

01 Jan 2005

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Recommended Citation

Q. Yang et al., "Block Phase Correlation-Based Automatic Drift Compensation for Atomic Force Microscopes," *Proceedings of the 5th IEEE Conference on Nanotechnology (2005, Nagoya, Japan)*, Institute of Electrical and Electronics Engineers (IEEE), Jan 2005.

The definitive version is available at <https://doi.org/10.1109/NANO.2005.1500773>

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Block Phase Correlation-based Automatic Drift Compensation for Atomic Force Microscopes

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Abstract – Automatic nanomanipulation and nanofabrication with an Atomic Force Microscope (AFM) is a precursor for nanomanufacturing. In ambient conditions without stringent environmental controls, nanomanipulation tasks require extensive human intervention to compensate for the many spatial uncertainties of the AFM. Among these uncertainties, thermal drift is especially hard to solve because it tends to increase with time and cannot be compensated simultaneously by feedback. In this paper, an automatic compensation scheme is introduced to measure and estimate drift. This information can be subsequently utilized to compensate for the thermal drift so that a real-time controller for nanomanipulation can be designed as if drift does not exist. Experimental results show that the proposed compensation scheme can predict drift with a small error. Future work is aimed at reducing the error even further through temperature feedback.

Keywords – nanomanipulation, Atomic Force microscope, drift, Phase-Correlation Method, Neural Network

I. INTRODUCTION

Nanomanipulation, which aims at manipulating nanometer size objects with nanometer precision, has become a recent topic since 1990 [1]. By accurately controlling atoms, molecules, or nano scale objects, numerous applications of nanotechnology can be cited in the area of molecular biology and genetics, solid-state physics, chemistry, material science, computer industry and medicine. By reducing the object size from micro meter to nano meter, new sensors, tera-byte capacity memories, DNA computers, man-made materials, etc., would be possible within the near future [2].

Today, manipulation of particles with 10nm in diameter using Atomic Force Microscopes (AFMs) is being investigated by many researchers. However, for new nanotechnology products, there are still many challenges to be solved. When operated in ambient conditions without stringent environmental controls, nanomanipulation requires extensive user intervention to compensate for the spatial uncertainties associated with AFM and its piezoelectric drive mechanism, such as hysteresis, creep, and thermal drift.

Mainly due to temperature change, the tip drifts by thermal effects at a speed of about one atomic diameter per second, even when the voltage inputs for controlling the tip position are held constant. Drift can be greatly reduced by placing an AFM in a temperature-controlled environment, which will be expensive and difficult. Furthermore, other uncertainties such as instrument noise will be introduced, and their effects are similar to that of the thermal drift.

Among these uncertainties, hysteresis can be reduced by scanning in the same direction while creep effects almost vanish by waiting a few minutes after a large scanning motion [3]. However, the effect of drift will increase with time and it cannot be compensated. Typically, it will take hours for an experienced operator to construct a pattern through the manipulation of several nano particles using AFM. To efficiently and successfully accomplish such tasks or even more complex ones, automated manipulation is desirable. For an automated nanomanipulation, drift compensation is the first step.

II. PROBLEM STATEMENT

Due to thermal changes in ambient conditions, drift usually appears in successive AFM scans of a sample even when the scanning parameters are not altered. In the x-y plane, drift can be observed as a translation between different images, as shown in Fig. 1. From the height data of the sample, it can be observed that drift is present even in the z direction. The drift velocities on the x-y plane are reported to vary from 0.01~0.1 nm/s [3]. So the drift between two images taken at 256 sec interval can be as much as 25.6 nm, which is larger than the diameter of the particles that are normally manipulated. In our experiments, drift in the z-direction is about 0.005 nm/s.

Because the topographic data provided by an AFM are

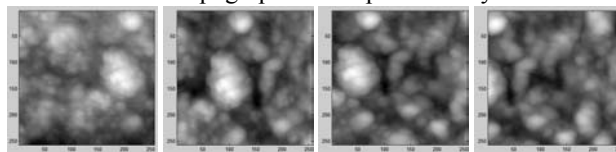


Fig. 1. Image sequences taken at 256 sec intervals showing drift on the x, y plan. The scanned area is 512×512nm².

