron probe, the maxima/minima position shift can only show up in the presence of specimen tilt. In the following simulation, we start from the results obtained for convergence and collection semi-angles used in our experiments, applying 5 mrad specimen tilt, which is on the high side of typical mistilts. Then we investigate the

<table>
<thead>
<tr>
<th>Tilt</th>
<th>$\alpha$ (mrad)</th>
<th>$\Delta x$ (pm)</th>
<th>$\sigma_{\Delta x}$ (pm)</th>
<th>$\Delta y$ (pm)</th>
<th>$\sigma_{\Delta y}$ (pm)</th>
<th>$\Delta$ (pm)</th>
<th>$\sigma_{\Delta}$ (pm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 ($\sim$0)</td>
<td>20.4 (Fig. 3b)</td>
<td>7.5</td>
<td>2.7</td>
<td>2.2</td>
<td>3.3</td>
<td>8.7</td>
<td>1.6</td>
</tr>
<tr>
<td>2 ($[k_x, k_y]$)</td>
<td>20.4 (Fig. 3e)</td>
<td>4.6</td>
<td>3.8</td>
<td>20.3</td>
<td>7.6</td>
<td>21.2</td>
<td>7.4</td>
</tr>
<tr>
<td>3 ($[-k_x, -k_y]$)</td>
<td>28 (Fig. 3h)</td>
<td>$-15.6$</td>
<td>4.4</td>
<td>0.1</td>
<td>4.5</td>
<td>16.2</td>
<td>4.4</td>
</tr>
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</table>
convergence and collection angle dependence of specific deviations separately, and finally, results for different tilt amounts are presented. In the following, unless otherwise mentioned, deviation means the shift of maxima/minima in HAADF/ABF images from the true atomic positions.

4.2. Correlating simulation with experimental results

Fig. 4 shows the deviations of HAADF and ABF atom positions from the true positions (deviation = 0) along the direction parallel to the shift direction of the Laue circle center. For the simulation of the ABF images, the same convergence and collection semi-angles were used as in the experiment, for HAADF images the same convergence semi-angle was used, but smaller collection semi-angles (71–100) mrad than in the experimental set-up to save computing time. The specimen tilt was set to 5 mrad.

As shown in Fig. 4a–d, firstly, deviations from true atomic positions exist for minima positions in ABF as well as maxima positions in HAADF images. The deviations extend to much thicker specimen regions for ABF imaging (Fig. 4a and b) than for HAADF imaging (Fig. 4c and d). This is probably because the thickness dependence of the 1 s Bloch wave state, which is essential for HAADF imaging [20], is weaker than the complex image formation in ABF imaging [7]. Independent of the imaging mode, deviations extend to thicker regions for light element atom columns. This is most likely because of the weaker electron channeling of light element atom columns. Therefore, it is reasonable to select the heavy element atom columns in thicker specimen areas, e.g. above 15–20 nm for Zr, as the rigid reference system. Still, deviations in ABF images are significant even at large thicknesses and do not allow accurate determination of absolute or relative atom positions. Such determination seems only possible at very thin areas (< 5 nm) where

Table 2
Relative shift of minima positions (O) compared to “tilt 1” acquired with a 20.4 mrad convergence angle condition (Fig. 3e). Here $\Delta x$ is the average relative shift along the x direction, $\Delta y$ is the average relative shift along the y direction and $\Delta d$ is the total average relative shift vector length, where $\sigma$ is the parameter’s standard error.

<table>
<thead>
<tr>
<th>Tilt</th>
<th>$\alpha$ (mrad)</th>
<th>$\Delta x$ (pm)</th>
<th>$\sigma_{\Delta x}$ (pm)</th>
<th>$\Delta y$ (pm)</th>
<th>$\sigma_{\Delta y}$ (pm)</th>
<th>$\Delta d$ (pm)</th>
<th>$\sigma_{\Delta d}$ (pm)</th>
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</thead>
<tbody>
<tr>
<td>1 (0, reference)</td>
<td>20.4 (Fig. 3c)</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>$2</td>
<td>n_\parallel-b_s</td>
<td>$</td>
<td>20.4 (Fig. 3f)</td>
<td>0.5</td>
<td>0.1</td>
<td>0.7</td>
<td>0.2</td>
</tr>
<tr>
<td>$3</td>
<td>/C_{0}$, xy</td>
<td>28 (Fig. 3i)</td>
<td>1.4</td>
<td>0.8</td>
<td>1.1</td>
<td>0.6</td>
<td>1.5</td>
</tr>
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</table>

