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Optimal sampling and reconstruction of undersampled atomic force microscope images using compressive sensing

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ABSTRACT

Atomic force microscope (AFM) is an analytical instrument which is used to study the surface structure and morphology of materials. The AFM can measure and observe samples either in air or liquid environment. However, the standard AFM requires a long time to acquire accurate images and data. In our work, the compressive sensing (CS) was applied in order to reduce the imaging time, lower the interactions between the probe and the sample, finally avoid sample damage in AFM. Three samples (PAA film, TGG1 grating and BOPP film) were used as the testing samples. Different image reconstruction algorithms (l1-ls, TVAL3, GPSR and IHT) were employed to reconstruct AFM image with different sampling rate. And various sampling patterns (Random Scan, Row Scan, SRM, Spiral Scan and Square-shape Scan) were used to obtain the undersampling data. A large number of experiments show that the choice of sampling pattern and image reconstruction algorithm has significant impact on the quality of the reconstructed images in AFM. Subsequently the reconstruction results of sample topographic images were analyzed and evaluated by the image quality indicators (PSNR and SSIM). The CS method can be used to obtain accurate images by reducing measurement data. It finally improves the measurement speed of AFM without cutting down the quality of AFM image.

1. Introduction

Atomic force microscope (AFM) is a powerful instrument which is unique in its ability to observe nanometer-scale objects both in air and liquid environment. This unique capability also allows the AFM to be used in biological sciences as a nano-tool for various measurements under physiological solution environments [1,2]. Because the Nyquist–Shannon sampling theorem is used to obtain AFM images, the standard AFM requires a long time to obtain an accurate image. Its slow measurement speed has prevented expansion of its applications to observe dynamic behavior of active biomolecules. In addition, the probe tip exerts a small force on the surface of the sample, which can bring sample damage, especially the soft surface samples such as biological cells. It is important to improve measurement speed and reduce the tip–sample interaction force without sacrificing the imaging quality.

There are three main methods to realize high-speed AFM for reducing the imaging time. Firstly, to make AFM tip move faster on the sample and improve the imaging quality, hardware upgrades are an option [3]. Various physical designs have been proposed to achieve high-speed AFM, such as small cantilevers, micro resonators, scanning stages, scanners with high resonance frequencies, new actuators and so on [4,5]. However, the complicated hardware design and modifications of standard AFM will bring additional hardware costs. The second solution for tackling the imaging speed problem is to use novel controllers and algorithms such as a combination of feed forward and feedback control algorithms and iterative control methods [6,7]. To reduce image scanning time and improve AFM measurement accuracy, many other approaches have been proposed by altering scanning routine and sampling strategies [8–10]. The third approach for speeding the imaging time in AFM is applying compressed sensing (CS) to AFM. CS is a new type of sampling theory in the field of sampling digital signals [11–13]. Signal can be reconstructed from significantly fewer measurements than the Nyquist–Shannon sampling theorem requires, if the signal can be compressed [14]. In the surface metrology and AFM measurement, CS is considered as an effective method to reduce the imaging time by reducing the total number of samples [15–23]. An obvious benefit of applying CS to AFM is that sample damage and probe tip abrasion are greatly reduced. Many scan patterns have been proposed to undersample the topography information of sample surface, such as random pattern, row scan pattern and spiral pattern [16,17,23]. In order to reconstruct accurate AFM images, many reconstruction algorithms have been proposed in AFM image reconstruction. However, there are still many prob-

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lems to be solved in applying CS to AFM. Currently, there are no universally accepted scan patterns and reconstruction algorithms for CS in AFM. How to select the suitable reconstruction algorithm and determine the appropriate sampling rate are essential for applying CS to AFM.

In this paper, a series of simulation experiments were performed to illustrate the reconstruction capability of the CS in AFM. Various measurement matrices (scan pattern) were used to obtain the sampling data. Then, the obtained spare data were used to reconstruct AFM images by various of sparse reconstruction algorithms, such as l1-Regularized Least Squares (l1-ls), TV minimization by Augmented Lagrangian and Alternating Direction Algorithms (TVAL3), Gradient Projection for Sparse Reconstruction (GPSR) and Iterative Hard Thresholding (IHT). The reconstruction results of AFM images were discussed and analyzed. The measurement matrix and the sparse reconstruction algorithm are important factors which will impact the reconstruction results. Suitable measurement matrix and sparse reconstruction algorithms make many contributions to shorten the acquirement time of imaging and obtain the high-quality AFM images.

2. Compressive sensing in AFM

2.1. Compressive sensing algorithm

Consider an unknown signal x, with at most k nonzero components in N-dimension. It is called k-sparse. If it takes M times linear measurements to sample the signal x, it means it takes fewer measurements than signal dimension.

$$y = \Phi x \tag{1}$$

where y is the sampled vector with $M \ll N$ data point. Φ is an $M \times N$ measurement matrix. Since the process is non-adaptive, the measurement matrix is selected beforehand. CS can recover the signal x from significantly fewer measurements, only $M = O(K \log N)$, suggesting the potential of significant cost reduction in digital data acquisition.

