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Strategy for reliable strain measurement in InAs/GaAs materials from high-resolution Z-contrast STEM images

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Abstract. Geometric phase analysis (GPA), a fast and simple Fourier space method for strain analysis, can give useful information on accumulated strain and defect propagation in multiple layers of semiconductors, including quantum dot materials. In this work, GPA has been applied to high resolution Z-contrast scanning transmission electron microscopy (STEM) images. Strain maps determined from different g vectors of these images are compared to each other, in order to analyze and assess the GPA technique in terms of accuracy. The SmartAlign tool has been used to improve the STEM image quality getting more reliable results. Strain maps from template matching as a real space approach are compared with strain maps from GPA, and it is discussed that a real space analysis is a better approach than GPA for aberration corrected STEM images.

1. Introduction
GPA is a novel and widely applied technique that can be used for quantitative measurements of lattice strains in both high-resolution transmission electron microscopy (HRTEM) and atomic resolution high angular annular dark field (HAADF) STEM images. The method is based on the assumption that there exists a constant spatial relationship between the intensity maxima and the location of lattice planes in the studied material [1]. This relationship appears in the form of a spatial shift of the intensity maxima positions with respect to the lattice. With the development of probe aberration correctors in STEM, sub-Ångström resolution now can be achieved with relatively uniform contrast, providing precise atomic-column positions and clear contrast to map the strain field. Nevertheless, additional precautions must be taken in experimental images to avoid unwanted effects from the microscope or the specimen that can produce incorrect strains. Questions also remain on the best strategy for strain mapping, and in GPA also to which two *g* vectors should be chosen in the Fourier transform to create the strain maps [2].

2. Experimental Details
In the present work, the GPA technique is applied to experimental HRSTEM images of InAs/GaAs quantum dot (QD) based intermediate band solar cell (IBSC) materials. The aim is to study strain relaxation mechanisms during the growth process of III–V semiconductors. The IBSC utilizes multiple band gaps in order to increase the efficiency beyond the Shockley-Queisser limit [3]. A necessary but challenging step towards fabricating high efficiency QD based IBSCs is to precisely control the QD structures, including strain, which requires accurate structure information. The InAs/GaAs QD materials studied here were grown by molecular beam epitaxy (MBE), in the Stranski-Krastanov (SK) growth mode on [001] GaAs substrates. The lattice mismatch between two materials in SK growth is used to create the QDs. For pure InAs grown epitaxially on GaAs, the mismatch is 7.2%, and the mismatch is smaller when there is a mixing between In and Ga. Thus, the maximum strain is expected at 7.2%. This

strain can be a problem when growing multiple layers of QDs, due to formation of defects, which might act as recombination centers. To compensate for the inherent strain, one can introduce nitrogen in the spacer layers. The small N atoms are supposed to cancel out the strain introduced by the large In atoms. The experimental HAADF-STEM images in Figs. 1 and 4 were taken using a double Cs-corrected, JEOL ARM-200CF microscope, at 200 kV, and the HAADF-STEM image in Fig. 2 was acquired using a 300kV FEI Titan with a Cs probe corrector. All images were taken with the electron beam parallel to the crystallographic [110] direction.

3. Results and discussion

A major issue in using HAADF-STEM images for strain mapping is the scan noise due to the flyback errors in the STEM scanning coils. A strategy to reduce the scan noise, and also to improve the quality of HAADF-STEM images, is to use multiple images recorded with a short scan dwell time and at 0° and 90° scan directions. Fig. 1 compares the effectiveness of this strategy by comparing the ε_{yy} map obtained from a single HAADF-STEM image and the scan noise corrected HAADF-STEM image using the SmartAlign tool [4]. We have used a very short dwell time of 2 μs, and recorded up to 40 frames at 0 and 90° rotations. The SmartAlign tool [4] superposes this image stack into a single image. Much of the noise and horizontal, artificial strain lines seen in the strain map from a single STEM image acquired with the pixel time of 38.8 μs are removed in the strain map of the HAADF-STEM image after applying SmartAlign with 90° rotation between every image in the stack that is shown in Fig.1 (b). We observe in Fig. 1 (d) that the systematic lines are removed from the strain map.
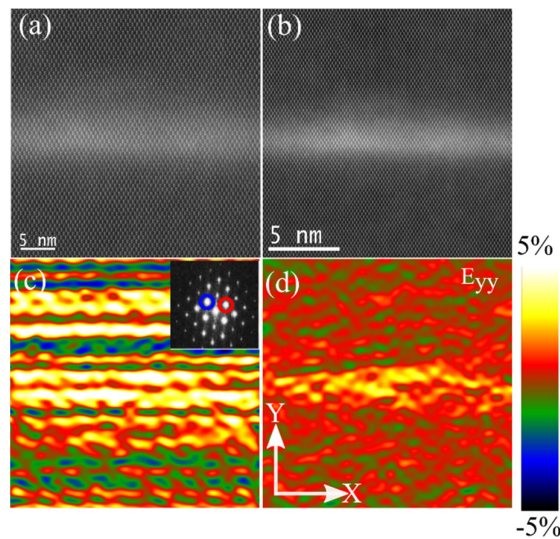

