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ATOMIC POSITIONS FROM HIGH RESOLUTION TRANSMISSION ELECTRON MICROSCOPY IMAGES OF GRAIN BOUNDARIES

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ABSTRACT

High resolution transmission electron microscopy images are constituted by diffuse spots which correspond to atomic columns of the observed crystal. In the case of grain boundaries including defects, the atomic positions accounting for the elastic distorsions of the crystals can be calculated. In order to compare calculated and experimental positions, it is necessary to extract the "centers" of the spots from experimental images. A simple method is proposed here, involving two steps: first, the identification of spot zones, with individual masks, then calculation of intensity weighed center of each spot inside each mask. The method was tested on a simple image and applied on a Ni_3Al-Ni_3Nb grain boundary, showing satisfactory agreement between predicted and experimental atomic positions.

Key words: high resolution transmission electron microscopy (HRTEM), interfaces, centroid, position measurement.

INTRODUCTION

The study of interfaces by high resolution transmission electron microscopy (HRTEM) now involves quantitative analysis of images (Ernst *et al.* 1996). The images can therefore be quantitatively be compared to computed images. In the case of perfect interfaces, periodicities allow to use global comparisons from cross correlations (Ernst *et al.* 1996), FFT (Hÿtch and Gandais 1995) or shift detections through averaging (Lay *et al.* 1996).

In the case of defects at interfaces, computed atomic positions are available from elasticity calculations (Bonnet and Loubradou 1997), which predict the inhomogeneous field of deformations, so that direct comparisons of positions should be used. The present paper proposes a simple method to extract positions from experimental HRTEM images using automatic image analyser.

METHOD

The atomic columns of the observed crystals appear on HRTEM images (Fig. 1) as diffuse spots. A significant noise can be present, so that the atomic positions cannot be directly obtained as a simple maximum of intensity. Among the various methods to get a center (West and Clarke 1990) the "standard first order moment", *i.e.*, the center of gravity using the intensity of the image as weighing function, is a simple and convenient way to get a satisfactory centroid. The ability of the method to achieve subpixel accuracy is generally accepted (West and Clarke 1990, Patwardhan 1997).

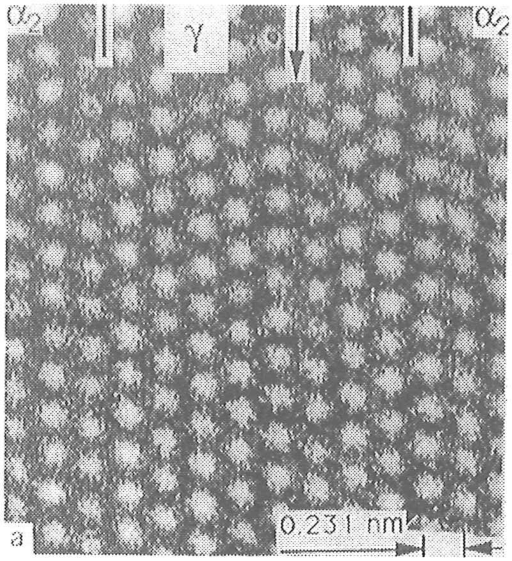

Fig. 1. HRTEM image of a Ti-30%Al alloy showing alternated α_2 and γ layers (courtesy R. Bonnet and M. Loubradou). The image is 505X554 pixels, with 6 10^{-3}nm/pixel.

In the present case, the problem is only to determine, for each spot, the extension of the area in which the calculation of the centroïd must be performed. A template image, constituted by zones which individually mark each spot region, is used here.

