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Automation

Development of SPM Quantitative Micromorphology Analysis Software

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Abstract: Scanning Probe Microscope (SPM) has great advantages in quantitative micromorphology analysis because of its convenience in obtaining micromorphology information of materials on nanometer or atomic scale under control of a computer. Based on an established SPM quantitative micromorphology analysis model, an SPM image analysis software which can calculate both two- and three-dimensional micromorphology parameters is developed.

Key words: SPM; quantitative micromorphology; analysis software

With rapid development of modern science and technology, more studies require high resolution and quantitative morphology information [1], especially in the field of nanotechnology, ultrafine powder processing, microelectronics, *etc.*. Conventional surface analysis methods can no longer meet this ever-growing demand. Scanning Probe Microscope (SPM) [2], a newly developed surface analysis technique, has the ability to obtain quantitatively micromorphology information on nanometer or atomic scale. However, for lack of a proper software, this ability of SPM has not been put to full use in related studies [3]. Therefore, a powerful quantitative micromorphology analysis software for SPM [4] has to be developed. This paper introduced an SPM Image Analysis Software (SPMIAS) developed in C^{++} language based on a data process model established by the author.

1 Data Process Model of SPMIAS

Micromorphology information obtained by means of SPM is voltage signals or gray scale signals collected at each scanning point and correspond to the altitude of surface. These signals are saved as image files in a computer. To calculate micromorphology parameters, a data process model is established in **figure 1**, which includes the setting up of a suitable coordination system, calculation of surface and profile departure, determination of points on a given line on SPM image and transformation of voltage signals or gray scale signals to nanometer values (*i.e.*, signal scaling). A brief explanation of each part of this data process model is presented later in the paper. Among all of these data process steps, the setting up of the suitable coordination system and the signal scaling are the most important.

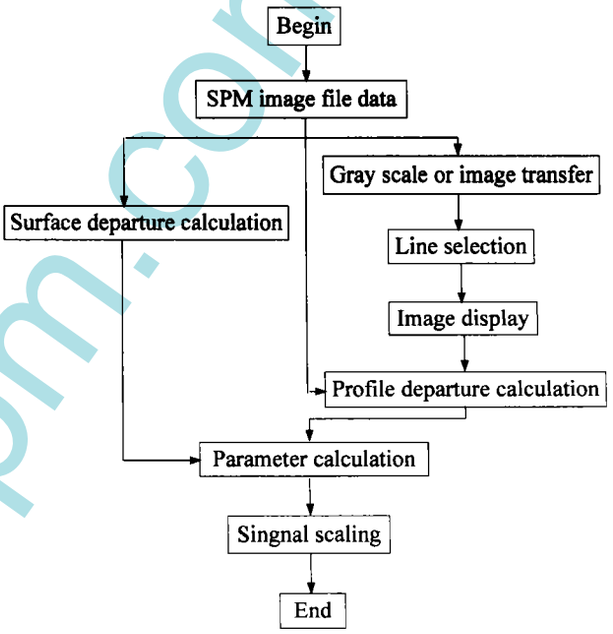

Figure 1 Data process model of SPMIAS.

2 Calculation of Surface Departure

Surface departure H_{ij} is the departure of sampling points from the reference plane. Three-dimensional micromorphology parameters are calculated based on H_{ij}. To calculate H_{ij}, a reference plane is to be found. This can be done by least square method, but before any calculation, a coordinate system must be established. In this study, the coordinate system is so chosen that its origin is at the left upper corner of the image, X and Y axes coincide with the vertical and horizontal edges of the image respectively and Z axis is perpendicular to the image. $Z(x,y)$ is the value along Z axis at point (x,y). Because sampling points of SPM are dispersed, $Z(x,y)$ can be denoted by Z_{ij}, $i,j=1,2,3,\cdots,n$. Then the

formula of the reference plane is

$$Z(x,y)=Ax+By+C,$$

least square method yields the equation

$$\Sigma\Sigma\,[Z_{ij}-(Ax+By+C)]^2=\mathrm{MIN}.$$

This equation can also be written in the following form:

