

Surface Reconstruction Through Microscopy Data Fusion

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Abstract:

Reconstructing the surface microtopography through data fusion from a range of microscopies offers a way to provide considerably more information than any one technique alone. This thesis explores several methods for combining the information from different kinds of microscopes including height data, electron images and optical images.

Each microscopy has distinct advantages and disadvantages that can be considered in terms of data leakage in the transfer function from the actual sample topography to any individual dataset. These leakage paths are identified for a range of microscopies including atomic force microscopy, scanning electron microscopy and white light interferometry. Existing techniques for reconstruction from multiple image datasets, such as shape-from-shading and stereomicroscopy are evaluated, again in terms of information leakage.

A new approach is presented which attempts to minimize leakage by identifying a pathway of data fusion which first isolates the most reliable information in each dataset, and then maintains this information as the datasets are combined. The identification of the most trusted data requires knowledge of each imaging mechanism, while the final reconstruction is based on iterative matching between the datasets and a simulated image. Hence the final reconstruction incorporates both the datasets from the microscopes and their imaging physics to suppress data leakage.

This approach is first validated with a model micromachined sample using a combination of height interferometer data together with back-scattered and secondary scanning electron microscope images. It is then applied to particulate samples to demonstrate the capabilities of the approach.

Beyond the examples presented, it is hoped that this work provides a rational basis for combining a range of microscopies with minimal data leakage to reconstruct surface data of maximum fidelity.

Declaration:

All other results reported in this thesis are primarily due to the author, except for background results and some samples, which are clearly referenced.

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Nomenclature:

Abbreviations:

AFM: Atomic force microscope

BSE: backscattered electrons

DRIE: Deep reactive-ion etching

ETD: Everhart-Thornley scintillator photo multiplier detectors

FM: Facet Model

ICP: Iterative Closest Point

L-DAP: Lunar Dust Analysis Package

LM: Levenberg-Marquardt

LOM: lensless optical microscope

MC: Monte Carlo simulation

MEMS: micro-electromechanical systems

MFM: Magnetic force microscope

OM: Optical microscope

OP: Optical profilers

QBSD: Quadrant backscattered detector

PI: Path integration

RIE: Reactive ion etching

RMS: Root-Mean-Square

SED: Secondary electron detector

SEM: Scanning electron microscope

SFS: Shape-from-shading

SPM: Scanning probe microscope

SSI: Simulated SEM image

STM: Scanning tunnelling microscopes

STS: Surface Technology Systems

TEM: Transmission electron microscope

WLI: White light interferometer.

Variables:

λ : the wavelength of light

ξ the angle between surface normal and direction of collection.

N : surface orientation

S : source direction

χ_N : azimuth relative to the x-axis.

S_A, S_B : signals of the BSE detectors,.

d_{xy} : distance in the coordinates obtained from the two images

ρ : normalized cross-correlation

δd_{xy} : disparity precision

K_{+n} : maximum principal curvatures

K_{-n} : minimum principal curvatures

G : gradient magnitude

Chapter 1: Introduction

A range of microscopes have been developed for the surface topographic study over the years. Different types of the information can be provided and the nature of them is complementary. There have been many approaches to combine or deduce from the information of various microscope images to produce an improved elevation map of the topography of the sample. The elevation map of the sample is an important data set for many research fields. For instance some nature surface such as particles can provide the geological information. The elevation map of the particle can hint towards the climate history, how the particle is formed [1] [2]. Also the topographic map of cells provides important morphological characteristics for biology study [3] [4]. For the manufacture field the roughness of the surface is an important indicator such as the optical device where the surface should be very flat [5] [6].

The techniques producing the height information can be separated into two categories. The first way is directly using a mode that output elevation information. For instance an atomic force microscope (AFM) uses a tip to probe surfaces [7] and produce height images of material surfaces and interferometers can measure height variations to output surface topographies using the wavelength of light as the ruler [8]. In the second category, techniques produce geometric images of surfaces but not elevation maps. From those images height images including re-entrant elevation images can be deduced out. For instance based on the shape-from-shading (SFS) algorithm intensity, images obtained by an optical microscope (OM) can be transformed to the height image of the sample surface [9] and scanning electron microscope (SEM) stereo algorithms produce elevation maps of sample topographies via SEM images [10].

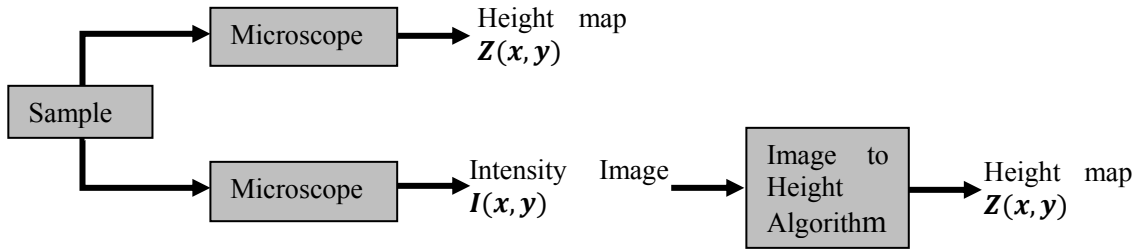


Figure 1-1: *Two basic ways that can produce elevation maps of sample*

Whichever of the two pathways is taken to obtain a height map, there will inevitably be a loss of information such that the derived height map does not fully reflect the surface of the sample. This loss can be regarded as a leakage of information from left to right of fig. 1-1. This leakage can occur either in the instrument, or within the algorithm, and the development of microscopy can be regarded as increasingly sophisticated attempts to minimise this information loss. One formalism to quantify this leakage is through the identification of a transfer function of a microscope, which maps the transfer of spatial frequencies, in both amplitude and phase, between a sample and an image. For example, beyond the resolution limit of a particular technique, the amplitude of the transfer function approaches zero and no higher spatial frequencies can be transmitted, corresponding to complete leakage of information below this limit. Any algorithm can be viewed in a similar fashion, with leakage of information corresponding for example to incomplete knowledge of image formation.

To control the information leakage we have to know how the height information is produced by the direct determination and indirect methods, both in the instrumentation and the algorithms. What follows is a survey of the major techniques used to image surfaces and determine surface topography at the microscopic level, followed by a selection of algorithms used to extract height information from image data. Although not exhaustive, this survey includes all of the approaches used in this thesis.

1.1 Microscopic surface imaging techniques

Microscopic imaging of surfaces has been dominated by light microscopy. However, to overcome the fundamental resolution limits of imaging with photons electron microscopy has been the major advance of the last one-hundred years. The much stronger interaction of the electron with matter requires electron imaging at reduced pressures, but also opens up a broader range of imaging modes. Optical and electron microscopy will now be presented in turn.

1.1.1 Optical microscopes

The classic microscope is an optical microscope (OM) using visible light and a system of lenses to magnify images of small samples [11] [12]. The schematic diagram of the simplest optical microscope is shown below.

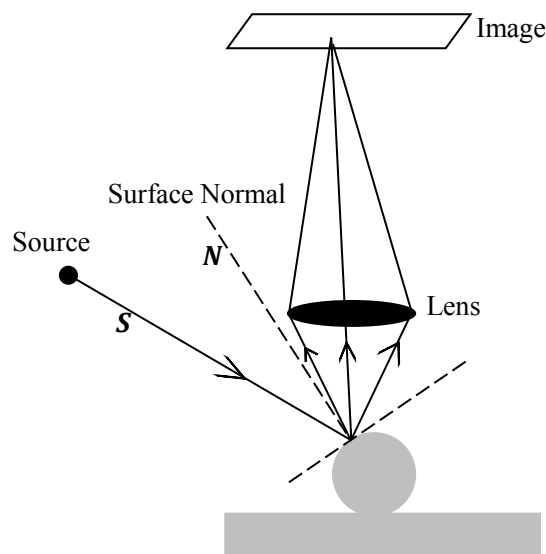


Figure 1-2: *The schematic of OM*

The lens is, at its simplest, a very high powered magnifying glass with a very short focal length. This is brought very close to the specimen being examined so that the light from

the specimen comes to a focus inside the microscope tube. This creates an enlarged image of the subject [13].

The image maps the intensity of the light that is scattered at the surface. This scattering is dependent on the surface orientation, source direction and surface reflectance. Surface reflectance can be separated into two categories, specular and diffuse reflection [14]. Specular reflection is the mirror-like reflection of light from a surface, in which light from a single incoming direction is reflected into a single outgoing direction, while diffuse reflection is the reflection of light from a surface such that an incident ray is reflected at many angles rather than at just one angle as in the case of specular reflection [15] [16] [17]. Common materials, even when perfectly polished, usually give not more than a few percent specular reflection. For an ideal diffusely reflecting surface, the intensity of the image to an observer is the same regardless of the observer's angle of view and obeys the Lambertian mode [18] [19]. The image irradiance in the model is

$$I(x, y) = K(x, y) \mathbf{N}(x, y) \cdot \mathbf{S} \quad (1-1)$$

Where $\mathbf{N}$: surface orientation, $\mathbf{S}$: source direction, K : constant, which depends on the source brightness, optical system and surface albedo which will not be varied over the surface for a signal-material sample [20] [21].

