Measuring strain on HR-STEM images: application to threading dislocations in Al$_{0.8}$In$_{0.2}$N

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Abstract. The Geometrical Phase Analysis (GPA) is an efficient method to measure strain from High Resolution Transmission Electron Microscopy (HRTEM) images. Here we show that it can also be applied efficiently to High Resolution Scanning Transmission Electron Microscopy (HR-STEM) images, which have several advantages: (i) patterns in HR-STEM do not change with thickness and chemical composition (ii) thicker samples can be analysed and (iii) strain and composition can be simultaneously determined. In many situations, the distortions due to the scanning of the beam can be corrected. The strain fields around different threading dislocations in an AlInN layer have been determined from plan view samples prepared by focus ion beam (FIB). Experimental strain maps were compared to analytical calculations that take into account the strain field of dislocations and of the In segregation. Mixed type dislocations are always terminated by an inverse hexagonal pyramidal pit, at the sample surface. The edges of the inverse pyramid are indium rich. The dislocation core is not situated at the centre of the inverse pyramid, which is indium-rich, but slightly shifted.

1. Introduction
Determining the strain locally is in many cases important as strain can change the physical and chemical characteristics of the material. For instance, microelectronics devices use stress to enhance their transport properties. Consequently, it is important to develop tools to measure locally at a nanometer scale strain to fully understand the property of materials. GPA is an effective technique to analyse HR-TEM images [1,2,3,4]. Recently it has been tested on HR-STEM images [5,6,7] as this technique is becoming more popular. In this paper, we report some advantages of using HR-STEM images to measure strain and apply the technique to a 100 nm thick Al$_{0.8}$In$_{0.2}$N layer lattice matched on top of a GaN buffer layer.

2. Experimental details
HR-STEM images were acquired at 300kV on a TITAN microscope equipped with a probe Cs-corrector. Image analysis was performed in Digital Micrograph, by using home made scripts. GPA was used and provided an easy way to correct the distortions due to scanning. The studied sample is a 100 nm thick Al$_{0.8}$In$_{0.2}$N layer nearly latticed matched to a 2 µm thick GaN buffer layer grown on a sapphire substrate. Layers were grown along the c-axis using the conditions reported in [8]. Plan view samples were prepared by focused ion beam (FIB). HR-STEM images, imaging only the remaining top AlInN layer, were realised around different threading dislocations coming from the GaN buffer.
layer. Edge dislocations, mixed type dislocations and screw dislocation having respectively Burgers vectors equal to \(a=1/3[2,-1,-1,0]\), \(a+c=1/3[2,-1,-1,0]\) and \([0001]\) were analysed.

3. Correction of scanning distortions

As stated in [6] and as can be seen in figure 1, the main source of error in strain measurement of HR-STEM images is the shift that can happen between different scanned lines. For instance, the phase image of figure 1b, obtained with the \(g = (1,0,-1,0)\) beam, contains horizontal broad lines that correspond to shift in the STEM images, as phase is proportional. In figure 1c, a phase shift of \(2\pi\) corresponds to a displacement of one \((1,0,-1,0)\) interplanar distance, i.e. 0.2741 nm. At the bottom of figure 1b, i.e. right part of figure 1c, the peak corresponds to a phase shift of \(\pi/2\), i.e. to a shift in the image of 0.7 nm. As proposed in [6], one solution to minimize these scanning errors is to align the scanning direction parallel to the principal axis of the strain and select frequencies that are close to the scanning direction. For instance, in the case of epitaxial layers, the growth direction and the scanning direction should be parallel.

Here we propose a simple way to correct for these scanning errors. It can be applied when the image has a large region that can be used as a reference, which is generally the case. Firstly the scanning direction should be chosen such that the reference region covers at least a narrow vertical strip in the image. In the case of epitaxial layers, this happens when, as before, the growth direction and the scanning direction are parallel. In figure 2b, the reference region we used is outlined by a dotted rectangle. Secondly the phase jumps in the vertical strip should be suppressed either by changing the origin of the phase or by unwrapping the phase. Thirdly, the average profile over this vertical strip should be calculated (figure 1c) and extended uniformly along the scanning direction (figure 1d). Finally, this last image should be subtracted from the original phase. As can be seen in figure 1e, most of the horizontal lines have been suppressed. Figures 1d and 1e show that by using the corrected phase, the strain \(\varepsilon_{gg}\) parallel to the selected g-vector contains few scanning errors. In [6], these scanning distortions are attributed to “flyback error” of the electron beam when the electron beam moves from the end of a line to the beginning of the next one. They could also be correlated to mechanical/thermal instabilities.

