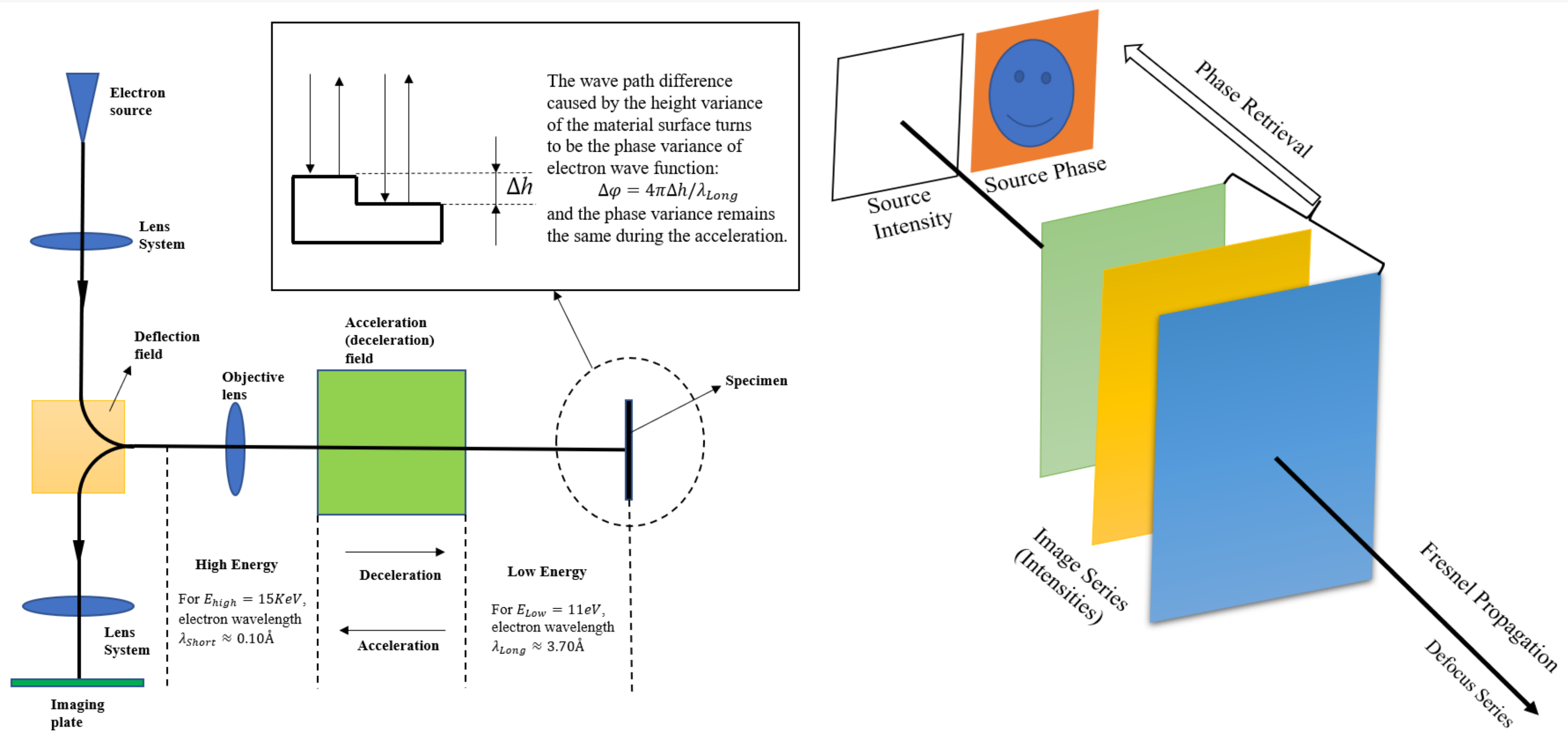
Phase retrieval in Low Energy Electron Microscope by Transport of Intensity Equation

Xian Li and Changlin Zheng
Department of Physics, Fudan University, Shanghai 200433, China

Introduction

Low energy electrons have been applied to surface physics researches since a long time ago. And one of such techniques is low energy electron microscope (LEEM), which reflects the morphological properties with high spatial resolution. However, phase information of electrons is usually lost because only electrons intensity is recorded. In this research, we apply transport of intensity equation (TIE) to LEEM, and successfully retrieve the phase of electron wave function from the recorded electrons intensity images. The surface morphology is further reconstructed.