The resolution of a microscope is taken as the ability to distinguish between two closely spaced Airy disks which are descriptions of the best focused spot of light that a perfect lens can make, limited by the diffraction of light. Generally, the optical resolution can be estimated as $\lambda/2NA$, where λ is the wavelength and NA is the numerical aperture of the lens which characterizes the range of angles over which the system can accept or emit light [22] [23] [24]. NA can be defined by $n \cdot \sin(\alpha)$ where n is the index of refraction of the medium in which the lens is working and α is the half-angle of the maximum cone of light that can enter or exit the lens. Based on the discussion above for white light, the average wavelength is approximately $0.55\mu\text{m}$. The best resolution is thus

a few hundred nanometres. The information below the resolution cannot be acquired by the OM causing the information leakage [25] [26].

Also some kinds of optical microscopies enable the reconstruction of three-dimensional structures directly such as confocal microscopy and holographic microscopy. The confocal microscopy uses spatial pinhole which is placed in front of the detector and eliminate out-of-focus signal. The microscopy requires the collection of data over a certain volume in the specimen, followed by a suitable two-dimensional visualization procedure in which the desired image is produced. The holographic microscopy records the light wave emitted from the object as a hologram and the object image is calculated by using a numerical reconstruction algorithm.

1.1.2 Scanning electron microscopy

The scanning electron microscope uses a focused beam of high-energy electrons to generate a variety of signals at the surface of solid specimens. The signals derived from electron-sample interactions can reveal geometrical information about the sample. In most applications, data are collected over a selected area of the surface of the sample, which ranges from approximately 1 cm to 1 micron in width [27] [28] [29].

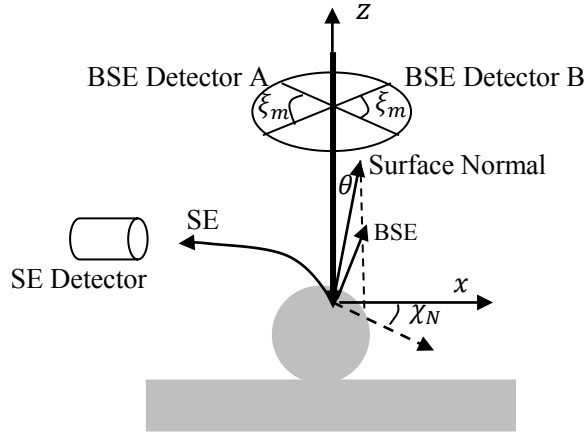


Figure 1-3: *The signals derived from electron-sample interactions, including the primary backscattered electrons, secondary electrons, auger electrons, and x-rays.*

The SEM is operated by applying a voltage on the sample surface which should be grounded. Electrons are emitted from the filament to the sample. The beam current and the final spot size determine the resolution and depth of field for the image. Depending on the beam parameters and sample type, the electrons interact with the sample over a range from a few nanometres to several microns of the surface. The backscattered electrons (BSE) or secondary electrons (SE) are then emitted from the sample. The secondary electrons are so named because some energy from the beam electrons is transferred to the conduction band electrons in the sample, providing enough energy to escape from the sample surface; thus they are not primary electrons but secondary electrons. Further, they are low-energy electrons (<50 eV), which means that only the first few nanometres of the sample surface have the energy necessary to allow secondary electrons to escape. [29] [30] [31].

These electrons will be detected when they escape from the sample surface. Everhart-Thornley scintillator photo multiplier detectors and solid-state BSE detectors are generally used for detection [32] [33] [34]. The E-T detector is both a SE and a BSE collector, consists of a scintillator inside a Faraday cage. To attract relatively low-energy secondary electrons, a low positive voltage is applied to the Faraday cage. The low

voltage cannot attract other electrons within the specimen chamber that will reach the detector only if the direction of travel takes them there.

The solid-state BSE detector uses a large silicon diode specially fabricated for electron detection. BSE with energies above about 3 keV produce electron-hole pairs in a junction diode. These charge carriers are collected by an applied voltage and amplified to produce image signal. The detector is usually placed just below the lens pole piece so that specimen can be brought close to the detector, giving very large acceptance angle and area. Finally, the SEM image is formed based on the intensity of the electron emissions from the sample at each x,y data point [35] [36] [37] which means that each pixel is synchronized with the position of the beam on the specimen in the microscope, and the resulting image is therefore a distribution map of the intensity of the signal being emitted from the scanned area of the specimen [38].

SEM images can be used for the geometric study and the topographic irradiance contrast of the SEM image dependences on the detector used. The topographic contrast in the E-T images contains both SE and BSE contributions [39] [40]. The SE yield $\delta(\theta)$, which depends on the tilt angle θ of the local surface normal relative to the incident beam, results in the surface-tilt contrast. When an E-T detector is on the side, shadowing contrast is superimposed on the surface tilt contrast. The topographic contrast also depends on the BSE, which is decided by the azimuth angle χ of the surface normal. Both backscattered and emitted secondary contributing to the Everhart-Thornley detector signal in unknown proportions, so it is difficult to quantify the relationship between the topography and the intensity [41]. However the BSE detector can offer a way to quantify the relative contributions, as will be presented in Chapter 4

By using the solid-state BSE detector, the irradiance of the image can be defined by the geometry of the sample and electron beam (see fig 1-3) [43] [44]. The electron beam direction onto the sample is the z-axis. The component of the line between the two BSE detectors perpendicular to the z-axis defines the x-axis [45]. The sample surface normal

has an angle θ to the z-axis, an azimuth of χ_N relative to the x-axis, and a topography described by $Z(x, y)$. The signals of the BSE detectors, S_A and S_B , depend on both the tilt and the azimuth χ_N of the surface normal with respect to the detector pair orientation. For standard quadrant detectors where $\xi_m = \pi/2$,

$$S_{A,B} = \frac{\eta}{2} (\cos\theta \pm \sin\theta \cos\chi_N) \quad (1-2) \quad [42]$$

The image limited by the shadowing effect for higher aspect ratio samples where the backscattered electrons are only collected at one detector. The information leakage happens due to the shadowing effect [46] [47] [48]. These effects will be discussed and quantified in great detail in chapter 4.

1.2 Direct height mapping

The two major techniques used to directly determine the surface topography are atomic-force microscopy (AFM) and optical profilometry. These are considered in turn.

1.2.1 Atomic force microscopes

The AFM is a standalone high-resolution imaging tool for the micro- and nano- scales. The general principle of AFM observation can be described as follows. An extremely fine sharp tip located at the free end of a cantilever comes into contact or very close proximity with the sample. The sample is then scanned by the tip. Either attractive or more usually repulsive forces will act on the tip, causing deflections of the cantilever [49] [50].

Typically the deflections are measured using a laser spot reflected from the top surface of the cantilever into an array of photodiodes. Other methods that are normally used are capacitive sensing or piezoresistive AFM cantilevers. By measuring and processing these deflections, the elevation of that point is obtained. In most cases a feedback mechanism is

employed to adjust the tip-to-sample distance to maintain a constant force or distance between the tip and the sample during the scanning [51] [52] [53].

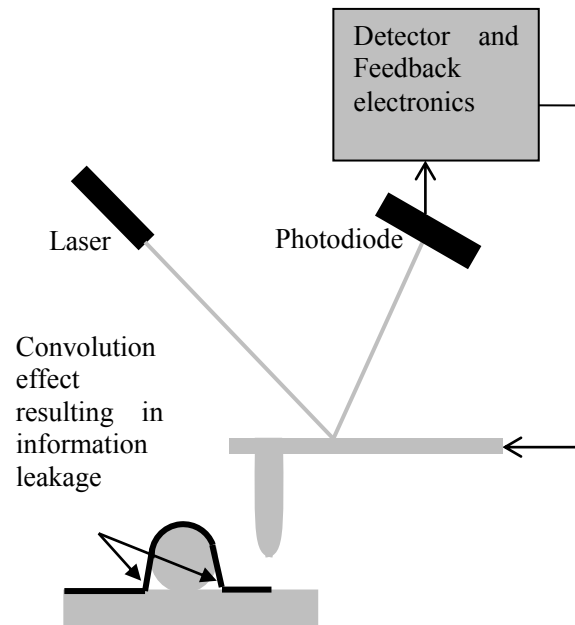


Figure 1-4: *The schematic of AFM scanning and the related information leakage*

Though the AFM is a common tool for studying the structure of specimens at a micro-scale, it also has some limitations. One limitation is the single-scan image size, which can image a maximum height on the order of only 10 to 20 μm and a maximum scanning area of about $150 \times 150 \mu\text{m}^2$. The scanning speed of an AFM is also a disadvantage. The relatively slow rate of scanning during AFM imaging often leads to thermal drift in the image. This is exacerbated by the non-linearity and hysteresis of the piezoelectric scanners. The combination of drift, hysteresis and nonlinearity mean that it is challenging to produce undistorted images in the AFM [54].