$$\begin{bmatrix}\Sigma\Sigma\, i^2 & \Sigma\Sigma\, ij & \Sigma\Sigma\, i\\ \Sigma\Sigma\, ij & \Sigma\Sigma\, j^2 & \Sigma\Sigma\, j\\ \Sigma\Sigma\, i & \Sigma\Sigma\, j & \Sigma\Sigma\, 1\end{bmatrix}\begin{bmatrix}A\\B\\C\end{bmatrix}=\begin{bmatrix}\Sigma\Sigma\, iZ_{ij}\\ \Sigma\Sigma\, jZ_{ij}\\ \Sigma\Sigma\, Z_{ij}\end{bmatrix}.$$

By solving this equation, A, B, C in the reference plane equation can be obtained. Then the surface departure H_{ij} at sampling point (i,j) can be calculated through

$$H_{ij}=\frac{Z_{ij}-(Ai+Bj+C)}{\sqrt{1+A^2+B^2}}.$$

3 Determination of the Points on a Given Line

If N_x is the number of sampling points in X direction, and N_y the number in Y direction, then x and y range from 1 to N_x and 1 to N_y respectively. $Z(x, y)$ is the profile value at point (x,y). If (x_1,y_1), (x_2,y_2) are two points on a given line AB, the coordinates of any other point (x_i,y_i) on line AB can be calculated in the following way.

If $|x_1-x_2|\geq|y_1-y_2|$ and $x_1>x_2$,

$$\begin{cases}y_i=\dfrac{y_1-y_2}{x_1-x_2}\times i+y_2-1\\ x_i=x_2+i-1\end{cases};$$

If $|x_1-x_2|\geq|y_1-y_2|$ and $x_2>x_1$,

$$\begin{cases}y_i=\dfrac{y_2-y_1}{x_2-x_1}\times i+y_1-1\\ x_i=x_1+i-1\end{cases};$$

If $|x_1-x_2|<|y_1-y_2|$ and $y_1>y_2$,

$$\begin{cases}x_i=\dfrac{x_1-x_2}{y_1-y_2}\times i+x_2-1\\ y_i=y_2+i-1\end{cases};$$

If $|x_1-x_2|<|y_1-y_2|$ and $y_2>y_1$,

$$\begin{cases}x_i=\dfrac{x_2-x_1}{y_2-y_1}\times i+x_1-1\\ y_i=y_1+i-1\end{cases}.$$

Then, the profile value on a given line at a given point (x_i,y_i) can be calculated as

$$Z_i=Z[y_i\times Ny+x_i],\ i=1,2,\cdots,N$$

4 Calculation of Profile Departure

Profile departure H_i is the distance between the profile and the reference line at the sampling point. $Z(x)$ is the profile value at point x. Because the sampling points are dispersed, $Z(x)$ can be denoted by Z_i, $i=1,2,3,\cdots$, n. The equation of the reference line is $Z(x)=Ax+B$. Least square method yields

$$\sum_{i=1}^{n}[Z_i-(Ax+B)]^2=\mathrm{MIN}.$$

This equation can also be written in the following form:

$$\begin{bmatrix}\Sigma i^2 & \Sigma i\\ \Sigma i & \Sigma 1\end{bmatrix}\begin{bmatrix}A\\B\end{bmatrix}=\begin{bmatrix}\Sigma iZ_i\\ \Sigma Z_i\end{bmatrix}.$$

A, B can be obtained by solving this equation. Then profile departure H_i can be calculated through

$$H_i=\frac{Z_i-(Ai+B)}{\sqrt{1+A^2}}.$$

5 Signal Scaling

Signal scaling is the process to transfer voltage signals or gray scale signals in X, Y and Z directions of the image to nanometer values. A standard sample is employed in signal scaling usually. Graphite and grating (standards for sample scaling in X, Y and Z directions, in current study, a 3 μm×3 μm×100.0 nm grating is used) are often served as standard samples. In this study, signal scaling is done in following steps: (I) Scanning the standard sample and the experimental sample under the same experiment conditions using SPM. (II) Scaling the scanning range in X and Y directions (counting the atom number of graphite or the track number of grating in X and Y directions respectively and multiply them by the interatomic distance of graphite or the grid width of grating). (III) Scaling signals in Z direction by multiplying the image signals of the experimental sample by a transfer factor T_Z. T_Z is the difference between the maximum and the minimum signal value in Z direction divided by the step height of the standard sample (grating).