Figure 1. HAADF-STEM image of InAs/GaAs QD, before (a) and and after (b) applying the SmartAlign with 90° rotation, (c) ε_{yy} strain measured from (a), (d) ε_{yy} strain measured from (b). The Bragg spots highlighted in the inset FFT in (c) are used to create strain maps.

The GPA requires two independent Bragg spots as a pair in the Fourier spectrum. The choice of the pair could have a large impact on the GPA results. In Fig. 3, GPA has been applied on different pairs in the fast Fourier transform (FFT) of the single HAADF-STEM image in Fig. 2. Strain maps obtained from (004)/(220), (002)/(220) and {111} pairs (a-c) using GPA show that in case of (004)/(220) the noise is doubled compared with {111}, and that {111} reflections give the best result from GPA in this case. The (002)/(220) pair gives a somewhat different strain map. The (002) reflection in InGaAs/GaAs is composition sensitive, while the (004) reflection is strain sensitive. In principle, the (004)/(220) pair is a good choice since these two reflections are orthogonal to each other and thus provide the most

information. However, the problem with the use of (004)/(220) in the case of Fig. 2 is noise. A single STEM image is too noisy for the low intensity reflections, such as (004). The scanning noise is a kind of high frequency noise and (004) is also affected. So, the overall noise of (004) in a single HAADF-STEM image is high.
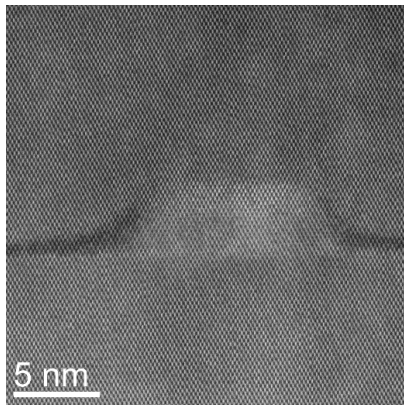

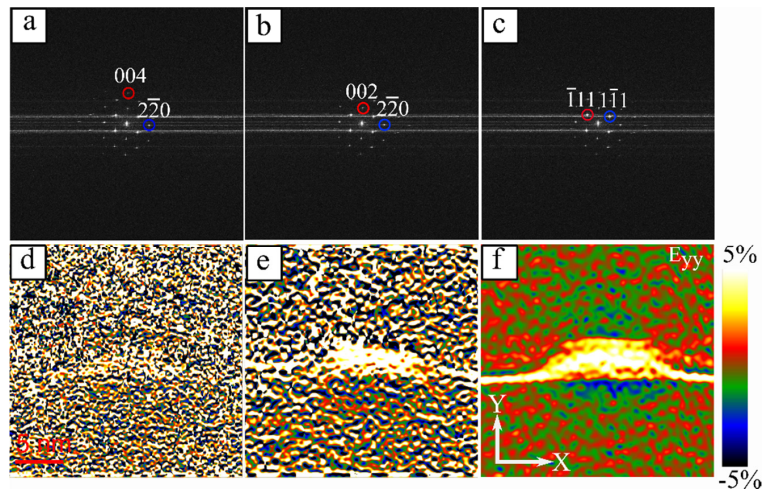**Figure 2.** High resolution HAADF STEM image of InAs/GaAs QD.