The key to AFM measurements is interaction between the probe and the sample. Some special tips can achieve some more complex measurement. For instance, the use of flared tip and bi-directional servo control in some AFM has made it possible to image structures of general shapes with undercut (re-entrant) surfaces. However, the major cause of information leakage is also due to the interaction between the tip and the sample. If the tip

were a stand-alone single atom capable of tracing all possible surface geometries, it could produce a height mapping of the sample with no information leakage above the atomic scale. Such a tip is not physically realisable as even if the force interaction is constrained to a single atom, that atom needs to be supported. For micro-machined tips, that support is normally formed by the facets of an etched crystal though the more open geometry of a nanotube-based tip has been studied. However, any support will inevitably cause information leakage by tip-sample convolution. Fig.1-4 shows a model of a probe tip scanning over a spherical particle placed on a flat surface. The black line is the data that the AFM records. The result of this convolution effect is illustrated. Due to the convolution the lateral resolution (around 5 nm) of the AFM is lower than its vertical resolution (around 0.5 nm) [55]. This is because AFM images are distorted representations of sample surfaces due to the convolution produced by the finite size of the tip. Obtaining the tip shape and eliminating the affection of the convolution is one of the main AFM supporting algorithm for correcting tip distortion [56] [57] [58].

1.2.2 Optical profilers

Optical profilers (OP) are interference microscopes which are used to measure height variations such as surface topography using the wavelength of light as the ruler [59] [60] [61].

A broadband white light source is used to illuminate the test and reference surfaces. A beam splitter separates the light into reference and measurement beams. One beam is reflected from the Reference Mirror, and the other one is reflected or scattered from the test surface. These two beams are recombined by the beam splitter to interfere. The returning beams are relayed by the beam splitter to the CCD image sensor where the two images are superimposed and form an interference pattern of the test surface topography that is spatially sampled by the individual CCD pixels [62] [63] [64].

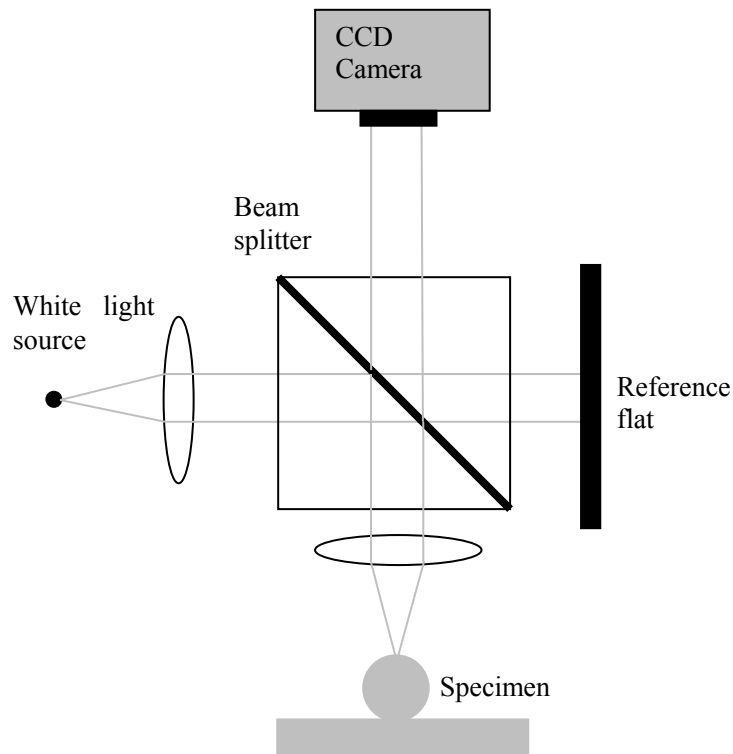


Figure 1-5: *The schematic of OP and the related information leakage*

The interference occurs for white light when the path lengths of the measurement beam and the reference beam are nearly matched [65]. By changing the measurement beam path length relative to the reference beam, a correlogram, interference signal, is generated at each pixel. Each pixel of the CCD samples a different spatial position within the image of the test surface. The correlogram of a pixel has maximum modulation when the optical path length of light impinging on the pixel is exactly the same for the reference and the object beams. Therefore, the z -value for the point on the surface imaged by this pixel corresponds to the z -value of the positioning stage when the modulation of the correlogram is greatest [66] [67] [68].

Though the profiler can be used to measure micro-scale surface variations, there is a limitation of the optical profiler, where the light is reflected away from the objective. This can result in some defects in the image. The vertical resolution depends mainly on the accuracy of the positioning stage, which is normally $<1 \text{ nm}$. The lateral positions of the

height values depend on the same factors of the optical microscope which is normally around 0.55 μm . [69] The following Table is a summary for the microscopes introduced above: [70] [71]

	SEM	OM	AFM	OP
Imaging Source	Electrons	Photons	-----	Photons
Mechanism for sample	Scattering	Scattering	Coulomb force	Scattering
resolution	lateral	5nm	500nm	5nm
	vertical	N/A	N/A	0.5nm
Resolution limited by	Interaction volume	Diffraction limitation	Tip geometry	Diffraction limitation
Main cause of information leakage for elevation mapping	Converting $I(x, y)$ to $Z(x, y)$	Diffraction Limitation & Converting $I(x, y)$ to $Z(x, y)$	Tip-sample dilation	Lateral stage control

Table 1: *the summary of the microscopes*

1.3 Approaches for extracting height data from images

Although it is evident from inspection of microscopic images that height information is present, extracting an elevation map from such image data requires the development of algorithms which themselves have limitations with regard to information leakage. Here we present the three most common algorithms to extract height information from microscopic images. The first two, stereoscopy and photometric stereo require two or more images. The third, shape from shading combines image and height data.

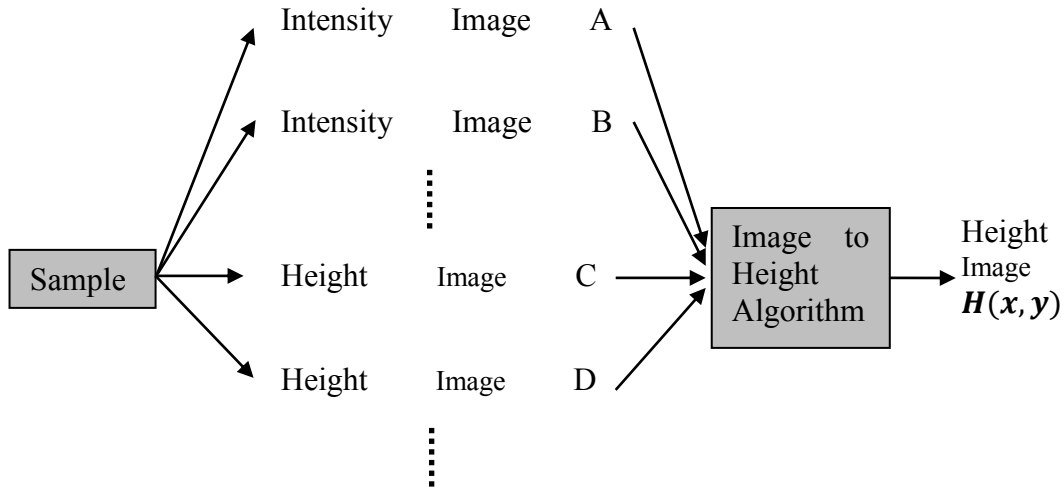


Figure 1-6: *Basic ways for data fusion to produce height images*

1.3.1 Stereoscopy

Stereoscopy is a technique for creating 3D images using a pair of intensity images which is binocular vision [72] [73].

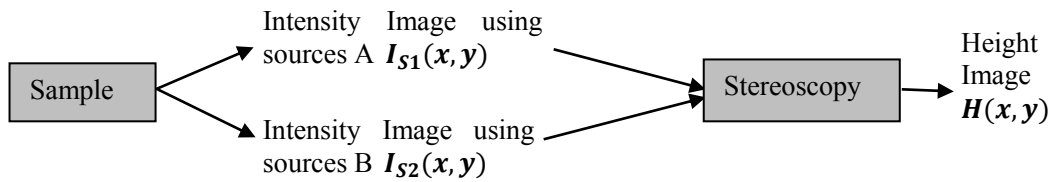


Figure 1-7: *the basic idea for stereoscopy to produce height images*

For SEM applications the stereoscopy is normally archived by tilting the sample. The following figure shows a sample which is imaged before (a: solid line) and after (a: dashed line) titling and the titling angle is θ . The corresponding images (b and c) are also shown. A is a point on the sample and the elevation of A is Z . A' is the corresponding point after titling [74] [75] [76].

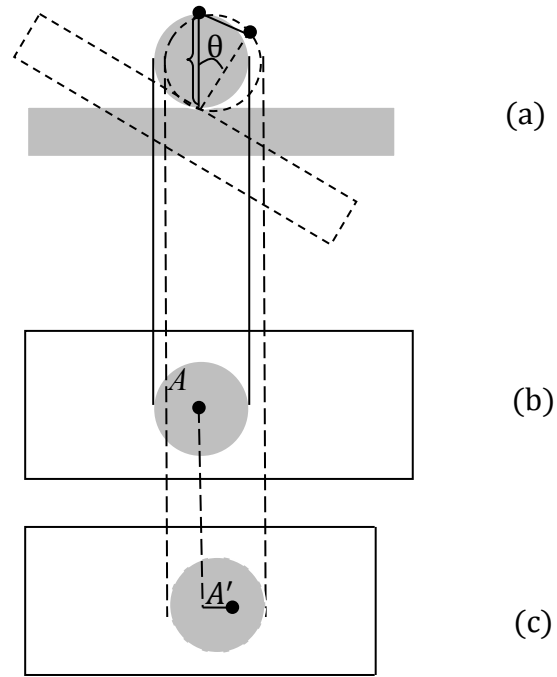


Figure 1-8: *The schematic of the stereo method. a: the titled sample b: image obtained before tilting c: image obtained after tilting*

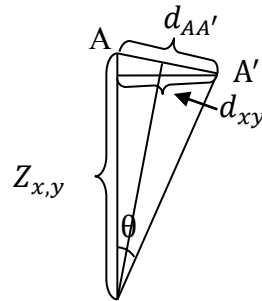


Figure 1-9: the diagram of the stereo method.