The first step of image analysis is therefore to build this template image (Fig. 2) from the following sequence, involving thresholding and transformations of mathematical morphology (Serra, 1982):

- a simple thresholding of the grey level image (Fig. 2a), limited to the higher intensities, roughly locates the zones of interest (Fig. 2b). Small unsignificant dots are eliminated using an adapted opening and artificially separated areas are connected using a closing (Fig. 2c). At this step, some hand made corrections can be necessary, depending on the image quality. Holes are eliminated by way of a "holefill" filter;
- the geodesic center of each zone is calculated using homotopic thinnings (Fig. 2d). This rough approximation of the centroid is not suitable for accurate measurements;
- from these centers, the template zones (Fig. 2e) are build using thickening (for instance, 4-connexity "L-skeleton" thickening), the size of the thickening being adapted so that the areas contain most of spot information;
- the areas in contact with the edge of the image are removed to avoid biases due uncomplete information (Fig. 2f).

This procedure ensures to get one, roughly isotropic, separated area for each spot on the image.

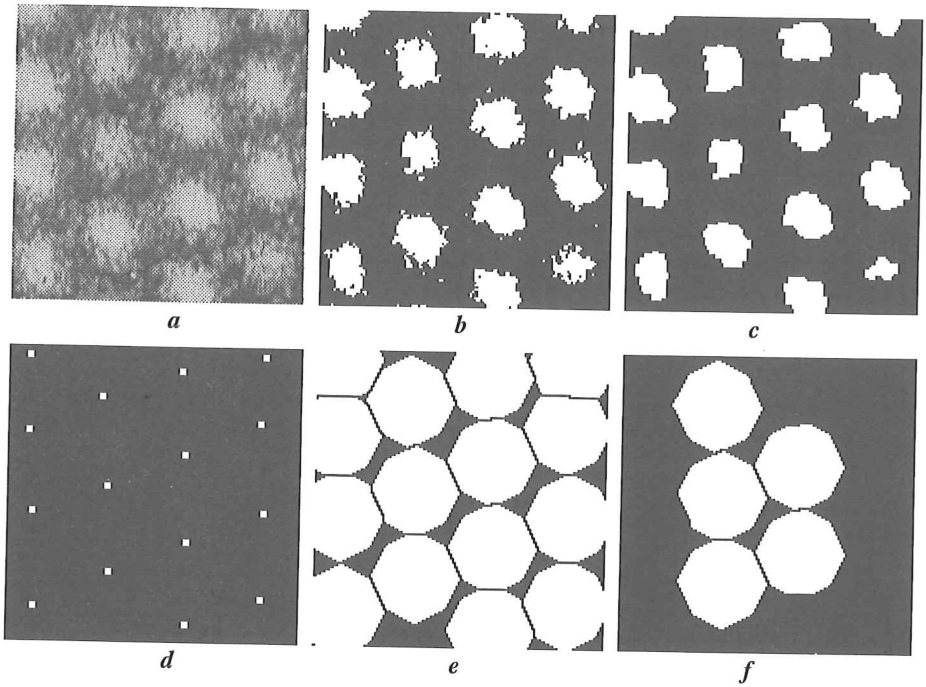

Fig. 2. Illustration of the sequence for building a template image, on a small 100X100 pixels image. a. initial image; b. thresholded image; c. after opening and closing by a 3X3 square; d. geodesic centers (dilated to be seen on the figure); e. thickened image, mask areas; f. final template image after border removing

Using this image, the second step is simply to get, for each template area, the centroid inside the area (Fig. 3).

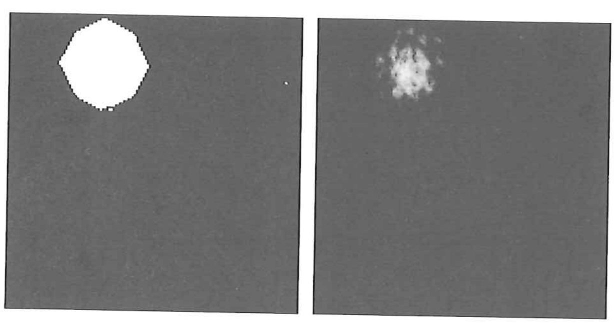

Fig. 3. Use of an area from Fig. 2f as template to compute the center of gravity of a spot.