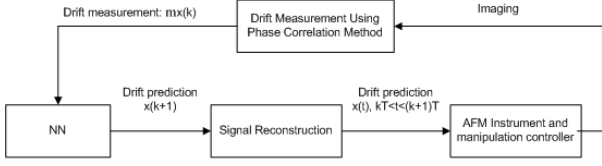


Fig. 2. Block diagram of the proposed drift compensation

actual height information in terms of discrete points on the sample surface, measuring drift in the z direction precisely will be difficult or impossible. A drift compensation scheme can be developed to estimate and compensate for the drift in the x and y directions under the influence of the noise from the z axis so that nanomanipulation can be performed as if drift does not exist. Fortunately, experiments show that the drift in x and y directions can be seen as a translational movement, not rotation. And, there is negligible correlation between the two. Hence, ideally, the height data between the two consecutive collections can be written as

$$h_{k+1}(x, y) = h_k(x + \Delta x_k, y + \Delta y_k) + \Delta z_k \quad (1)$$

where Δx_k , Δy_k and Δz_k denote drift in the x, y and z axes respectively between time instants k and $k + 1$.

To compensate for the horizontal drift, several methods have been proposed [3–8]. All of them are based on sequencing images of an unmodified sample. However, the topography in the scanning region usually has to be changed during the tasks of manipulation or fabrication. Moreover, available techniques [4–8] require that the drift velocity is constant for proper compensation. Though in [3], a Kalman filter based compensator is introduced, a user has to select a tracking window and appropriate model parameters which are very difficult in changing environmental conditions.

In this paper, drift measurement will be accomplished by block-based phase correlation method, which can work smoothly even when some areas of the sample have been manually modified. Taking diverse working conditions into account, an artificial neural network (NN) will be utilized for predicting drift at the next sampling interval.

III. COMPENSATOR SYSTEM

The block diagram of the proposed compensation system is depicted in Fig. 2. For simplicity, the drift in the x direction is shown.

D. AFM Imaging.

As mentioned in the last section, drift in the z direction will include some measurement error from the x and y directions. To minimize this error, gradient will be used for drift measurement, which is computed as

$$g_k(x, y) = h_k(x, y) - h_k(x - 1, y) \quad (2)$$

Substituting (1) into (2) yields

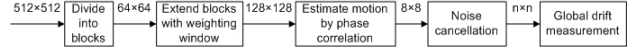


Fig. 3. Schematic diagram of block phase correlation

$$\begin{aligned} g_{k+1}(x, y) &= h_{k+1}(x, y) - h_{k+1}(x - 1, y) \\ &= h_k(x + \Delta x_k, y + \Delta y_k) + \Delta z_k - (h_k(x + \Delta x_k - 1, y + \Delta y_k) + \Delta z_k) \\ &= g_k(x + \Delta x_k, y + \Delta y_k) \end{aligned}$$

where the effect of z-axis drift is eliminated. Moreover, measurement results with gradient-based image interpretation will be better than that of the original height data.

B. Block Phase Correlation Method

The drift measurement problem is similar to the motion estimation (ME) and compensation (MC) in the area of signal processing. Among various techniques, phase correlation method measures the motion directly from the phase correlation map, so that it can give a more accurate and robust estimate of the motion vector and a motion field with much lower entropy [9]. Additionally, phase correlation method is computationally very efficient. In particular this method shows a better performance on translational and large-scale motion since these are the characteristics that are normally observed in AFM drift.

On the other hand, block-based motion estimation and compensation schemes are quite popular in practice due to their robust performance and they do not require object identification. Moreover, they allow some objects in the image to be moved while not influencing the motion estimation of other blocks. This feature makes it possible to estimate the drift of the whole image even when some particles in the vision have been moved which will be usually encountered in nanomanipulation.

In the proposed block-based phase correlation scheme (Fig. 3.), a 512x512 gradient frame is divided into 64x64 pixel blocks and phase correlation calculation is performed for each block. There will be 64 blocks for a 512x512 image. For correctly estimating the cross correlation of corresponding blocks, we extend the blocks to 128x128 pixel in size, centered around the formerly defined 64x64 blocks to calculate phase correlation. It can be readily found that, with bigger blocks, the overlapping area will be larger, and their correlation might be high even with a large amount of drift. Subsequently, a two-dimensional raised cosine window is applied to each 128x128 block to put more weight on our formerly defined 64x64 region, to which a motion vector will be assigned.