According to the [77], as shown in fig.1-9 the elevation (Z) at the point (x, y) can be calculated as below:

$$Z_{x,y} = \frac{C_{scale}}{2 \sin\left(\frac{\theta}{2}\right)} d_{AA'}$$

If the θ is small, $d_{AA'} \approx d_{xy}$, so

$$Z_{x,y} = \frac{C_{scale}}{2 \sin(\frac{\theta}{2})} d_{AA'} \approx \frac{C_{scale}}{2 \sin(\frac{\theta}{2})} d_{xy} \quad (1-3)$$

where C_{scale} is the scale factor to convert pixels to micrometres, based on magnification, θ is the total change in tilting angles, d_{xy} is the spatial distance between points A and A' . d_{xy} is the distance in the coordinates obtained from the two images, respectively [78].

Following the equation an entire elevation map for the specimen surface can be calculated by a sufficient amount of coordinate pairs, but the reconstruction image resolution will be limited by the correspondence problem which consists of finding a unique mapping between the points belonging to two images of the same scene. Such matching is almost impossible since many pixels have similar intensity or colour. To reduce the correspondence possibilities for a pixel to a single possibility, regions around that pixel must be used along with additional continuity or smoothness assumptions about the scene depth. Enforcing smoothness without a prior knowledge of depth discontinuities (segmentation) will inevitably lead to errors, especially near the discontinuities, so that the information leakage will happen. Also the information leakage results from the half-occluded regions in a stereo pair which a set of pixels in one image representing points in space visible to the detector only, and not to the other, which means some information that is not present in both images [79] [80] [81].

1.3.2 Photometric stereo

Though stereoscopy is a main approach towards three-dimensional (3D) surface reconstruction, this approach is suitable for surfaces with a sufficient amount of distinguishable details, which can be identified in both images [82] [83].

An alternative method evolved from the group of photometric methods, which is a technique for estimating the surface normal of objects by observing that object under different lighting conditions [84] [85].

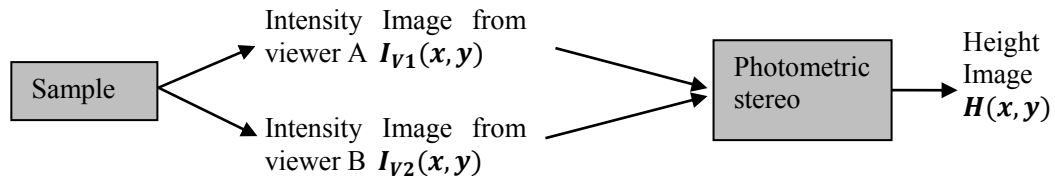


Figure 1-10: *The basic idea for photometric stereo to produce height images*

It is based on the fact that the amount of light reflected by a surface is dependent on the orientation of the surface in relation to the light source. By measuring the amount of light reflected into a camera, the space of possible surface orientations is limited. Given enough light sources from different angles, the surface orientation may be constrained to a single orientation. However the photometric stereo technique is limited to a single viewpoint the information leakage resulting from the half-occlusion [86].

One of its variant applicable is in SEM, which can also allow extracting information about local topography. For the optical microscope the technique requires several different sources from different angles but for the SEM it requests several different detectors at different angles. One of the established approaches to reconstruct height image from SEM images is based on the angular dependence of the backscattered electron yield. This is most easily achieved by positioning the detectors at equal but opposed scattering angles to the specimen along the scan direction [87].

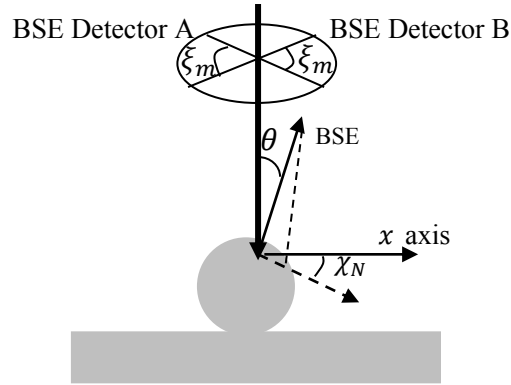


Figure 1-11: *The schematic of the SEM photometric stereo method.*

Based on equation (1-2)

$$S_A + S_B = \frac{\eta}{2} \cos \theta \quad (1-4)$$

$$S_A - S_B = \frac{\eta}{2} \sin \theta \cos \chi_N \quad (1-5)$$

Dividing

$$\frac{S_A - S_B}{S_A + S_B} = \tan \theta \cos \chi_N \quad (1-6)$$

which is the slope of the sample in the detector-pair axis direction,

$$\frac{dz}{dx} = \tan \theta \cos \chi_N \quad (1-7)$$

This can provide a specimen topography profile if integrated along a scan line in the x -direction. Though the method is rapid and fully automatic, it is limited by the shadowing effect for higher aspect ratio samples where the backscattered electrons are only collected at one detector [88] [89].

1.3.3 Shape-from-shading method

Another popular method used for reconstruction is shape-from-shading (SFS), a special case of photometric method, which uses the gradual variation of shading in the image to recover the shape of the surface. In SFS only a single image is needed, as well as an initial guess [90] [91].

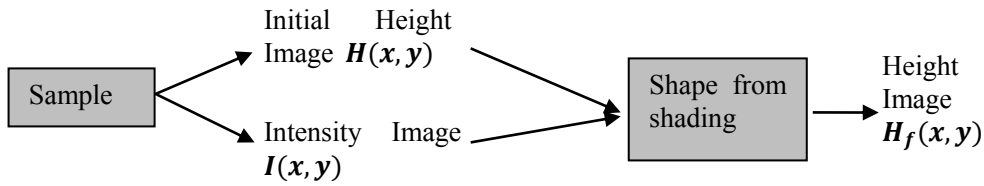


Figure 1-12: *The basic idea for shape from shading to produce height images*

Brightness minimisation based SFS is a commonly used method to identify a solution that minimises the simulated and the acquired brightness of the image. The brightness constraint requires that the reconstructed shape produces the same brightness as the input image at each surface point [92] [93] [94].

$$\iint (I - R)^2 dx dy \quad (1-8)$$

where I is the intensity from the measurement and R is the brightness from the reconstruction.

The smoothness constraint refers to an assumption that pixel values will change slowly in any direction and will likely be close in value to their neighbours. For the SFS method the smoothness should be over the recovered 3D position, which will stabilise the convergence to a unique solution. In our project, smoothness was achieved by adding a median filter [95] [96] [97].

However, several limitations still have to be addressed in SFS systems. Currently, depth can only be recovered up to an unknown scale factor determined by an intensity

simulation algorithm. Moreover, numerical methods for solving out the final results tend to be sensitive to initial conditions [98] [99].

Jones and Taylor presented a method that can reconstruct the 3D topography of SEM images obtained by an E-T detector using an SFS minimisation approach [100]. In theory, this method could be adapted for use with Monte Carlo (MC) simulation [101]; however, this would require the simulation of thousands of SEM images, which would be time consuming and impractical. Therefore, the feasibility simulation of SEM intensity is obtained from a function of the slope of the surface, and the reconstructed surface topography can be determined through an inverse process (SFS minimisation). The SEM signal used in the method consists of multiple components, including BSE and SE, which have different interaction scales with the specimen; therefore, the estimates of the slope must be at multiple scales to predict the SEM signal. Seeger and Haussecker described an alternative approach for simulating SEM images by taking into account both the slope and curvature of the surface to improve the accuracy of the result from the multi-component SEM image [102].

1.4 Aim of the thesis and the outline of the related chapters

Microscopy of various forms offers a range of approaches to quantify the topography of samples at the micro- or nano-scale. The relevant algorithms and techniques have been addressed above, however information leakage limits what can be achieved. BSE images are influenced strongly by shadows in which information is lost. Also, SEM images obtained from an E-T detector will also be influenced by the BSE. The AFM image is limited by the tip-sample convolution, while the OP has relatively low resolution. 3D stereoscopy will cause the resolution reduction when the corresponding points cannot be matched, while half-occluded regions will result in information leakage, an effect also seen in photometric stereo. The resolution of SFS is limited by the intensity simulation method and forcing image smoothness will also cause information leakage. If the source

of the information leakage cannot be properly handled in the algorithms that combine image datasets, the result can be even worse than the individual data sets.

The objective of our work is to improve existing methods by addressing their disadvantages and making better use of the reliable characteristics and parts of the images by exploiting their strengths to control the information leakage and extract accurate details of the sample for morphology research.

Several different methods have been tried and will be presented in the following chapters. Chapter 2 provides an initial comparison and assessment of the microscopes. Chapter 3 presents several methods such as the stereo-pairs method and SFS minimisation that have not been fully adopted but which help form the basic ideal of the final algorithm. The final proposed method combines the minimisation and propagation methods to complement each other in suppressing the defects. This method will be introduced in chapters 4 and 5.

