

# High Resolution Peak Measurement and Strain Mapping using Peak Pairs Analysis

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## BIOGRAPHY

Pedro L. Galindo graduated in computer science and received his PhD in artificial intelligence from the Polytechnic University of Madrid. He is now an associate professor at the University of Cadiz and the head of the 'Intelligent Systems' research group. His research interests include strain mapping in materials, STEM-HAADF, electron microscopy image simulation, and supercomputing in materials science.



## ABSTRACT

Strain mapping is a numerical image-processing technique that measures the local shifts of an image with respect to the ideal positions in the bulk. Peak Pairs is a recently introduced real space algorithm for strain mapping. A new plug-in for DigitalMicrograph™ implementing Peak Pairs Analysis has been developed by HREM Research. It features high-resolution peak detection, image filtering, displacement and strain map calculation, atomic column and/or continuous strain maps, histogram and lattice point's analysis and geometric distortion determination and correction.

## KEYWORDS

transmission electron microscopy, high-resolution electron microscopy, image analysis, image processing, strain mapping, peak pairs analysis, peak finding methods, materials science

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## INTRODUCTION

High-resolution transmission electron microscopy (HRTEM) combined with image analysis is a very useful tool for the structural analysis of materials, whose behaviour is in many cases controlled by interfaces and/or defects. Strain mapping can be used to analyze materials at the atomic-column level, measuring local displacements and strain, and so revealing lattice translations, dislocations and/or rotations. Recent advances in digital imaging have offered the possibility of locally determining the elastic strain of materials from HRTEM images very precisely (on the order of a 1% displacement of an atomic column), enabling the detection of the slightest changes in structure that cannot be seen by the naked eye in an HRTEM image.

Several methodologies have been described in the literature to determine strain field mapping from HRTEM images, either in real space (peak finding) [1] or in Fourier space (geometrical phase analysis, GPA) [2]. Here we describe a recently introduced real-space algorithm for strain mapping called Peak Pairs Analysis [3].

## MATERIALS AND METHODS

### Materials and Preparation

The HRTEM image shown and analysed in this paper corresponds to an InAs/GaAs interface of a InAs/GaAs double layer heterostructure, grown by atomic layer molecular beam epitaxy at 350°C on a (001) GaAs substrate, in the Institute of Microelectronics of Madrid by Y. González et al. Specimen was thinned down to electron transparency for HRTEM study by conventional mechanical procedures and ion milling.

### Transmission Electron Microscopy

HRTEM images were taken with a top-entry JEOL 2000-EX transmission electron microscope at 200 kV with the electron beam aligned along the [110] axis of the specimen.

### Analysis

All analyses described here were made using the Peak Pairs Analysis software, which is a plug-in for DigitalMicrograph (DM) developed by HREM Research with the collaboration of the original developer, Pedro L. Galindo from the University of Cádiz.

Strain determination from TEM images is based on the assumption that there is a direct relationship between the intensity maxima in the image and the position of atomic columns in the sample. A diagram of the usual steps involved in the strain mapping analysis is shown in Figure 1.

## HRTEM Image Requirements

HRTEM images should have enough resolution so that the intensity maxima are clearly visible. The distance between adjacent maxima will directly affect the resolution of the results. In order to be able to apply strain mapping, a reference area should be defined. Therefore, the image should contain non-deformed areas far away from defects so that they can be taken as a reference. Contrast changes due to changes in sample thickness should be avoided. Additionally, the microscope transfer function affects the phases of the diffracted beams differently depending on their position in Fourier space, giving rise to strain artifacts. In the case of strained heterostructures, the effect of column bending needs to be carefully considered.

