Micron 110 (2018) 18–27

Contents lists available at ScienceDirect

Micron

journal homepage: www.elsevier.com/locate/micron

Correcting sample drift using Fourier harmonics

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ARTICLE INFO

Keywords:
Drift correction
Image distortion
Fourier analysis
Harmonic analysis

ABSTRACT

During image acquisition of crystalline materials by high-resolution scanning transmission electron microscopy, the sample drift could lead to distortions and shears that hinder their quantitative analysis and characterization. In order to measure and correct this effect, several authors have proposed different methodologies making use of series of images. In this work, we introduce a methodology to determine the drift angle via Fourier analysis by using a single image based on the measurements between the angles of the second Fourier harmonics in different quadrants. Two different approaches, that are independent of the angle of acquisition of the image, are evaluated. In addition, our results demonstrate that the determination of the drift angle is more accurate by using the measurements of non-consecutive quadrants when the angle of acquisition is an odd multiple of 45°.

1. Introduction

Images of crystals obtained in a scanning transmission electron microscope (STEM), using a High Angle Annular Dark Field (HAADF) detector, provide a relatively uniform image contrast peaked at atomic columns that depends on the atomic number (Z-contrast) (Nellist and Pennycook, 2000; Pennycook and Jesson, 1990a, 1990b). The analysis of atomic displacements that can be carried out directly in real o reciprocal space is a useful tool to obtain strain maps that reveal the stress state of the materials. However, systematic displacement produced by sample drift during image acquisition in scanning microscopes could introduce distortions, expansions, compressions and shears of the lattice positions that invalid them to perform quantitative strain analyses (Braidy et al., 2012; Nakanishi et al., 2002; Rečnik et al., 2005). Despite efforts to reduce vibration, air flow/fields, and temperature fluctuations in STEM laboratories, some sample drift affecting the final image is very often inevitable (Muller and Grazul, 2001; Sang and LeBeau, 2014; von Harrach, 1995).

Over the years a number of software-based solutions designed to drift analysis have been developed. Real space approaches to identify drift rely on the statistical measurement of the distances between the nearest atomic columns in the whole image. The work of Zuo et al. (2014) for example, applies template matching for quantitative lattice analysis achieving a precision of few picometers in the calculation of lattice displacements. In general current proposals have been successfully addressed to both, drift detection and drift correction, by using series of images assuming uniform drift rates. Indeed, Rečnik et al. (2005) based his method on finding the displaced vertices in STEM images and warping to geometrically correct the reference grid of the object. Saito et al. (2009) pointed out that each frame should be acquired using a short probe dwell time at each pixel, since a high-speed multiple imaging can be more effective to accuracy improve the signal-to-noise ratio (SNR). Jones and Nellist (2013) used a defect-free zone of the image with a real space iterative method to determine the affine transformation that corrects the image and more recently (Jones et al., 2015) they have presented a distortion correction technique based on non-rigid registration of serial microscopy data, whereas Sang and LeBeau (2014) developed the revolving STEM method, RevSTEM, based on rotating the scan coordinate system between successive frames during the acquisition process of the whole series. They demonstrated that this series can contain the information necessary to analyse sample drift rate and direction, and they used histograms of the distances between the atom neighbours to identify drift. Ophus et al. (2016) developed an algorithm to correct all linear and nonlinear drift distortions using kernel density estimation and a Fourier weighting scheme to further reduce error and correcting the scanline origin positions from several images. Other approaches, from simple registration and averaging (Berkels et al., 2012) to more reliable alignment and restoration methods (Binev et al., 2012; Jones et al., 2015; Yankovich et al., 2014) have been proposed, including super-resolution, that provides enhanced images and more accurate quantitative analysis (Bárcena-González et al., 2016, 2017).

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https://doi.org/10.1016/j.micron.2018.04.004
Received 23 January 2018; Received in revised form 13 April 2018; Accepted 13 April 2018