Chapter 2: Initial comparative evaluation of microscopic imaging

Before combining the information from different microscopes images to reconstruct a new elevation map, it is necessary to assess the information obtained from the main techniques, AFM and SEM. This evaluation of the ability and the characteristics of the microscopes will inform the subsequent development of any surface reconstruction.

The chapter provides an initial comparison and assessment of the microscopes. Firstly an overview of the equipment used for the work in this thesis is presented including resolutions, scanning ranges and scanning times. The AFM and SEM are evaluated against a model particle sample. To improve the performance of AFM, micromachined silicon substrates are used to immobilise the particles. The experiments show the advantages, disadvantages and complementarity of the microscopes, and suggest what might be an possible routes to combine information in a surface reconstruction.

2.1 Description of the microscopes, the sample and the micro-machined Si substrates

2.1.1 AFM

In this thesis, all the AFM images are taken by the “EasyScan” AFM. The complete system (scanning head and electronics) is portable. This built around an electromagnetic scanner rather than the more normal piezoelectric actuator producing a compact microscope with a large scan range: scan sizes up to $70\mu\text{m}$ laterally and $10\mu\text{m}$ vertically can be realized. Two magnifying glasses display a top view and a side view of the cantilever to aid the initial positioning of the cantilever near to the sample surface [103] [104].

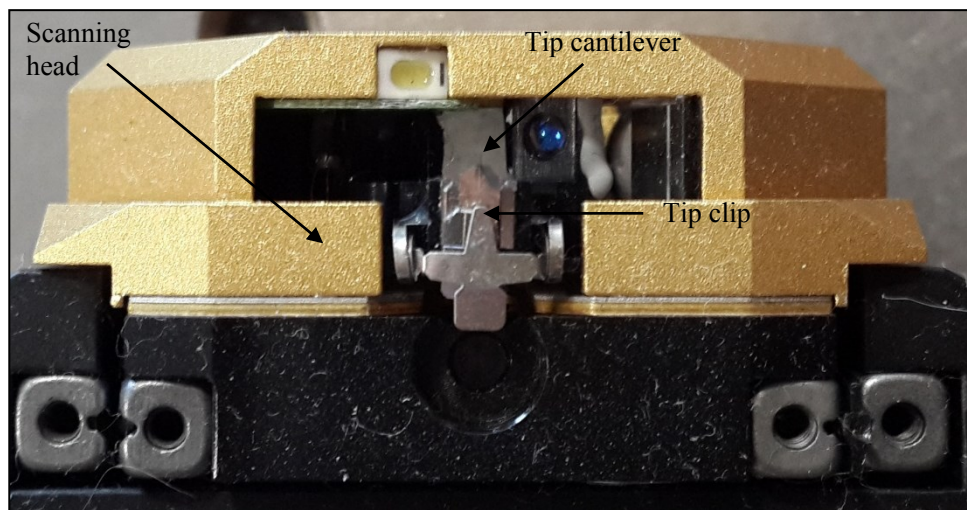
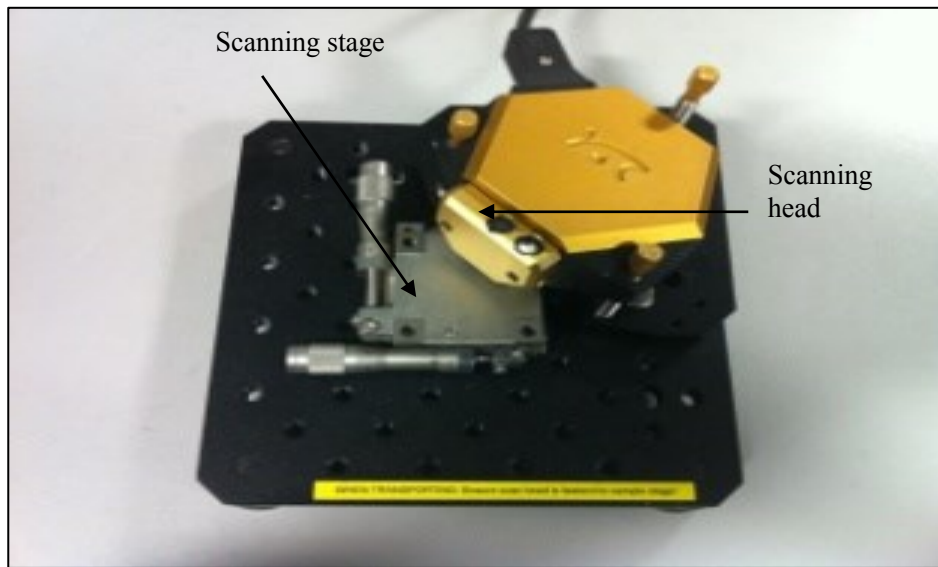


Figure 2-1: *The EasyScan AFM and the head of the AFM which has two magnifying glasses display a top view and a side view of the cantilever.*

2.1.2 SEM

In this thesis, all the SEM images are taken by the LEO 1455VP scanning electron microscope which can work in variable pressure and high vacuum modes and can be used for both imaging and qualitative X-ray analysis. The magnification is from 20× to

60,000 $\times$ and the image output is 8-bit TIFF, up to 3072 x 2304 pixels. The large chamber capability is up to approximately 15 $\times$ 15 $\times$ 15cm. [105] [108]

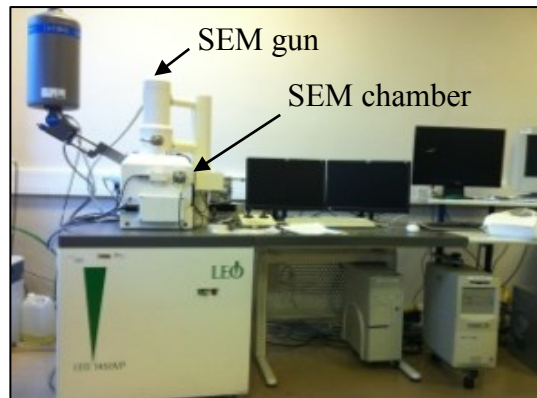


Figure 2-2:*The LEO 1455VP SEM that can work in variable pressure and high vacuum modes to be used for both imaging and qualitative X-ray analysis*

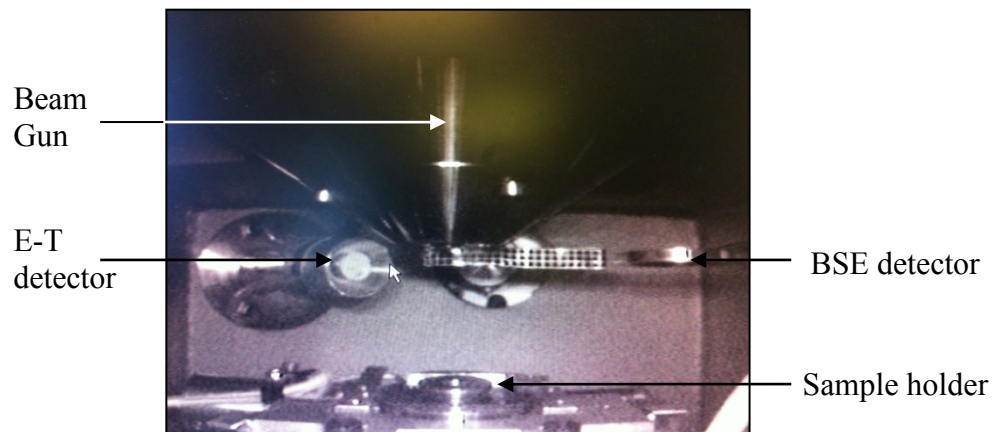


Figure 2-3:*The chamber of the LEO 1455VP SEM*

Microscopes	Resolution	Measurement regain/ Magnifications	brand
AFM	0.21nm (vertical)	70 μ m (scan range)	EasyScan
	1.1nm (lateral)	14 μ m (z-range)	
SEM	5 nm	$\times 20$ - $\times 60,000$ (Magnifications)	LEO 1455VP

Table 2: Summary of microscopes performance. [103] [105]

2.1.3 Sample description

For our comparison we focus on imaging of particles. We are surrounded by a huge number of particles in our lives which are composed of a variety of materials. Microstructural imaging of particle surfaces is critical in understanding their formation and interactions. For example, air pollution is caused by large amount of particles derived from vehicular emission, industrial fumes and burning large amounts of coal within a city. The smog is toxic to human being and can cause severe sickness, shortened life or death.

More generally, the whole universe is also full of particles of different components, from cosmic dust to the surface particles of a planet. No matter where the particles are located, their texture and surface morphology (particle size, surface materials, etc.) are closely related to the climatic factors (wind speed and moisture, etc) and in the case of Earth by human activities such as factory emissions. Therefore, the study of particle shape, size, surface texture and topography contributes in many directions, such as air pollution control, dust toxicity and planetary exploration, to name just three areas. We choose the diameter of the particles smaller than 10 μ m to test the ability of AFM and SEM as well as the reconstruction algorithm in our research, with the best hope that our research could contribute to more general studies of particles in a broad range of areas.

2.1.4 Micromachined Si substrates

There are two main challenges for AFM measurement of particles. Firstly AFM may move the particles during scanning if there were no special method applied to improve adhesion between dust particles and the substrate. In addition, the typical AFM tip height is about 10 μm ; so if some particles greater than 10 μm were deposited around the region of interest, the cantilever would be subjected to potential risks such as being broken or hampered when it collides with those ‘dangerous’ particles without the usual feedback control used to maintain the particle-tip distance [109] [110] [111].