## Image Filtering

Image filtering is needed not only to reduce noise in the image but also to smooth the image around the peaks, greatly improving the precision at which the intensity maxima are determined. Currently, there are several approaches to HRTEM image filtering. Different algorithms may be used, having different properties and complexity levels depending on the necessities of the researcher. Bragg filtering is considered as the most efficient algorithm in usual applications, but low-pass

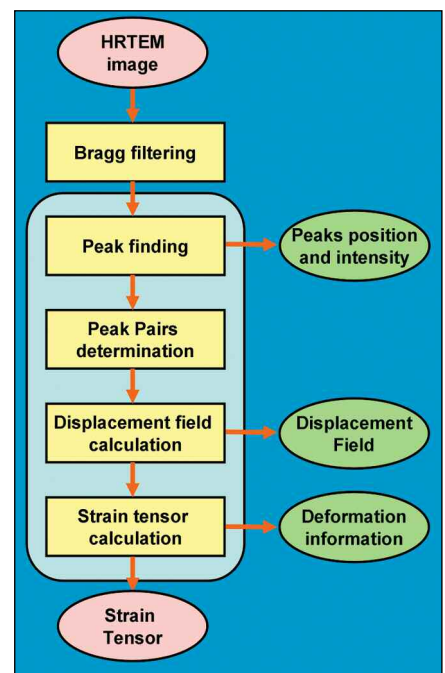


Figure 1: Schematic of the steps involved in strain mapping using Peak Pairs Analysis.



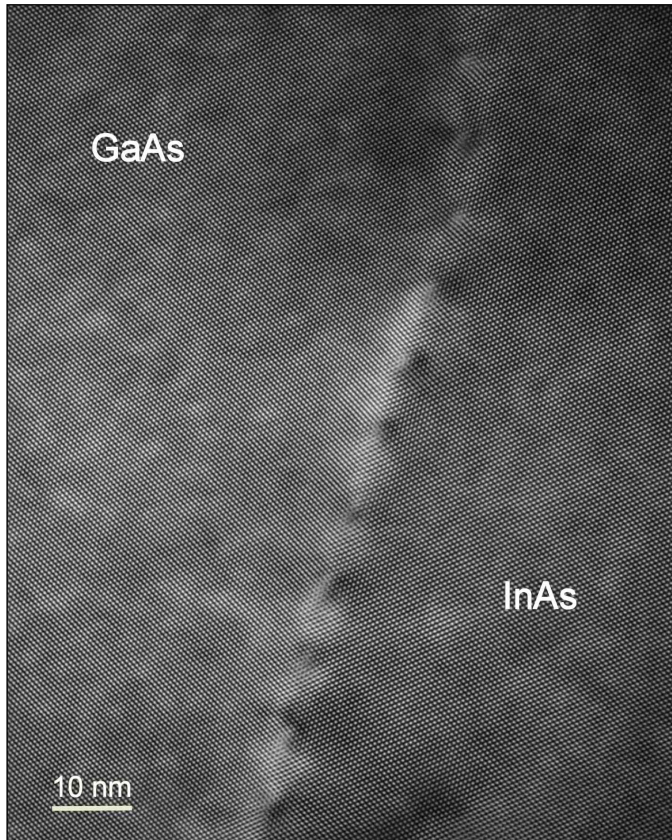


Figure 2:  
High-resolution transmission electron microscope (HRTEM) image of an InAs/GaAs (001) interface taken with a JEOL 2000 EX TEM at 200 kV. Point resolution = 0.21 nm.