LEEM instrument and TIE



(a) (b)

Fig. 1 (a) Schematic diagram of LEEM instrument and the relation between surface morphology and electron phase; (b) the principle diagram of TIE: three intensity images are recorded at a defocus series of $z-\Delta z$, z, $z+\Delta z$, this set of intensity images are used to approximate the intensity gradient along z, which is the key of TIE phase retrieval.

Propagation of electrons in LEEM:

The transfer function of the objective lens in LEEM is written as

$$\Psi_{out}(x,y) = F^{-1}T(\boldsymbol{k})F\Psi_{in}(x,y)$$

where $\boldsymbol{k}$ is the reciprocal vector, F and F^{-1} denote the Fourier transform and inverse Fourier transform respectively, and $T(\boldsymbol{k})$ is the transfer function in reciprocal space:

$$T(\boldsymbol{k}) = \varepsilon(\boldsymbol{k})\exp(i\pi\Delta f\lambda k^2 + \frac{i\pi C_s\lambda^3k^4}{2})$$

where $\varepsilon(k)$ is the chromatic-aberration damping envelope and is unity in an ideal case, Δf is the defocus and C_s is the spherical aberration.

Phase retrieval using TIE:

$$\phi(x,y) = -\frac{2\pi}{\lambda}\nabla_{xy}^{-2}\nabla_{xy}\cdot\left(\frac{1}{I(xyz)}\nabla_{xy}\nabla_{xy}^{-2}\frac{\partial}{\partial z}I(xyz)\right)$$

Where intensity

$$I(xyz) = |\Psi(x,y;z)|^2.$$

In a practical case, the intensity gradient is usually approximated with at least three images:

$$\left.\frac{\partial I}{\partial z}\right|_{z=z_0} \approx \frac{I|_{z=z_0+\Delta z} - I|_{z=z_0-\Delta z}}{2\Delta z}$$

Gradient calculation and inverse Laplacian are realized using the differential and integral properties of Fourier transform.

Reference

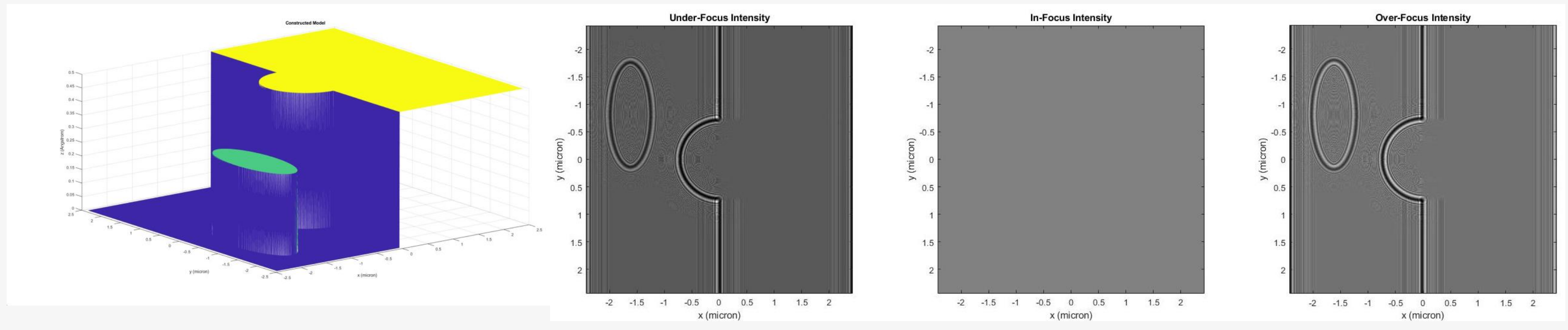
[1] Yu R P, Kennedy S M, Paganin D M, et al. Phase retrieval low energy electron microscopy [J]. Micron, 2010, 41(3): 232-238.

[2] Ishizuka K, Allman B. Phase measurement of atomic resolution image using transport of intensity equation[J]. Journal of electron microscopy, 2005, 54(3): 191-197.

Acknowledgement

Thank Dr. Changxi Zheng (Monash University) to provide us the experimental LEEM images.