Fig. 4. Simulated deviations of the minima positions of (a) Zr and (b) O in ABF imaging from true positions, simulated deviations of the maxima positions of (c) Zr and (d) O in HAADF imaging from true positions, and relative shift of the minima positions in ABF images to the maxima positions in HAADF images of Zr (e) and O (f) as a function of sample thickness.
the specimen can be treated within the (weak) phase-object approximation [16] and thus deviations for both atom species are found to be similar. The difference between different convergence semi-angles becomes less as thickness increases and is most pronounced for Zr atomic columns where no differences are detectable above 25 nm thickness, while in the case of O atomic columns the difference is still pronounced up to a thickness of 60 nm. This behavior is related with the decreasing fraction of tilt (5 mrad) versus amount of convergence. The oscillatory variation of deviations with thickness is quicker for Zr than for O, most likely owing to the smaller extinction length for the heavy element.

In the following, we study the convergence semi-angle and collection semi-angle dependence separately.

### 4.3. Convergence and collection angles

In Fig. 4 data are shown where the ABF signal was calculated over the full range (11–23 mrad). We will now have a more detailed look how deviations vary across this range. Fig. 5a and b shows the deviations in ABF images at 3 different collection angles (15, 17, and 19 mrad) integrated over 1 mrad width for Zr and O, respectively. The convergence semi-angle is 20.4 mrad. As shown in Fig. 5a and b, a larger collection angle leads to a quicker variation of the oscillatory deviation with thickness. Moreover as noted above (Fig. 4), Zr shows a quicker variation with thickness compared to O. It is interesting to compare Fig. 4a and b, which is an integral over the entire angular range, with Fig. 5a and b. The integrated signal shows significantly smaller deviations because the signals contributing from different collection angles tend to cancel each other. This effect is more significant for Zr.

Different from the minima position deviations in ABF images, the corresponding maxima position deviations in HAADF images are always positive, i.e. along the tilting direction, and are less dependent on the collection angle (Fig. S1a and b). After an initial increase of the deviation with increasing thickness, the deviation values decrease monotonically with increasing thickness. There is only very limited influence of the deviations from the collection angle.

Comparisons for different convergence semi-angles (20.4 mrad and 28 mrad) at constant collection semi-angles are shown in Fig. 5c and d for Zr and O, respectively. The collection semi-angle range is fixed to be 19–20 mrad. There are close similarities at these two convergence semi-angles for both elements. More data from different convergence semi-angles and collection semi-angles were calculated, which also confirm this aspect. In general, larger convergence angles lead to smaller deviations because the specimen tilt becomes a smaller fraction of the probe-forming convergence angle as the latter is increased. These results indicate that the thickness dependence of the deviation is mainly due to variations of the collection angle, while the convergence angle modifies the deviations only slightly. For very thin samples the convergence angle almost does not influence the deviation. We observed that to get minimum deviations at atom column positions, a larger convergence semi-angle requires a larger inner collection semi-angle, especially for light elements.

Fig. 5. Collection angle dependence of the deviation in ABF imaging with 5 mrad tilt along the shift direction of the Laue circle center for (a) Zr and (b) O using a convergence semi-angle of 20.4 mrad in the simulation. Convergence angle dependence of the deviation in ABF imaging with 5 mrad tilt along the shift direction of the Laue circle center for (c) Zr and (d) O using a collection semi-angle of 19–20 mrad.