DISCUSSION

The above procedure was implemented on a Windows 95 workstation, using the image analysis software Aphelion™ produced by ADCIS S.A.(France) and Amerinex Applied Imaging Inc.(USA).

Tests have been performed on the simple image of Fig 1, in order to evaluate the sensitivity of measurements with respect to image acquisition (digitizing) and template building. Two different digitized images (I1 and I2) of the same micrograph were grabbed, using or not the "quality improving" option of the numerical scanner. Two template images (T1 and T2) were also defined from image I1, using two different thresholds and the above template building procedure. Three sets of 136 centroïd positions were calculated, using the three (image+template) following couples: (I1+T1), (I1+T2), (I2+T1). The sensitivity of the center evaluation to image acquisition was analysed by comparison of results of (I1+T1) and (I2+T1) (two images, one template). The sensitivity to template building was analysed from (I1+T1) and (I1+T2) (one image, two templates).

In each case, the difference between the two evaluations of each of the 136 spot center positions (x,y) was calculated ($\sqrt{\delta x^2+\delta y^2}$). The statistical analysis results are shown in Table 1.

Table 1. Statistical analysis of differences (euclidean distance) between center positionss due to acquisition and template, from the 136 spots of the micrograph of Fig. 1.

	Acquisition: (I1,T1) and (I2,T1) (pixel unit)	Template: (I1,T1) and (I1,T2) (pixel unit)	Template: (I1,T1) and (I1,T2) (nm)
mean difference	0.019	0.35	0.02
standard deviation	0.012	0.34	0.02
max difference	0.071	1.50	0.09

The effect of the different acquisitions is quite negligible (about 0.02 pixel). The difference due to the template appears larger, as maximum differences up to 1.5 pixel are denoted. However, it must be noticed that only a small fraction of points show more than 0.5 pixel difference (Fig. 4), and that the mean value and standard deviation remains small. The larger differences have been obtained for particles close to the edges of the image, in which the labels and arrows drawn on the original image (Fig. 1) introduced abnormal biases on the template areas. It must also be noticed that 1 pixel is only 0.006 nm on the actual image, so that the sensitivity with respect to template building remains small (last column of Table 1).

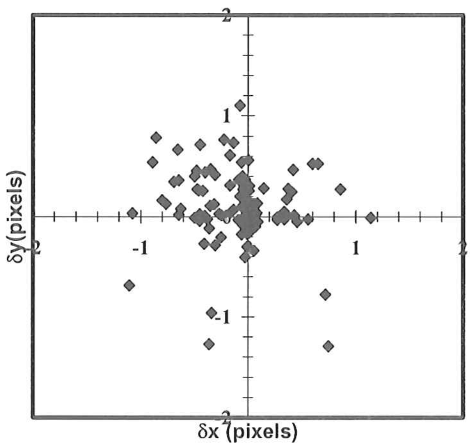

Fig. 4. Scattering diagram showing the difference δy in y coordinate vs. the difference δx in x for each point, measured using 2 template images obtained from two different thresholds. Most of the 136 points are packed in the center zone of the diagram.

R. Bonnet and M. Loubradou (1997) have compared experimental positions obtained from the present method (267 centers) with their own calculations in the case of a Ni_3Al-Ni_3Nb heterointerface, around a 90° misfit dislocation. Their histogram of distances between calculated and measured positions shows a mean value around 0.03 to 0.035nm, with only about 2% values larger than 0.05nm, which is quite satisfactory.

CONCLUSION

The present method is simple and easy to implement on a classic image analysis software. The tests performed here and by Bonnet and Loubradou (1997) show that it can give accurate enough results, although, of course, the quality of the results always depend on the quality of the image.

Its application could help to answer some questions such as the difference between atom centers positions and spot positions on the images: measurements on simulated images based on calculated positions are easy and should be performed. The exploitation of the obtained data should also be developed, for instance finding a pertinent quantitative comparison of calculated and experimental images which contain heterogeneous deformations.

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