To immobilise or eliminate large dust particles during AFM scanning and have better results, Vijendran developed several kinds of micromachined Si substrates that have been successfully applied in the Phoenix project for Mars exploration in 2008 [112] [113]. On the substrates, micron-scale pits are patterned and serve as traps to enhance the AFM scanning stability of particles wedged in the pits. In addition, the diameter of the pits can determine the size of particles to be captured and reduce adhesion for the larger dust particles, so that when the dust is deposited on the substrate and then tilted the substrate stand the substrate up to filter out unwanted large particles with the help of gravity. The substrate is shown in fig. 2-4 with a height of 5 μm .

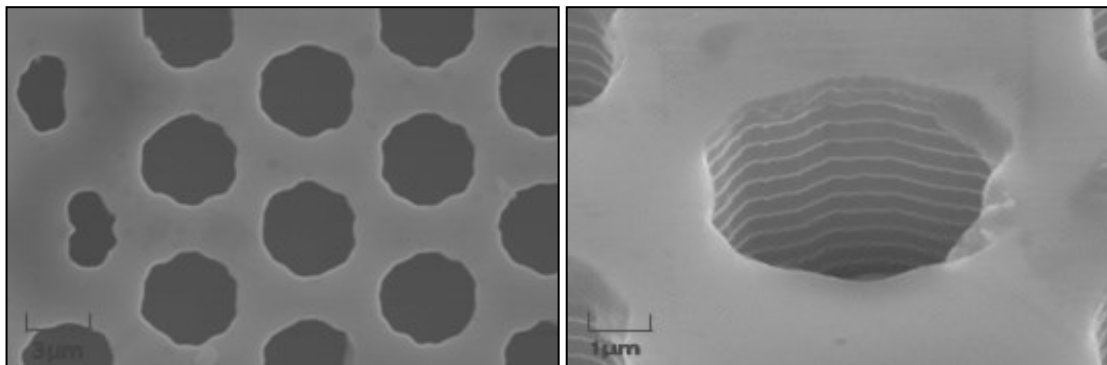


Figure 2-4: *The pattern of the pits on the micromachined Si substrate with 5 μm diameter and 5 μm height. Left: top view. Right: 45°side view.*

2.2 Evaluation of AFM and SEM particle imaging

2.2.1 Large area imaging

Both the SEM and AFM are used to image the same area of the micromachined substrate, which is shown in fig 2-5.

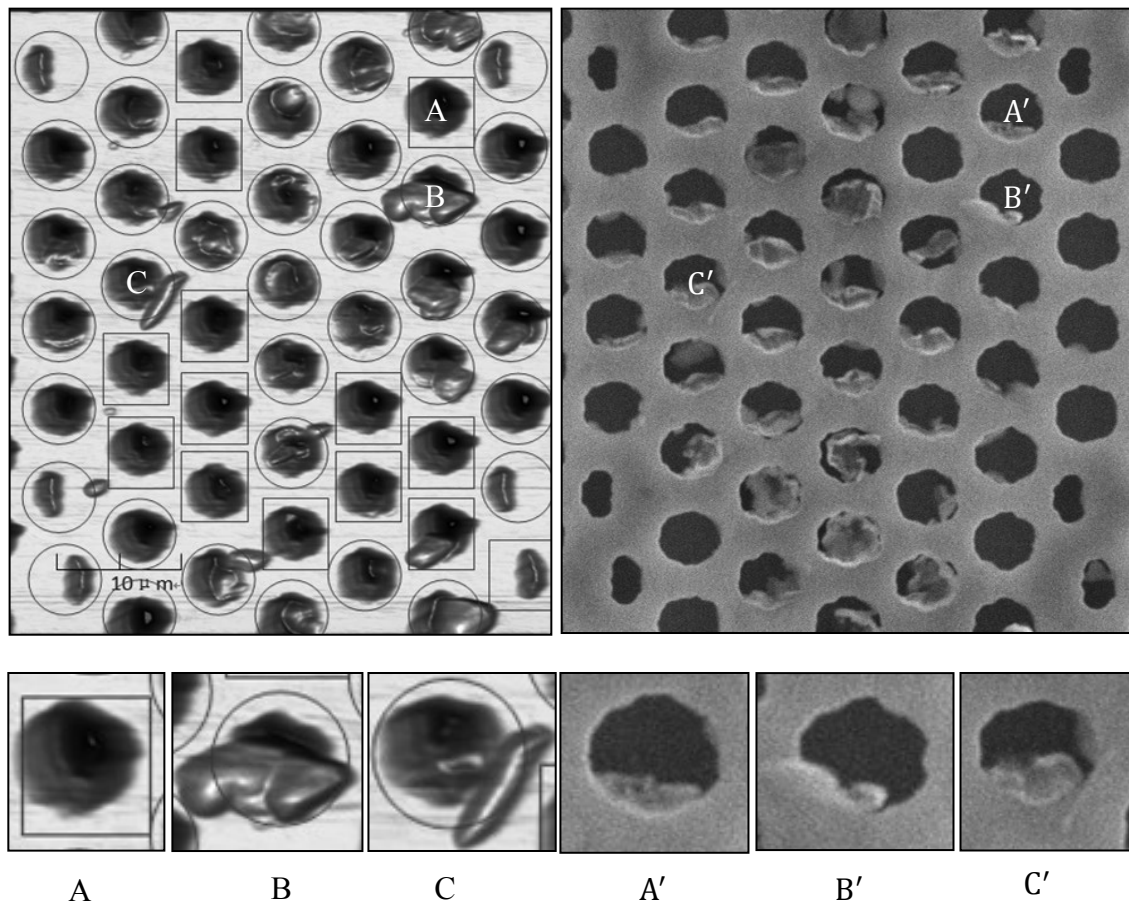


Figure 2-5: *AFM (left) and SEM (right) images*

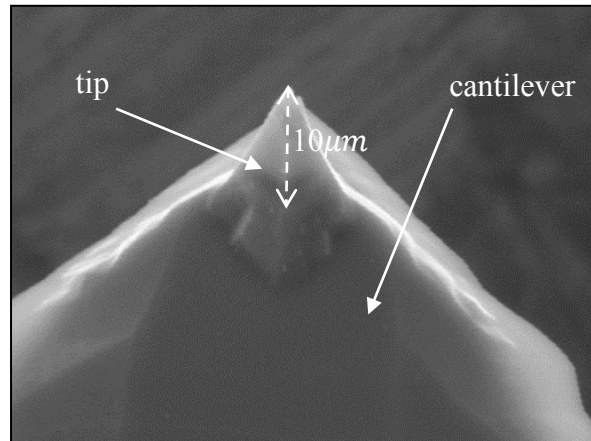


Figure 2-6: *AFM tip used*

This area is approximately $42 \times 52 \mu\text{m}^2$ and include 52 pits. The 38 circles on the AFM image show the similarities between the AFM and SEM images, and the 14 squares reveal the differences. By comparing the different parts, the particles that were completely inside the pits could be easily imaged by the SEM, but the AFM had difficulty in recognising them. This may result from the $5 \mu\text{m}$ depth of the pits, which could be deeper than a particle size, making the particles inaccessible to the AFM tip during scanning. For example in the SEM image we can clear recognize that there is a particle glued to the wall of the pit A, but in the AFM image only a small part of that particle can be found because the tip is unable to access the surface across.

AFM will also introduce the tip-sample convolution in the imaging result. Such as particles B and C, in the AFM image it is obviously shown a wider result than that of SEM image, which is caused by the convolution effect. The shape of the tip is shown in figure 2-6. The bottom of the tip is around $4 \mu\text{m}$ and the height of the tip is $10 \mu\text{m}$, so the tip angle is around 20° .

2.2.2 Individual particle imaging

To reveal the surface texture and shape of the particles, a single pit containing two particles is chosen for scanning. Both SEM images and AFM images are taken (see fig 2-7).