The phase correlation method measures the movement between two blocks directly from their phases. The basic principle is briefly given next. Assuming a translational shift between frames k and $k + 1$, the gradient can be written as

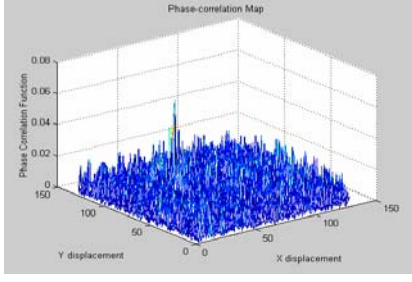


Fig. 4. Phase correlation function between two blocks.

$$g_k(x, y) = g_{k+1}(x + \Delta x, y + \Delta y) \quad (3)$$

The 2-D Fourier transform on (3) is given by

$$G_k(f_x, f_y) = G_{k+1}(f_x, f_y) \exp[j2\pi(\Delta x f_x + \Delta y f_y)] \quad (4)$$

Therefore drift in the spatial-domain is reflected as a phase change in the frequency spectrum. Further, the cross-correlation between the two frames can be written as

$$c_{k,k+1}(x, y) = g_{k+1}(x, y) g_k^*(-x, -y) \quad (5)$$

whose Fourier transform is given by

$$C_{k,k+1}(f_x, f_y) = G_{k+1}(f_x, f_y) G_k^*(f_x, f_y) \quad (6)$$

After normalizing the cross-power spectrum by its magnitude and getting rid of the luminance variation influence during our phase analysis, we obtain its phase as

$$\Phi[C_{k,k+1}(f_x, f_y)] = \frac{G_{k+1}(f_x, f_y) G_k^*(f_x, f_y)}{|G_{k+1}(f_x, f_y) G_k^*(f_x, f_y)|} \quad (7)$$

By substituting (4) into (7), we have

$$\Phi[C_{k,k+1}(f_x, f_y)] = \exp[-j2\pi(\Delta x \cdot f_x + \Delta y \cdot f_y)] \quad (8)$$

whose 2-D inverse transform is given by

$$c_{k,k+1}(x, y) = \delta(x - \Delta x, y - \Delta y) \quad (9)$$

where (9) is an impulse function in the x-y plane. As a result, by finding the location of the spike in (9), we are able to estimate the displacement, which is represented as the motion vector. In practice, since the motion between any two blocks is not pure translational, usually we will get a phase correlation map similar to what is depicted in Fig. 4. In practice, the phase correlations of the blocks in consecutive frames are calculated by 128x128 FFTs.

The highest peak in the phase correlation map usually corresponds to the best match between frames. However, for our 64x64 pixel block, due to several moving objects in the blocks due to different displacements or noise, several peaks can be appearing in the correlation map. In this case several candidates will be selected instead of the one with the highest peak, and then deciding which peak best represents the displacement vector for the object block. Once these candidates are selected, each of these peaks will be examined using image correlation with mean squared error (MSE) criterion. The candidate resulting in

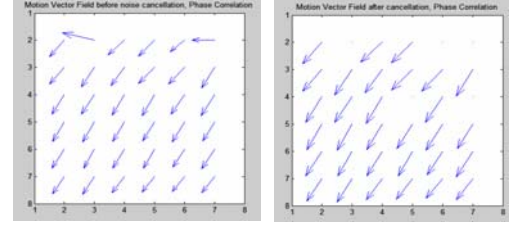


Fig. 5. Motion vector field before and after noise cancellation.

the highest image correlation is identified, and its displacement will be selected as the right motion vector for the object block. (Note that a maximum drift of +/- 64 pixels is determined in order to make sure there is overlapping area between corresponding blocks). In case the drift is too large, we may increase the block size.

Finally, after the motion vectors of all blocks are computed, we can obtain a drift measurement of the whole frame by simply calculating the mean. However, as we have stated before, because of some particles or some parts of the sample having been moved, or pixels corrupted by noise, some blocks will have considerably different motion vectors from others, as shown in Fig. 5. Thus appropriate ones are selected by checking their motion vectors with the mean, and obtaining a better drift measurement by computing the mean of motion vectors of the left blocks.

In practice, a specified constant threshold δ is used for noise cancellation. If the difference between the motion vector of one block and the mean of all the blocks is larger than δ , that block will be removed from the calculation of the final global drift measurement of the whole image. Otherwise, the block will be selected as valid for the final measurement.

C. Time Series Prediction with Neural Networks

After obtaining the drift measurement at time instant k , the drift must be predicted for compensation. In other words, we need to predict the drift value at time instant $k+1$. Although Kalman filter can provide the best estimation based on maximum likelihood optimization, the model and parameters have to be identified under different running conditions.