![Figure 1](image_url)

**Figure 1.** a) Initial HAADF-STEM image. A pure edge dislocation is present at the center of the black ellipse. b) Initial phase image obtained by selecting the \(g = (1,0,-1,0)\) beam. c) Phase profile horizontally averaged in the vertical strip of figure 1b. So the horizontal pixels in figure 1c are vertical in figure 1b. d) Image made from the average profile of fig. 1c. The horizontal arrow points to a scan error that is pointed by a vertical arrow in figure 1c. e) Corrected phase image f) \(\varepsilon_{gg}\) strain image (grey scale in %) calculated from the initial phase. The scan errors are clearly seen. g) \(\varepsilon_{gg}\) strain image (in %) calculated from the corrected phase. h) Zoom into the dislocation core of figure 1a.
4. Application to Al$_{0.8}$In$_{0.2}$N

In the studied sample, threading dislocations with screw components terminate at the surface of the sample by inverse pyramidal pits that have hexagonal basis [9, 10]. On plan view images, these pyramidal pits look like hexagonal stars (figure 2 and 4) whose arms are elongated along the six $<$1,-1,0,0$>$ directions. In HAADF imaging these arms, which are in fact the edges of the inverse pyramid, are bright indicating that they are indium rich. Pure edge dislocation, which have a Burgers vector equal to 1/3$<$2,-1,-1,0$>$ do not form pits (figure 1a). The analysis of the strain fields around these 3 types of dislocations are summarized in figure 2, 3 and 4. In figure 2 and 3 the positions of the dislocation cores were found by locating either the extremity of the additional plane well defined in “$<$1,0,-1,0$>$ filtered images” (see figures 2b and 2c). It is found that in mixed type dislocation, the centre of the pit, which is In-rich, does not coincide with the dislocation core. As in pure edge dislocation, In tends to segregate on the tensile region of the dislocation. We applied a model presented in [10, 11] to calculate the In concentration around the dislocation core. For pure-edge dislocation taking into account the segregation of In, the calculated stress field reproduces quite well the experimental one, especially in the In rich region (figure 3).

**Figure 2.** a) Smoothed HAADF-STEM image of a mixed type dislocation ($a$+$c$) in Al$_{0.8}$In$_{0.2}$N. The edge component of the ($a$+$c$) Burgers vector is represented by the white $a$ vector. The two black spots, as determined in figure 2b and 2c, locate the dislocation core. b) Filtered image of figure 2a obtained by selecting the ($1,-1,0,0$) and ($-1,1,0,0$) spots. The place of the dislocation is determined by the upper black spot that is reported in figure 2a. c) Filtered image of figure 2a obtained with the ($1,0,-1,0$) and ($-1,0,1,0$) spots. d) $\varepsilon_{xx}$ strain map.

**Figure 3.** a) $\varepsilon_{xx}$ strain of the pure edge dislocation shown in figure 1a, which has been rotated in order that the Burgers vector $a = \frac{1}{3}[2,-1,-1,0]$ becomes horizontal i.e. parallel to the x-axis. b-c) Simulated $\varepsilon_{xx}$ strain fields of a pure edge dislocation in AlInN without (image b) and with (image c) In segregation. d) In concentration as determined by the analytical model.
Even for screw dislocations, a strain field was measured around a dislocation core. It is attributed to the variation of In concentration around the screw dislocation core, even though there are no really tensile or compressed regions, but mainly shear regions around the core. Indeed, our model indicates that shear components lead to In segregation (figure 4, [10]). Wider lattice parameters are found at the dislocation core and along the edges of the inverse pyramid, which is qualitatively in agreement with the contrast of STEM images that are bright, i.e In-rich, along these edges.

Figure 4.
(a) HAADF-STEM image of a screw dislocation. The star shape is due to presence of an inverse pyramidal pit at the surface of the sample.
(b) Calculated In-concentration around the dislocation core. The model described in [10] does not include the presence of the hexagonal pit and so the calculated concentration is symmetric around the dislocation core.
(c) $\varepsilon_{xx} + \varepsilon_{yy}$ strain field as determined from figure 4a.

5. Conclusion
By correcting the scanning distortions of HR-STEM images, we were able to determine the strain fields around 3 types of threading dislocations. Such analysis would have been more difficult with HR-TEM images due to the thickness variations around the dislocation cores that have a pyramidal pit and because the studied areas were rather thick. The Z-contrast of STEM images, that gives the In-content, was qualitatively correlated to the measured strain fields. Further work would be needed to determine more quantitatively from the Z-contrast the In-content around threading dislocations. In principle, HR-STEM images allow to measure simultaneously, quantitatively and independently, strain and composition, which is not the case of HR-TEM images.

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