LEEM phase retrieval by Simulation



(a) (b) (c) (d)

Fig.2 : (a) a constructed surface model which is composed of an oval pillar of 0.3Å, a step of 0.5Å and a semi-circle step of 0.5Å attached to the square step; (b) the under-focus image taken at $\Delta f = -400\mu m$; (c) the in-focus image taken at $\Delta f = 0$; (d) the over-focus image taken at $\Delta f = 400\mu m$. All the above images are simulated under the condition of 15 KeV LEEM high energy and 11 eV LEEM low energy. Simulation was realized in MATLAB.

Analysis of the simulation:

We build a sample containing steps of different height (Fig 2a). The simulated LEEM images with different defocus are shown in figure 2(b)-(d). By using TIE algorithm, the surface steps are successfully reconstructed in Fig. 3.

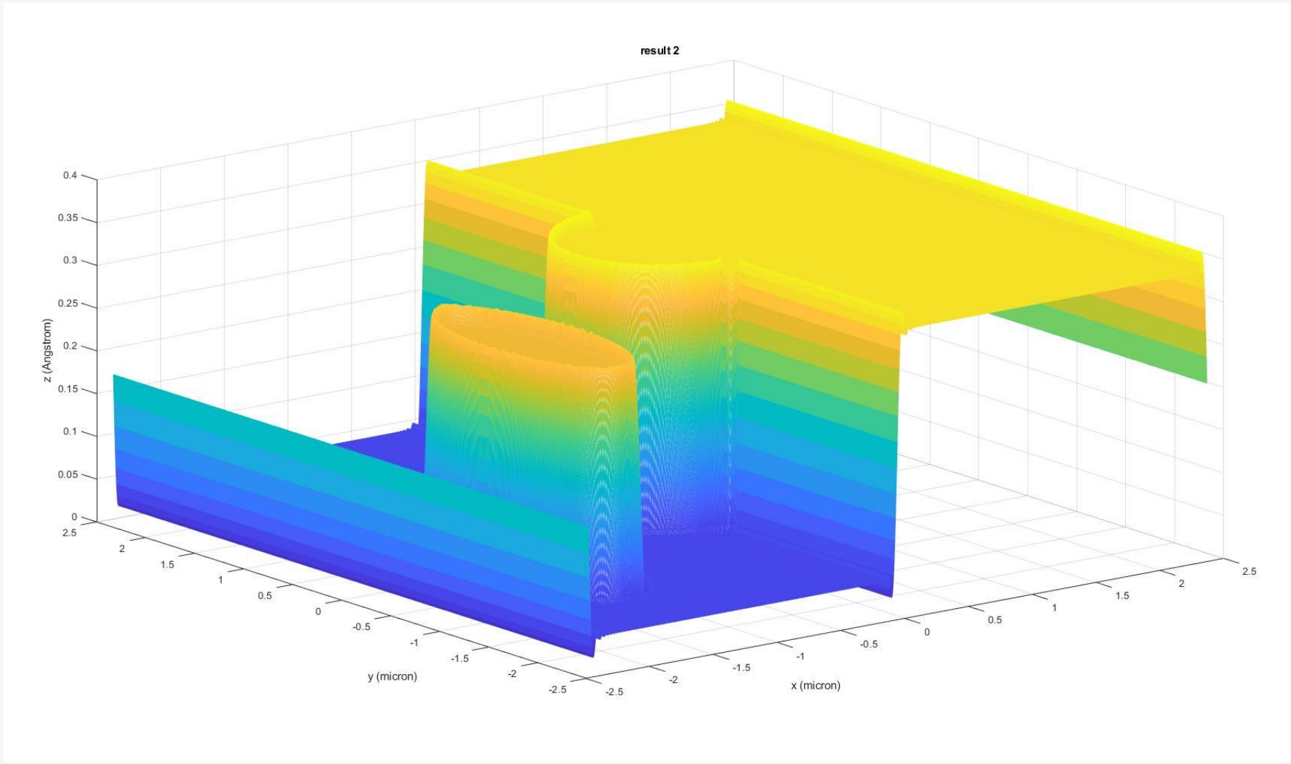
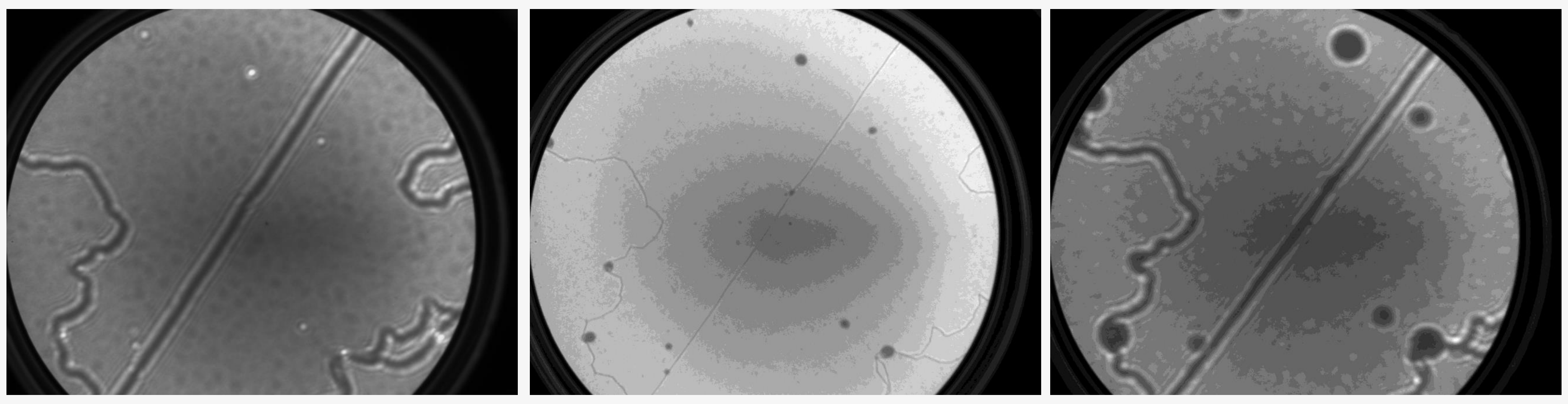