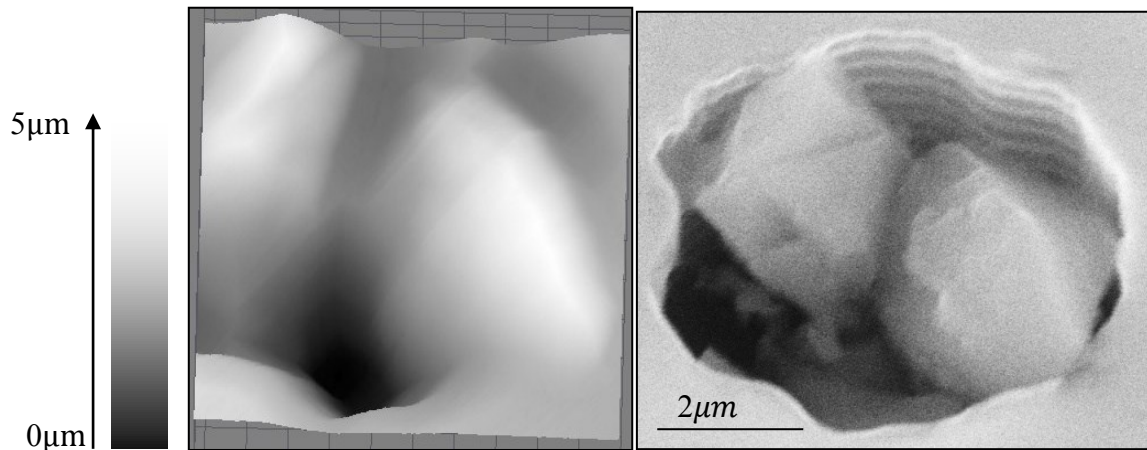
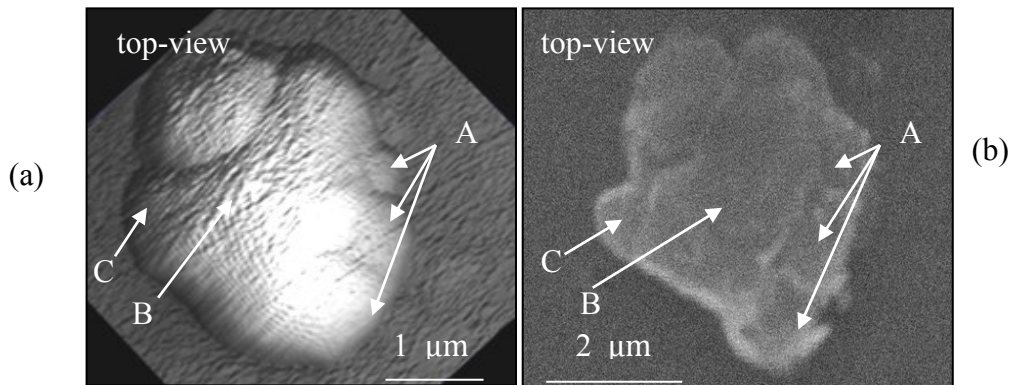


Figure 2-7: *AFM (left) and SEM (right) images of a single pit containing two particles.*

The top surface of the left particle can be recognised as a parallelogram with several inside scratches which can be seen and the top topography of the right particle can be generally described as an edge crossed by two steps, which are all seen in both the SEM image and the AFM image. The resolution of the AFM image is less than that of the SEM image. In addition the lower portions of both the left and right particles could not be measured by the AFM in detail. Also the shape of the particle shown on AFM image has some defects compare to the SEM image which is caused by the tip-sample convolution. The de-convolution technique [114] can be used to solve this problem which can eliminate the influence from the tip-shape., however only the part which can be touched by the tip is suitable for this method. For the parts such the bottom in the pit which cannot be touched by the tip at all, the AFM image of these parts cannot be improved even if de-convolution is applied, because there is no valid information obtained.

2.2.3 Comparison of AFM and SEM images [115]

To compare the consistency of the two approaches, the AFM images and SEM scans were also taken on the same particle. The sample is coated with a layer of gold (around 50 nm) and the diameter is around 5 μm . The SEM images are acquired from different angles to show the details that cannot be obtained from one angle. The AFM image $Z(x, y)$ represents a reconstruction of the surface limited by the inevitable effects of the dilation, and the avoidable information loss from a blunt tip. The SEM image gives a projection of this surface, in this case at two different angles, as marked in figure 2-8. The AFM result, $Z(x, y)$, and three SEM images $I_1(x, y)$, $I_2(x, y)$ taken from top-view and 45° side view respectively as shown in fig.2-8. For each SEM image $I_i(x, y)$, the AFM dataset $Z(x, y)$ was rotated to provide the best visual match between the two image pairs. To aid this comparison, the particle is divided into four different regions (A, B, C). In zone A there are 3 steps shown in both the SEM image and the AFM image. These steps can be shown clearer from the 45° side view images (fig.2-8 (c) and (d)). The SEM image shows that there is a small step between zone B and zone C; however in the AFM image this step is not as clear as that shown in SEM, which is caused by the geometric inability of the AFM tip to contact the surface in this region. The difference in information transfer for SEM and AFM makes a suitable alignment impossible. However, a comparison between two images illustrates graphically the challenges in combining these datasets.



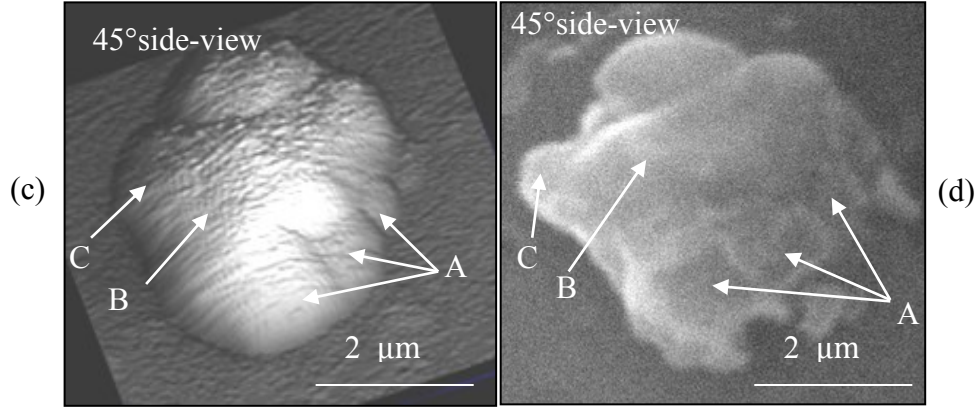


Figure 2-8: (a)(b): *AFM* , $Z(x,y)$, (left) and *SEM* $I_1(x,y)$ (right) top-view images
(c)(d): 45° side view *AFM* , $Z(x,y)$, (left) and *SEM* $I_2(x,y)$ (right) images.

Figure 2-9 illustrates the limitations and possibilities of AFM and SEM. $Z_0(x,y)$ represents the actual particle surface, $Z(x,y)$, the AFM image, is obtained through the transfer function of the AFM $Z(x,y) = T_{AFM}(Z_0(x,y))$. T_{AFM} includes convolution effects. In particular the inverse transfer function T'_{AFM} cannot map from the AFM data, $Z(x,y)$, back to $Z_0(x,y)$. This is because of the inevitable information loss in T_{AFM} , meaning that a unique $Z'(x,y)$ cannot be obtained.

The SEM images are obtained through the transfer function of the SEM, T_{SEM} . Although for a single image, T'_{SEM} will not be able to retrieve a surface reconstruction, $Z'(x,y)$, the addition information from multiple images might be able to constrain the inverse transfer function sufficiently to allow a unique reconstruction. One of the aims of this thesis is therefore seeking the solution $T'_{SEM}(I_1(x,y), I_2(x,y), I_3(x,y)) = Z'(x,y)$

From fig. 2-8 both AFM and SEM images can show the main patterns of the particle but compared to the SEM images, the AFM image is still influenced by the tip-sample convolution which has been discussed in the example above. The new thing can be found from this example is that the advantage of combining the SEM images, which

means that SEM image can illuminate the sample from different view containing complimentary information of the sample and these information can verify each other to provide a basis to reconstruct a 3D image by mathematical method such as stereoscopy discussed in chapter one, and also provide a information supplement to each other of the details of the sample, so this combination is a promising way to reconstruct the surface topography and will be discussed in the following Chapters.

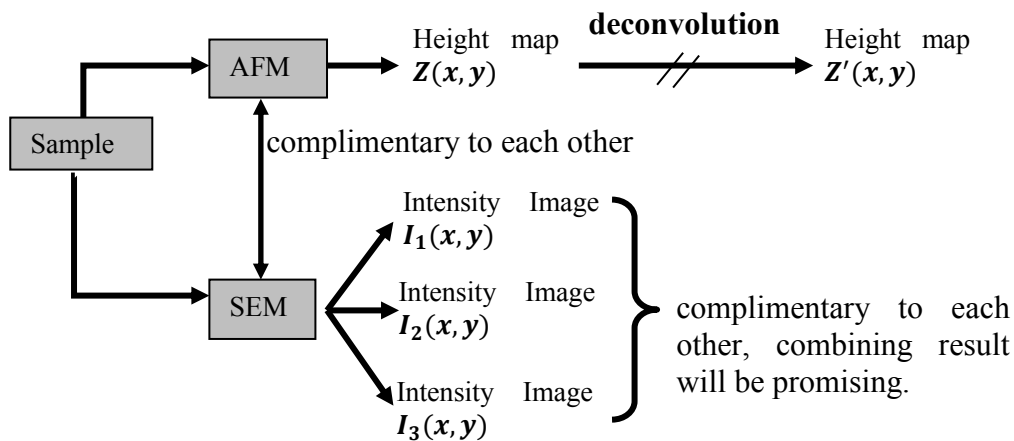


Figure 2-9:The promising to combine SEM image with *AFM image which are complimentary to each other*

2.3 Conclusion

These experiments have given an initial evaluation of a general idea about the ability of the AFM and the SEM to image particles, as shown in figure 2-9. With the help of a micromachined Si substrate, the AFM could achieve stable scanning, producing microscopic information about the upper part of a dust particle and display the shape and surface texture of particles clearly up to the nano-scale; however the quality of the AFM image is strongly related to the tip. A blunt tip will reduce the resolution of the image and even for a sharp tip it cannot obtain the height information of the bottom of the pit and introduce the tip-sample convolution defects especially on the edge of the sample.

SEM images can provide complimentary information. It can access the bottom of the pit and there is no tip-sample convolution causing the edge effect. In addition it can achieve a much quicker measurement than that of AFM.