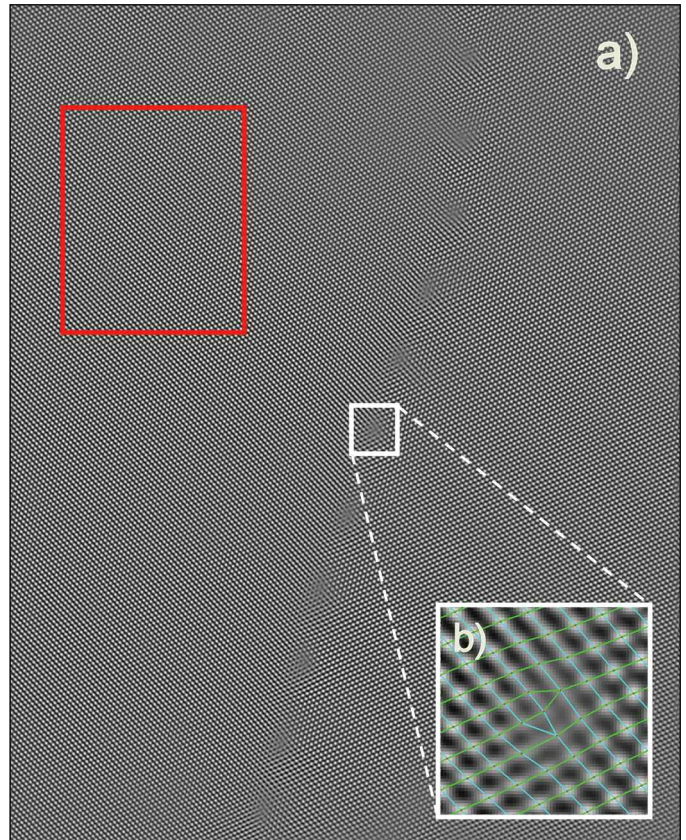


Figure 3:  
(a) Bragg filtered image. The red square indicates the region of the image taken as reference.  
(b) Grid details obtained by peak pairs analysis around a dislocation.

and/or adaptive Wiener filters are also often very useful. Bragg filtering consists of placing a mask around two or more Bragg peaks in the Fourier transform of the image and then applying an inverse Fourier transform. The size of the mask at each Bragg peak determines the range of frequencies that are preserved by the filter.

#### Peak Detection

Once the image has been filtered, all the intensity peaks are automatically located using 8-neighbourhood maxima detection at the pixel level. In order to get sub-pixel resolution, a 2D quadratic function is fitted using grey levels in the neighbourhood of each peak, and solving the resulting equations for the maxima.

#### Peak Pairs Detection

The software then searches for pairs of peaks that have a relative distance and direction. This process is done twice, using two different basis vectors whose magnitude and directions are determined directly from two of the peaks chosen by the user in the Bragg filtering stage. In order to reduce errors in the location of pairs, an affine transformation defined by a pair of basis vectors is applied. This transformation greatly reduces potential errors in the determination of pairs. Using all pairs of peaks, the displacement field is calculated at the positions of atomic columns using the difference between local peak pairs and basis vectors. Peak pairs can be safely found by using roughly estimated basis vectors, and the

initial displacement maps can be estimated.

Subsequently, using peak-pair information, displacement fields are evaluated along two basis vectors. Here, the displacement maps were evaluated using an average structure corresponding to approximated base vectors.

#### Strain Calculation

The accuracy of the strain map strongly depends on the accuracy of the basis vectors of the undistorted structure. The original basis vectors can be refined for a specified reference region with high accuracy by adjusting the initially estimated displacement maps. Thus, the displacement field, and hence the strain field, can be evaluated in terms of the selected reference structure in the image. At this point, by defining a region corresponding to a reference structure, we can update the base vectors and get refined displacement maps. The reference area should be taken on the same image, but far away from deformed regions. Using the refined displacement maps, the strain field is calculated with high accuracy after some mathematical treatments which are completely detailed in [3].

#### RESULTS

The HRTEM image shown in Figure 2 is of an InAs/GaAs (001) interface with a point resolution of 0.21 nm. This image was taken in a specimen area where thickness fluctuations were minimal.

Since an experimental HRTEM image is noisy, a Bragg filter was applied to the original image by selecting two main reflections and a

proper mask size in Fourier space (Figure 3a). Intensity maxima were automatically located with sub-pixel resolution, and pairs of peaks were searched along two predefined directions and distances defined by two basis vectors. The set of pairs described a grid across the material, where all distortions had been automatically identified on a local basis. Material defects such as dislocations could now easily be located, as shown in Figure 3b.