Fig.3: Reconstructed surface using TIE

Application in experimental data

LEEM images:



(a) (b) (c)

Fig.4 Real-space images of Ag(111) in LEEM: (a) under-focus image at $\Delta f = -400\mu m$; (b) in-focus image at $\Delta f = 0$; (c) over-focus image at $\Delta f = 400\mu m$. Diameter of the imaging scope is 6 μm, LEEM high energy is 15 KeV, and low energy is 11eV.

Image registration and selection of regions of interest:

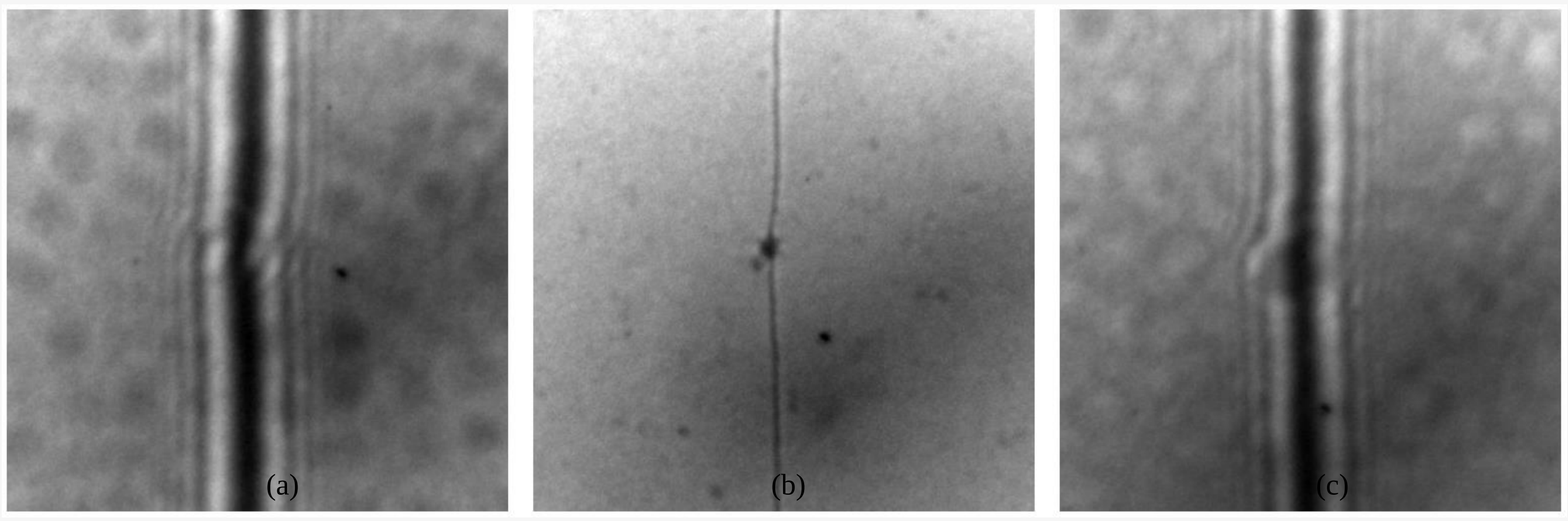
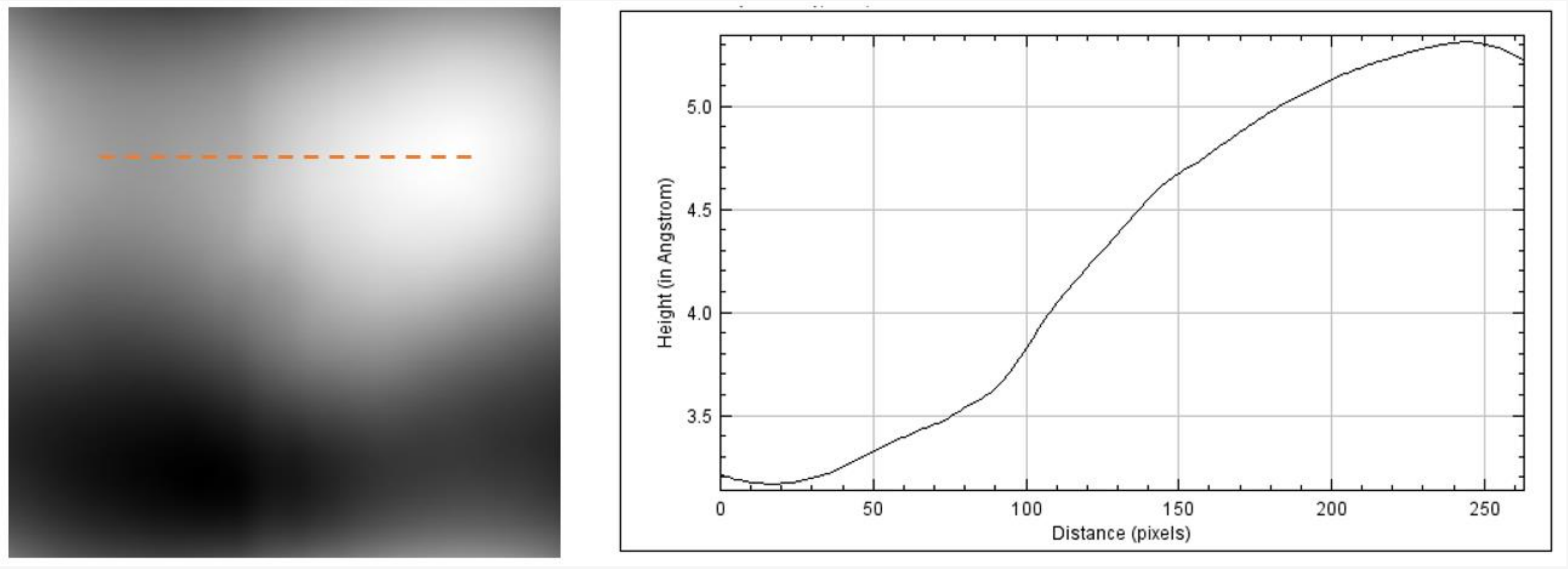


Fig.5 Experimental images are usually accompanied by misalignments, therefore it becomes quite necessary to correct such misalignments and this process is called image registration, which is mainly based on affine transformation. The above images are the regions of interest selected after image registration: (a) under-focus image; (b) in-focus image; (c) over-focus image.

Surface morphology reconstruction using TIE:



(a) (b)

Fig.6 (a) Retrieved surface height using TIE ;(b) profile along the orange dashed line, from which it is obvious that the structure corresponding to the vertical line in Fig. 5 is an atomic step and is about 2.5Å high.