As an alternative, multilayer neural networks (NN) can be used for drift prediction since neural networks can approximate any nonlinear temporal mapping. Assuming that the environmental conditions will not change much in a short time, neural networks can learn the statistical nature of the drift from historical data and other feedback mechanisms.

D. Signal Reconstruction Using Sinc Function

Since drift is a continuous function of time, and for any controller design, it is necessary to obtain a continuous function of drift with time from the discrete time series. Considering that the power spectra of the drift time series exhibit a bandwidth on the order of 0.001 Hz [3], we can

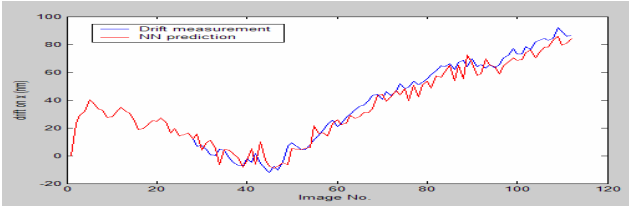


Fig. 6. Measured and predicted drift value.

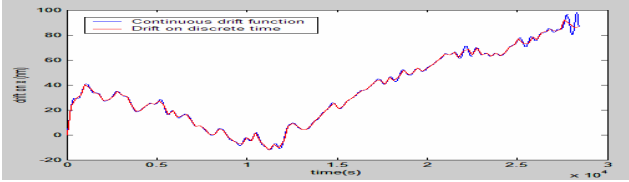


Fig. 7. Continuous drift function after signal reconstruction.

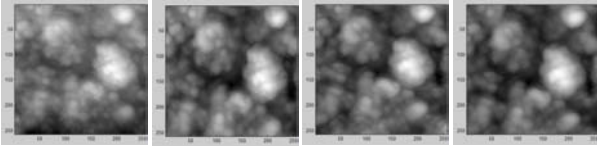


Fig. 8. Image sequences taken at 256 sec intervals with drift compensation ($512 \times 512 \text{nm}^2$).

get proper reconstruction results using sinc function, as long as the sampling duration between images are short enough. In our applications, the samples will be collected every 256 sec, which means the sampling frequency is about 0.004 Hz. Therefore it is reasonable to use sinc function to reconstruct the drift signal without much loss of information. In other words,

$$d(t) = \sum_{i=0}^{k+1} d_i \sin c \left(\frac{\pi(t - t_i)}{\Delta t} \right) \quad (10)$$

where $d(t)$ is the continuous drift function, d_i is the drift measurement or prediction on sampling time t_i , and Δt is the sampling interval.

IV. IMPLEMENTATION AND RESULTS

To verify our proposed work, the compensation system is implemented on a multimode scanning probe microscope (SPM) with NanoScope IIIa controller (Veeco Instruments). In our experiments, a sample with Au on mica substrate is imaged at a scan rate of 4 Hz with an imaging frequency of 0.004 Hz. At each scanning, a 512×512 height image representing $1 \mu\text{m}^2$ area is obtained. This implies that each loop takes about 256 sec and half of the time can be used for manipulation, fabrication and other tasks.

For NN-based drift prediction, a fixed time window of past eight values will be fed into the input layer of the NN. In our future work, an embedded thermal sensor in the tip for measuring temperature will be used as an additional input of the NN for accurate prediction. The two-layer NN consists of 50 neurons in the hidden layer. The initial

weights of all layers are selected uniformly within an interval of $[0, 1]$. The activation function of the first layer is selected as hyperbolic tangent sigmoid function and that of the second layer are taken as Pure linear functions. The first 20 sets of drift measurement data will be used for offline training by using Levenberg-Marquardt backpropagation algorithm. With any new data, online learning is utilized with at most the first 50 data points.

The following results were obtained on a MultiMode AFM operating in the tapping mode at the room temperature with humidity. Fig. 6 shows that the error between the measured and predicted values of drift in the x direction is quite small, which will be further reduced when we add the thermal sensor embedded in the tip. In Fig. 7, we can see the continuous function of drift after the signal reconstruction process. In comparison with Fig. 1, the sample images with compensation are shown in Fig. 8.

V. CONCLUSIONS

To realize full automated nanomanipulation and nanofabrication, nonlinearity effects and spatial uncertainties in AFMs have to be compensated in order to minimize user's intervention. This paper describes a novel compensation system for drift, which is a major cause of spatial uncertainty. The compensating scheme can be subsequently used in designing a nanomanipulation controller. Moreover, more efficient tools must be developed for other uncertainties, such as creep, hysteresis and so on.

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