Many signals are not sparse. They can be not directly used in compressive sensing. Fortunately, most natural signals are compressible, that is the signal x could be transformed into sparse form through sparse basis Ψ.

$$x = \Psi\alpha \tag{2}$$

where α is the sparse representation of signal x. Ψ is an $N \times N$ basis transform matrix. Then, the Eq. (1) changes into

$$y = \Phi x = \Phi\Psi\alpha = A\alpha \tag{3}$$

where $A = \Phi\Psi$ is $M \times N$ sensing matrix which should satisfy the *restricted isometry property* (RIP) [24].

2.2. Measurement matrices

In general CS case, the measurement matrix can be chosen as a dense matrix such as Gaussian random matrix, Bernoulli Matrices, Random Partial Fourier Matrices, etc. Each measurement of CS typically relies on a linear combination of many elements of the signal. However, they are difficult to be applied in the AFM application due to the point-like nature of the AFM probe tip. The AFM probe tip only measures a single pixel at a time. Therefore, we need a special designed measurement matrix to measure the sample of AFM. An identity matrix with some of its row removed is a good choice in AFM application as the measurement matrix Φ [16]. In each row of Φ, there is only a single one and zeros elsewhere. One possible realization is:

$$\Phi_{m\times n} = \begin{bmatrix} 0 & 1 & 0 & \cdots & 0 & 0 \\ 0 & 0 & 1 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 1 & 0 \end{bmatrix} \tag{4}$$

Such a measurement matrix ensures that only a single pixel of the image is required for each measurement. This unique measurement matrix could seem as AFM tip trajectory. The scan pattern of random sampling is shown in Fig. 1(a). The black points are the AFM probe tip scanning trajectory on the surface of sample.

Undersampling of raster scan is also a way to realize the CS measurement in AFM which means several rows of the raster is selected at random as the sampling data of CS. The row scan is shown in Fig. 1(b). Fig. 1(b) shows that the AFM probe tip has a relatively continuous scanning trajectory. The probe tip does not have to be lifted off the sample frequently, moved to the next point, and then re-engaged for the next measurement. Using raster scan, more sampling time can be reduced at the same sampling rate.

Structurally random matrix (SRM) has sensing performance comparable to that of a Gaussian random matrix. An SRM is defined as a product of three matrices [25]

$$\Phi = cDFR \tag{5}$$

where c is a scalar constant. R is either an $N \times N$ uniform random permutation matrix or an $N \times N$ diagonal random matrix. The diagonal entries R_{ii} of R are independent and identically distributed Bernoulli random variables with identical distribution $P(R_{ii} = \pm 1) = \frac{1}{2}$. F is a $N \times N$ orthonormal matrix and the popular fast computable transform is a good choice such as the Fast Fourier Transform (FFT) or the discrete cosine transform (DCT). If Ψ is dense and uniform, we can use the identity matrix for the transform F. A DCT matrix was chosen as the basis transform matrix Ψ. So F is taken to be an $N \times N$ identity matrix. D is an $M \times N$ subsampling matrix. In matrix representation, D is simply a random subset of M rows of the identity matrix of size $N \times N$. To reduce the sampling time, these M measurements need to be arranged into μ-paths, each of length q [19], that is, $\frac{M}{q}$ groups of rows of the $N \times N$ identity matrix are selected at random. The SRM scan with $q = 4$ are shown in Fig. 1(c). The μ-paths can be set to any suitable value. Longer μ-paths leads to faster sampling speed, but worse reconstruction capability.

A spiral trajectory is generated at a constant linear velocity [10]. The spiral scan pattern is plotted by mapping the sampling points along the spiral trajectory to points or pixels of the raster-scanned image. As shown in Fig. 1(d), the AFM probe tip is engaged the entire time. Compared with other scan patterns, the spiral scan pattern can reduce more sampling time. The square-shape scan pattern is shown in Fig. 1(e), it is similar to spiral scan pattern, and also has a smooth sampling path.

2.3. Scanning time estimation

In order to evaluate the performance of measurement matrices, the time cost of various data collection schemes should be reasonably estimated. For random scan and SRM, the sampling points are very scattered. When the probe moves between the two sets of sampling points, the probe needs to be lifted off the sample, moved to the next point, and then re-engaged for the next measurement. If the probe is doing this frequently, it will waste a lot of time. The scanning time when using random scan or SRM to collect data can be computed approximately as follows [26]:

$$t_{R,SRM} = a \times \left(t_{Zup} + t_{Zdown}\right) + \delta \times T \tag{6}$$