For a given experiment condition, T_Z is a constant. For different experiment conditions, T_Z is different. T_Z values for different experiment conditions can be obtained by scanning on a standard sample under these experiment conditions and put in a file TF. When a sample is studied, signal scaling can be conveniently conducted by indexing TF for a T_Z corresponding to the experiment condition used and multiplying the image data by this T_Z. Signal scaling in X and Y directions can also be done in the same way.

6 Functions of SPMIAS

Based on the above data process model and data process skills, micromorphology parameters can be calculated [5], such as

R_a, the arithmetical mean deviation of the profile;
R_q, the root-mean-square deviation of the profile;
R_p, the maximum height of profile peak;
R_m, the maximum depth of profile valley;
R_y, the height of the profile;
ADF, the amplitude distribution function of the profile;
BAC, the bearing area carve of the profile;
ACF, the auto-condition function of the profile;
PSP, the power spectral parameters of the profile;
R_{sa}, the arithmetical mean deviation of the surface;
R_{sq}, the root-mean-square deviation of the surface;
R_{sp}, the maximum height of surface peak;
R_{sm}, the maximum depth of surface valley;
R_{sy}, the maximum height of the surface:
SADF, the amplitude distribution function of the surface;
SBAC, the bearing area carve of the surface.

In addition, a software (SPMIAS) to accomplish this work is developed in C^{++} language and run on the Windows Platform. At present, SPMIAS works only on images obtained by CSTM-9000 type SPM. However, after a little modification, SPMIAS can work on any SPM image files. SPMIAS is easy to operate and powerful in function. It can calculate most two- and three-dimensional micromorphology parameters above-mentioned. The function frame of SPMIAS is shown in **figure 2**.

SPMIAS has been tested on a compact disk [5]. Results showed that SPMIAS works very well.

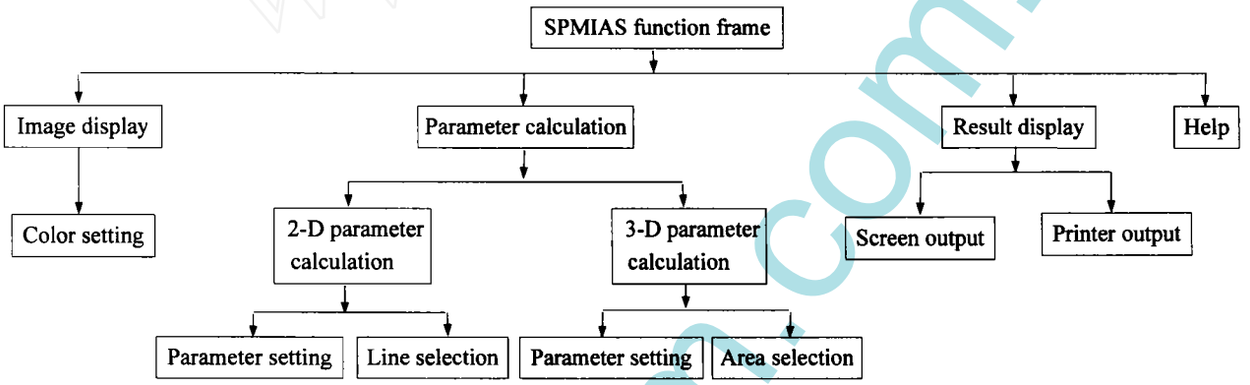

Figure 2 SPMIAS function frame.

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