Subsequently, using peak-pair information, displacement fields were evaluated along two basis vectors. Here, the displacement maps were evaluated using an average structure corresponding to selected Bragg peaks. A region-of-interest corresponding to the reference area was then defined by using a rectangle (shown in red in the upper-left corner of Figure 3), and used to refine the original displacement maps.

From the resulting displacement field, the strain field components  $\epsilon_{xx}$ ,  $\epsilon_{yy}$ ,  $\epsilon_{xy}$  and  $\epsilon_{yx}$  were finally calculated (Figure 4). The green colour in the strain images corresponds to the unstrained GaAs area, which was also the material defined as the reference and set to 0% strain. The orange area corresponds to the InAs material showing about 7% strain in reference to GaAs in the  $\epsilon_{xx}$  and  $\epsilon_{yy}$  maps, and 0% strain in the  $\epsilon_{xy}$  and  $\epsilon_{yx}$  maps. This situation is characteristic of two different materials, with the same crystalline structure and different lattice constants.

The  $\epsilon_{xx}$  and  $\epsilon_{yy}$  values show that the InAs was almost completely relaxed due to the existence of a misfit dislocation network just at



the InAs/GaAs interface. The existence of an array of regularly arranged misfit dislocations at the InAs/GaAs interface was clearly visible from the strain maps. Misfit dislocations compensate for differences in the lattice constants. Let us note that the dislocations were regularly spaced, following the typical dislocation configuration associated with the relief of the epilayer-substrate lattice misfit stress.

## DISCUSSION

Strain mapping is a very useful tool for the determination of distortions in an image, and can be applied not only to HRTEM images, but also to any type of lattice image (e.g. it can be applied to high resolution Z-contrast images).

When applied to HRTEM images the reliability of strain mapping is somewhat problematic due to some known effects, such as defocus, local crystal tilts, thin foil relaxation, local thickness variations and changes in the composition across the material, and so great care should be taken to ensure that a proper analysis is applied [4]. Only when all these factors are taken into account does the method offer a reliable way of extracting quantitative strain information at an atomic scale.

Peak Pairs Analysis is a recently developed method for strain mapping operating in image space, reducing memory and CPU requirements. With respect to other approaches, it achieves high resolution results, because more than two beams can be used to determine the strain, and its behaviour is unaltered in the presence of defects as well as in the strain mapping of nonhomogeneous surfaces. As an example, Peak Pairs has been used to identify critical regions in quantum dots structures [5].

Another advantage is that peak-pairs information can be used to automatically find atomic column positions equivalent to the specified atomic columns within a unit cell (a motif), and to evaluate all the equivalent peak intensities within a specified area.

Strain mapping is often used not only to identify defects and/or distortions in the image, but also to rectify distorted images. CTEM projector lens systems, STEM scanning systems, CCD cameras or scanners often distort the images they form. Fortunately, these geometric distortions are frequently systematic, and it is therefore possible to eliminate these distortions by measuring them using the image of an unstrained specimen, and using the information contained in the resulting displacement maps to define a warp function, that when applied to a distorted image restores the undistorted one [6].

## CONCLUSIONS

Recent advances in digital imaging have offered the possibility of locally determining the elastic strain of materials from HRTEM images very precisely. Several methodologies have been described in the literature, both in real and Fourier space. Peak Pairs Analysis is a real space algorithm for strain mapping, offering valuable advantages, such as its performance, accuracy and intuitiveness. It works on