0968-4328/

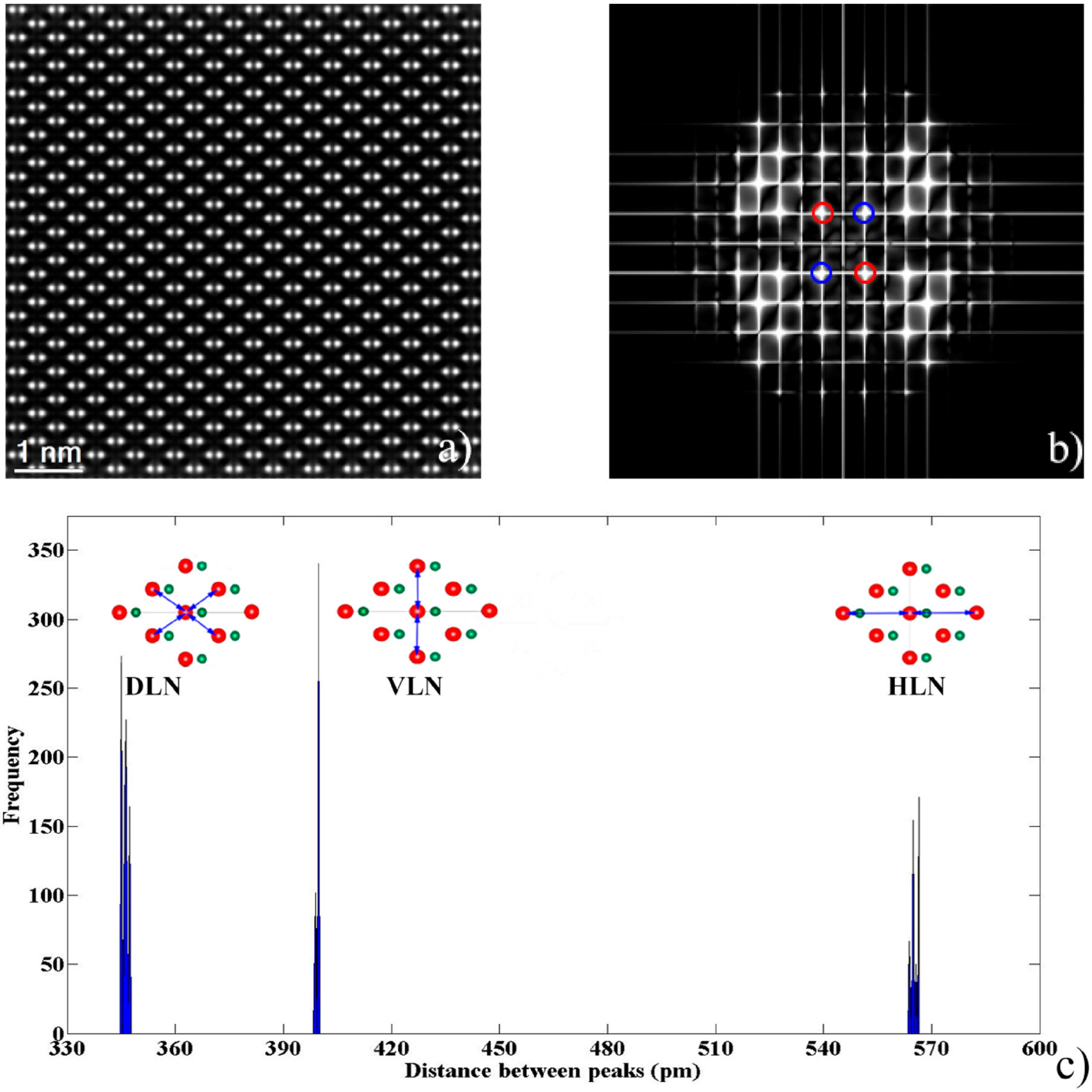

Fig. 1. a) Simulated image of Gallium Arsenide (GaAs) without drift effect (acquisition angle ϕ = 0° and drift angle α = 0°). b) Discrete Fourier Transform and c) VLN, HLN and SLN distance histograms calculated from peak locations determined by fitting atom column intensities to a Gaussian distribution.

In this work, we introduce a method to determine the drift angle that uses only a single STEM image. The determined drift angle could be used afterwards to make an inverse affine transformation obtaining a free-distortion image. Our method is based on the measurements of the angle that is formed by the second Fourier harmonics in the Fourier Transform image and the acquisition angle regarding a principal crystalline direction of the crystal. The method has been demonstrated on a mathematical derivation and probed in experimental images on several semiconductor images. As we can see in the follow, the accuracy of the method has a high dependence of the choice of this angle of acquisition.

2. Materials & methods

A supercell of Gallium Arsenide (GaAs) containing all the information about atom positions, compositions, site occupancy and Debye-Waller factors has been generated. This model together with the parameters of a 100 kV dedicated VG Microscope HB501UX STEM constitutes the input to the SICSTEM program (Pizarro et al., 2008). A set of 360 images oriented along the [110] direction are obtained by simulating a rotation of the acquisition angle (ϕ) from 0° to 360° in steps of 1° (defining the acquisition angle as the angle between the y direction of the image and the $[\bar{1}10]$of the crystal). In these simulated images of 701 × 701 pixels, where the x-direction is along the [001], we have added a linear drift effect. For it, each row of pixels in the image is shifted to the right a number of pixels that is proportional to the distance from the upper left corner of the image. In this way, the drift could be defined by a drift angle (α). In this paper, we have obtained five different series of images with different drift angle values of 1°, 3°, 5°, 7° and 10°.

Fig. 1a shows a simulated image of GaAs (acquisition angle ϕ = 0° and drift angle $\alpha = 0°$). Fig. 1b shows the discrete Fourier transform (DFT), using a real-space windowing (Hovden et al., 2015), where the peaks corresponding to the fundamental frequencies have been marked with red and blue circles. Fig. 1c shows, as proposed in (Sang and LeBeau, 2014), the histogram of the distances, where we can distinguish three slender peaks that corresponding with the distances between the closest atom columns in the vertical, horizontal and diagonal directions named as VLN, HLN and DLN, respectively.

In Fig. 2a, a simulated image with the same acquisition angle ϕ = 0° but with a drift angle, $\alpha = 5°$ is shown. This drift can be identified in the frequency domain (Fig. 2b) by different vertical displacements along the y-axis of the fundamental and harmonic frequencies in each