Figure 3. (d-f) ε_{yy} strain measured from Fig. 2 using the Bragg spots highlighted in the (a-c) FFTs.
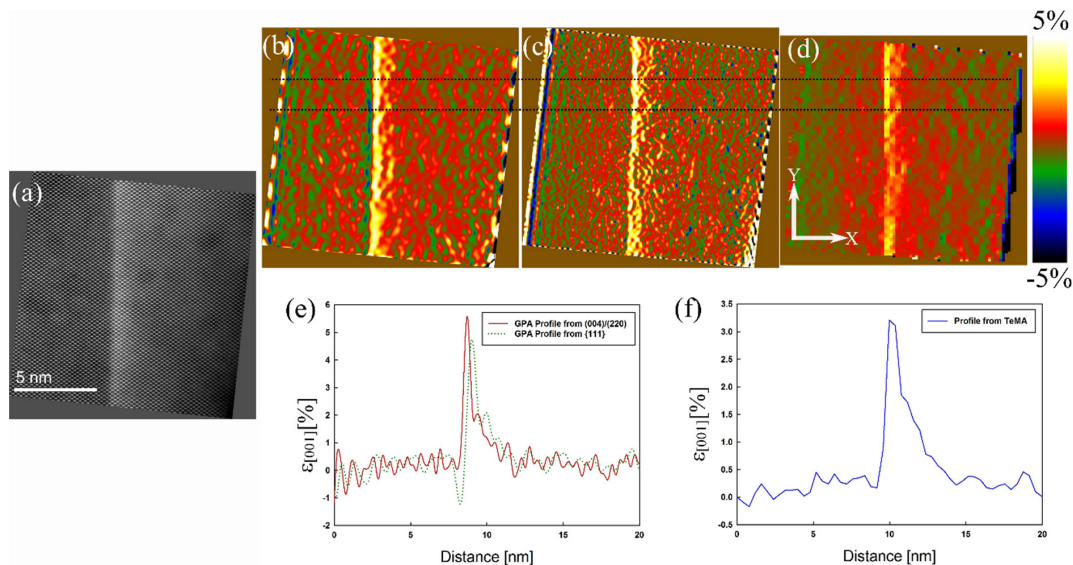

Figure 4. (a) HAADF STEM image of InAs/GaAs wetting layer after applying the SmartAlign, (b and c) ε_{xx} strain maps for strain parallel to the crystallographic [001] direction from (a) using the Bragg spots {111} and (004)/(220), respectively in the FFTs. (d) ε_{xx} strain map from TeMA, (e) The strain profile along a line crossing through the wetting layers shown with dashed lines in (b and c), (f) The strain profile along a line crossing through the wetting layers shown with dashed lines in (d).

An atomic resolution image contains multiple reflections or spatial frequencies, and GPA only uses two frequencies to calculate strain, as Fig. 3 demonstrates. While the approach used by GPA is advantageous for the analysis of HRTEM images of limited spatial resolution, ideally, the analysis of aberration

corrected STEM images should take the advantages of all frequencies, and this can be achieved using real space based methods based on atomic peak finding or template matching (TeMA) [5, 6]. In these methods, the position of the atomic columns is determined by the intensity distribution, which utilizes all information recorded in the image. Fig. 4a shows a HAADF STEM image a GaAs/InAs wetting layer after applying the SmartAlign algorithm. GPA and TeMA have been used to measure the strain in this image. Fig. 4 (b and c) show the strain map from {111} and (004)/(220) reflections, respectively, and Fig. 4 (d) is the strain map from TeMA. The profiles in Fig.4 (e and f) that are taken from Fig. 4(b-d) show that (004)/(220) is in closer agreement with the real space approach (TeMA), and {111} gives systematic noise and interfacial features that are not seen in (004)/(220). This could be a Fourier termination effect due to the stronger background in the FFT spectrum near the {111} reflections.

Finally, thin foil relaxation effects are not taken into account in the strain measurements since the dimensions of the QDs are small and the sample is not extremely thin. Together, we expect the relaxation happens mostly on the same surfaces [7].

4. Conclusions

In conclusion, we have demonstrated several strategies for improving the results of strain analysis by GPA of the InAs/GaAs quantum dot (QD) material, including

1) The image quality can be significantly improved by performing multiple scans with 0° and 90° rotations and by using SmartAlign to reduce noise and scan errors.
2) The choice of g vectors in the GPA procedure can have a large impact on the strain mapping results. The use of {111} reflections are the most effective in case of a single HAADF-STEM image. However, the same {111} pair applied to the improved HAADF-STEM image revealed artefacts at the wetting layer interface.
3) By using SmartAlign for a series of images to improve the signals at high frequencies, and as it is shown in Fig. 4c, the (004)/(220) reflections gave the best results when using GPA for strain measurements.

The data in this paper also shows that GPA analysis using only one pair of reflections has its limitations since it does not take advantage of all information recorded at atomic resolution. For GPA, the challenge is how to combine information obtained by using different Fourier pairs in order to obtain true strain information. With aberration corrected microscopes the resolution is much higher, and by using SmartAlign we get better atomic resolution images, which definitely improves the GPA analysis. However, still additional information can be picked up with real space approaches which use information from all frequencies and would be a better approach than GPA.

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