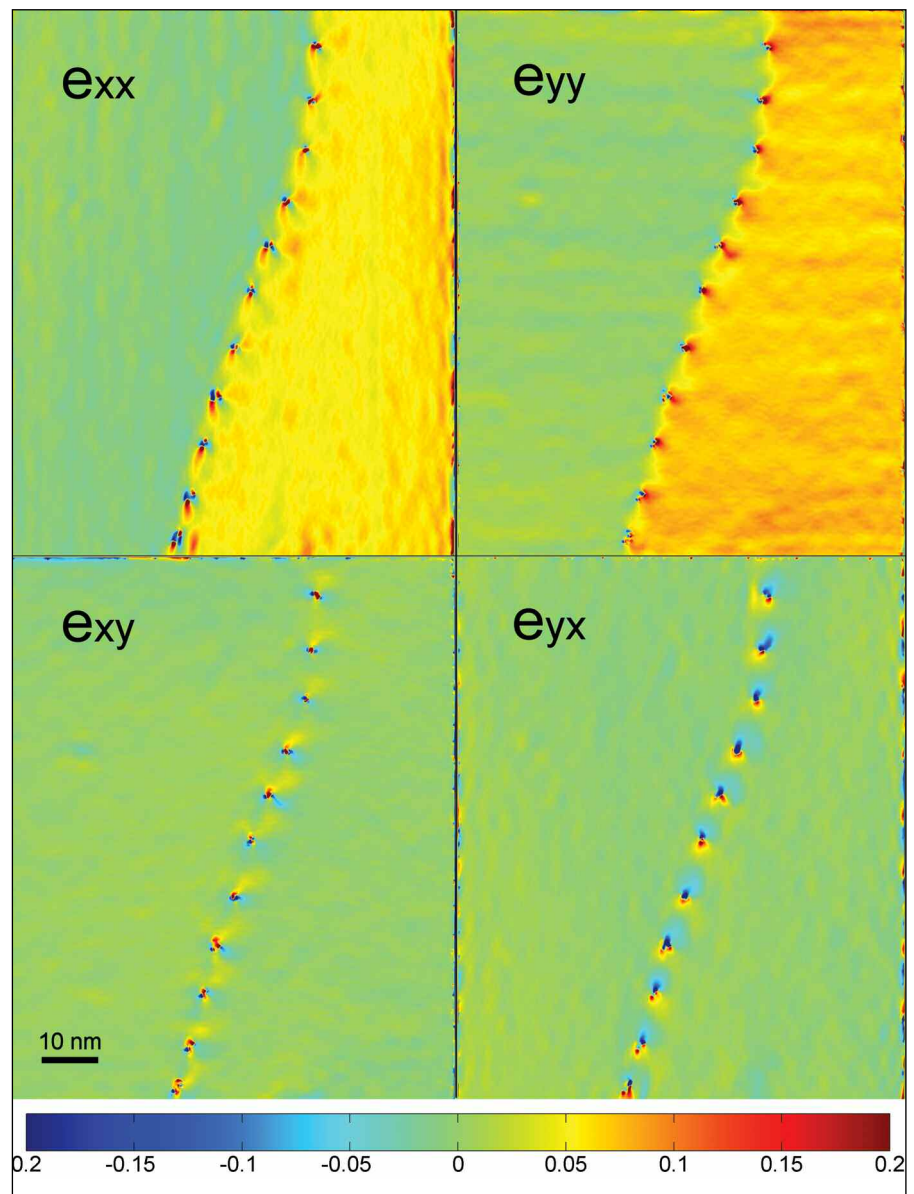


Figure 4:

Components of the strain tensors  $\epsilon_{xx}$ ,  $\epsilon_{yy}$ ,  $\epsilon_{xy}$  and  $\epsilon_{yx}$  showing the presence of two well-distinguished materials corresponding to GaAs and InAs and a misfit dislocation network just at the InAs/GaAs interface.

a filtered image by locating pairs of peaks along two predefined basis vectors. From the deformation of each pair across the image, it is possible to reconstruct the displacement field, and to calculate strain maps. Strain maps can be used to identify defects and/or quantify distortions in the image with respect to a reference area, offering the researcher a valuable tool to locate different phases or analyze defects and even to rectify distorted images.

Peak Pairs Analysis [7] has been implemented as a plug-in for DigitalMicrograph [8], the industry leading software for electron microscopy. Its integration provides the user with complete access to all the other powerful functions and useful features present in DigitalMicrograph.

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