### 4.4. Tilt amount

In general, with all the other conditions the same, larger specimen tilt gives larger deviation as shown in Fig. 6a (Zr) and b (O), with exceptions at those thicknesses at which the deviations are close to zero. Fig. 6c and d shows that the deviation of Zr and O atom columns is proportional to the tilt amount for thicknesses below...
about 6 nm for all the tilt amounts presented. Careful inspection of these two figures indicates a trend of non-linear relationship starting at smaller thickness value for larger tilt amount, i.e. the beginning thickness at which the difference value deviates from zero. This is more visible for light element O than for heavy element Zr. These observations can be correlated with the reduction of thickness value below which the weak-phase object approximation is valid caused by the increased specimen tilt [16,21,22].

5. Discussions

5.1. Influence on the measurement of bond angles

The case of measuring relative deviations between Zr and O positions, which is important for extracting information about the ligand coordination, is shown in Fig. 7. These results are extracted from the simulated data with the same convergence semi-angles and collection semi-angles as in the experimental section at a specimen tilt of 5 mrad. The expected angle from the structure model is $90^\circ$. However, the deviation causes the angle to vary between about $80^\circ$ and $97^\circ$ for 20.4 mrad convergence semi-angle, and between about $85^\circ$ and $93^\circ$ for 28 mrad convergence semi-angle as a function of thickness.

5.2. Summary of experimental and simulation results and suggestions to minimize errors

In order to minimize the quantitative error in the determination of the atom position by ABF imaging and to achieve a good
match between experimental and simulated results a number of suggestions are listed in the following:

1. Align the specimen as close as possible to the targeted zone axis with assistance of techniques like PACBED [18]. This may allow an alignment accuracy better than 1 mrad. However, this is often more difficult in thin specimen regions or in the case of large convergence angles, where the overlap of diffraction disks is large. Especially if one wants to determine atom positions with an accuracy of a few picometers, one should be aware of the fact that tilt deviations below 1 mrad can lead to errors larger than the required accuracy. In such cases, it is also not sufficient to use HAADF maxima of heavy element columns in thicker specimen areas as a rigid reference system, because even then the deviations of the lighter element atom columns can still exceed the required accuracy.

2. For an aberration-free electron probe, a change of position and shape of maxima/minima can only show up when specimen tilt exists. Therefore, observation of a position mismatch between HAADF and ABF images for the same element is an indication of a small amount of tilt.

3. For the same element, the collection semi-angle and tilt angle determine the thickness dependence of the atom column position deviation. The larger the collection angles and the smaller the tilting angle, the more rapid will the deviations vary with thickness. For very thin specimen regions, the convergence angle does not modify the deviation, while larger tilt angles result in larger deviations. In thicker specimen regions, larger convergence angles give smaller deviation while larger tilt angle not necessarily gives larger or smaller deviation. Thus, selection of larger convergence semi-angles and corresponding larger collection semi-angles can give smaller error in determining the relative positions or angles between different atom columns on average, but not for all thickness values.

4. For the same experimental conditions, the heavier the element, the smaller will be the overall deviation and the more rapid variations will occur with thickness.

5. To minimize deviations for small, unavoidable specimen tilt: For thin regions, use larger inner collection semi-angle; for thick regions, use a detector covering a larger angular range.

6. Change of convergence semi-angle, i.e. condenser aperture, can introduce a small amount of beam tilt. Therefore checking the diffraction pattern after changing condenser aperture is essential to avoid difficulties in correlating the deviations with diffraction patterns acquired with different condenser apertures.

6. Conclusions

In this paper, we investigated the reliability of atom position determination in ABF–STEM imaging in an aberration-corrected STEM through experimental HAADF and ABF imaging and simulation results. Deviations from the true atom positions are observed in both experiments and simulations. The deviations are quantitatively studied for different collection semi-angles, convergence semi-angles and tilt amounts with an aberration-free probe. Suggestions on minimizing the errors in the atom position determination by ABF imaging are given based on our experimental experience and the simulated data. The deviations from the true atom positions caused by minor un-avoidable specimen tilts are suggested to be taken into account when for the experimental results higher accuracy are pursued.

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Appendix A. Supplementary material

Supplementary data associated with this article can be found in the online version at http://dx.doi.org/10.1016/j.ultramic.2015.10.008.

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