Although we can register an AFM scan with an SEM image (fig 2-8), this cannot provide a quantified comparison or surface reconstruction directly, as the SEM can only provide a 2D image. However the combination of SEM images taken on the same sample from different angles provides a promising way to reconstruct 3D images from the 2D SEM datasets. Furthermore, the AFM can provide quantified information in the absence of image artefacts such as dilation. The two techniques are actually complimentary to each other and might provide an improved surface topography of the sample. The following chapters develop a new approach to achieve the goal, starting with the established technique of stereomicroscopy.

Chapter 3: Application and extension of existing methods

The objection is to develop a new technique that combines the advantages of the previous methods while avoiding their weaknesses, two approaches are introduced in this chapter.

In the first method, both SEM stereo reconstruction and AFM are applied to a particle sample of which the dimension is around 5 μm . However, it will be demonstrated that stereo microscopy has limited resolution. Furthermore, comparison with AFM images indicates that neither can provide height information for all sample surfaces. In an attempt to produce an improved combined dataset an algorithm for optimising the registration between two elevation maps is investigated using the iterative closest point (ICP) method. [116] [117]. The problem with such an approach is that it treats all the original data as being of equal value, and therefore the final fused dataset is not better, or even worse than, the selected parts of the original data.

To avoid such leakage of information, it is necessary to incorporate the physics of image formation into the algorithm to maintain the resolution during the processing. Based on the idea of the method, this is attempted by using an electron scattering model to produce simulated SEM data from the AFM elevation maps. These simulations are then incorporated into an iterative search for the best height reconstruction which can minimize the difference between the simulated and ordinal SEM. It is this approach that will provide the kernel for the final algorithm which will be presented in the following chapter.

3.1 AFM and stereo SEM

Combining AFM and stereo AFM was the first studied as a method of improving the 3D information extraction. Firstly the SEM stereoscopy is used to reconstruct a 3D image of a

particle sample of which the dimension is around 5 μm . Then the AFM image of the same sample is demonstrated. By comparing the results from the two different techniques, the advantages and disadvantages of each method is clear. Finally a data fusion method, iterative closest point, is applied to produce a new height data set containing the information from both the AFM and 3D-stereo image, however this method cannot be utilised to suppress the defects of the images and exploit their strengths. Though the result is not satisfactory, it provides the starting point for exploration of the algorithm.

3.1.1 SEM stereoscopy

SEM stereoscopy has been widely studied by many research groups and the software application StereoWorks developed by Victor Polillo was used for obtaining 3D Stereo result [118] based on the underlying principle introduced in Chapter one. By looking at image shift for features that can be recognized in two image of the sample taken under the different tilt angle, the coordinate pairs can be identified from both tilted images, and then an entire elevation map for the specimen surface can be calculated [119] [120].

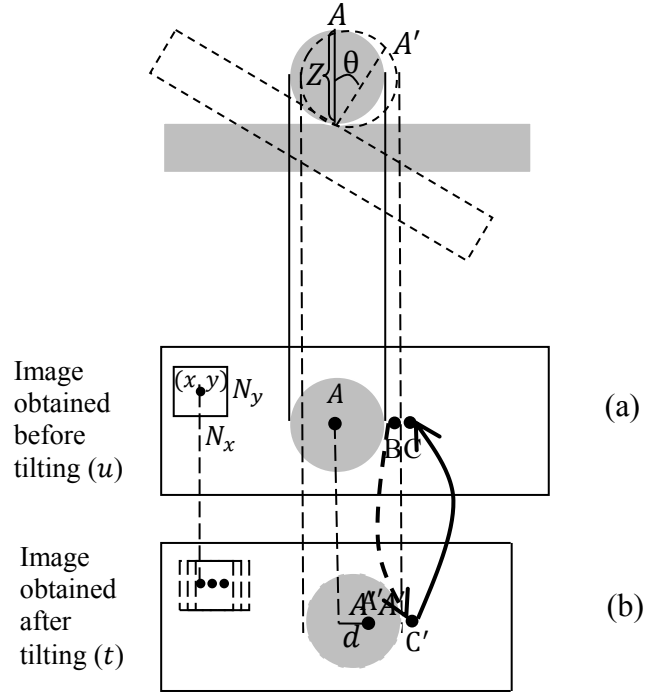


Figure 3-1: Left (u) –right ($\tilde{u}$) consistency. Point B which is occluded, is given C' as a match, but C' actually matches C rather than B . The pair (B, C') can be suppressed

More specifically the pair identification is based on a pattern recognition function which scans one region against successive regions extracted from the other image. Similarity scores are computed via normalized cross-correlation of the sequence of pairs. [121] The cross correlation, $\rho(d)$:

$$\rho(d) = \frac{\sum_{x,y} (u(x,y) - \bar{u}(d,0)) (t(x-d,y) - \bar{t})}{\sqrt{\sum_{x,y} (u(x,y) - \bar{u}(d,0))^2 \sum_{x,y} (t(x-d,y) - \bar{t})^2}} \quad (3-2)$$

where u is an part of the image and the size is $N_x \times N_y$. t is the corresponding part in the tilted image. $\bar{u}_{d,0}$ is the mean of $u(x,y)$ which means that $\bar{u}_{d,0}$ denotes the mean value calculated by

$$\bar{u}_{d,0} = \frac{1}{N_x N_y} \sum_{x=d}^{d+N_x-1} \sum_{y=0}^{N_y-1} u(x,y) \quad (3-3)$$

$\bar{t}_{d,0}$ is the mean of $t(x, y)$ in the region.

The displacement value is changing along with shifting the region on the right image. The final selected displacement value is the one that maximizes the normalized cross-correlating (ρ) of which the interval value is from 0 to 1, which means the region pairs in the two images is matched at that displacement [121] [122].

The displacement value that maximize the normalized cross-correlating is placed at the coordinates of the fixed window centre. By calculating the displacement value for each pixel the displacement map will be produced, so that the elevation value will be obtained based on the equation (1-4).

The theoretical depth resolution of a stereo camera $\delta Z_{(x,y)}$ at the point (x, y) can be calculated as below (this has been discussed in Chapter 1.3.1): [123] [124]

$$\delta Z_{x,y} = \frac{C_{scale}}{2\sin(\frac{\theta}{2})} \delta d_{xy} \quad (3-4)$$

where C_{scale} is the scale factor to convert pixels to micrometers, based on magnification, θ is the total change in tilting angles, δd_{xy} is disparity precision (the spatial distance between two corresponding points in images u and t respectively) [123].

If the two images are taken with a very small angle separately, the disparities obtained can be smaller than the pixel size. From equation (3-3) it can be seen that the depth resolution is linked to the disparity precision and the sub-pixel disparity estimation will be required in such cases. For instant let d be the disparity estimate of the normalized cross-correlating method for a certain pixel. Hence, changing the disparity by ± 1 yields an reduce the cross-correlating value. The maximum, however, may be located in between pixels and if a subsequent sub-pixel estimation step is adopted, the precision of the stereoscopic disparity comes to sub-pixel resulting in the improvement of the depth resolution and the depth accuracy [125] [126].

According to the method discussed above with sub-pixel precision the reconstruction is shown as below:

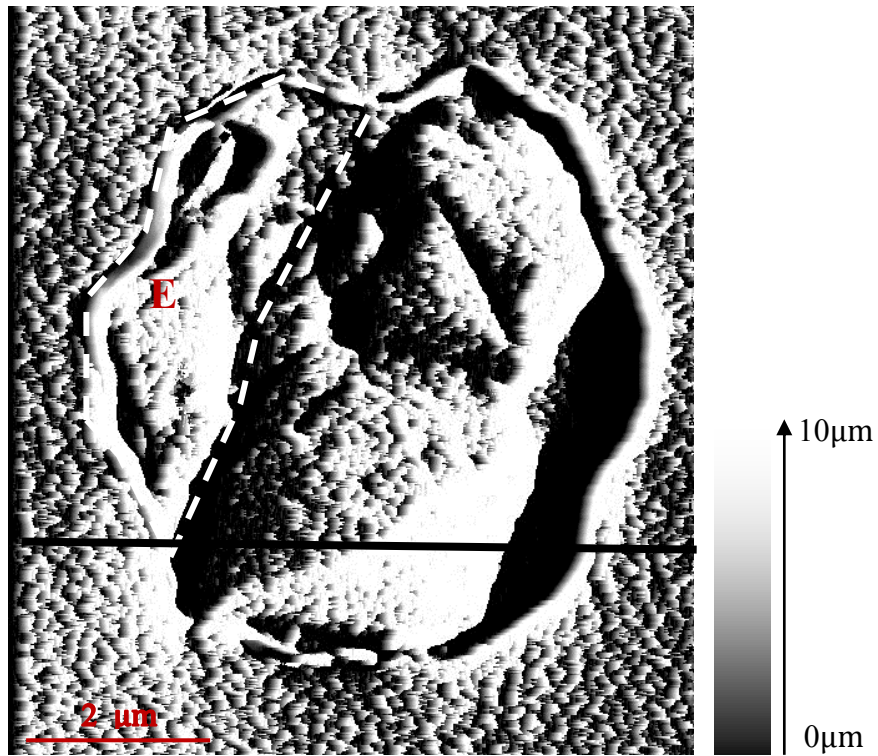


Figure 3-2: *The 3D reconstruction obtained by the stereoscopy*

The profile line along the black line is shown as below:

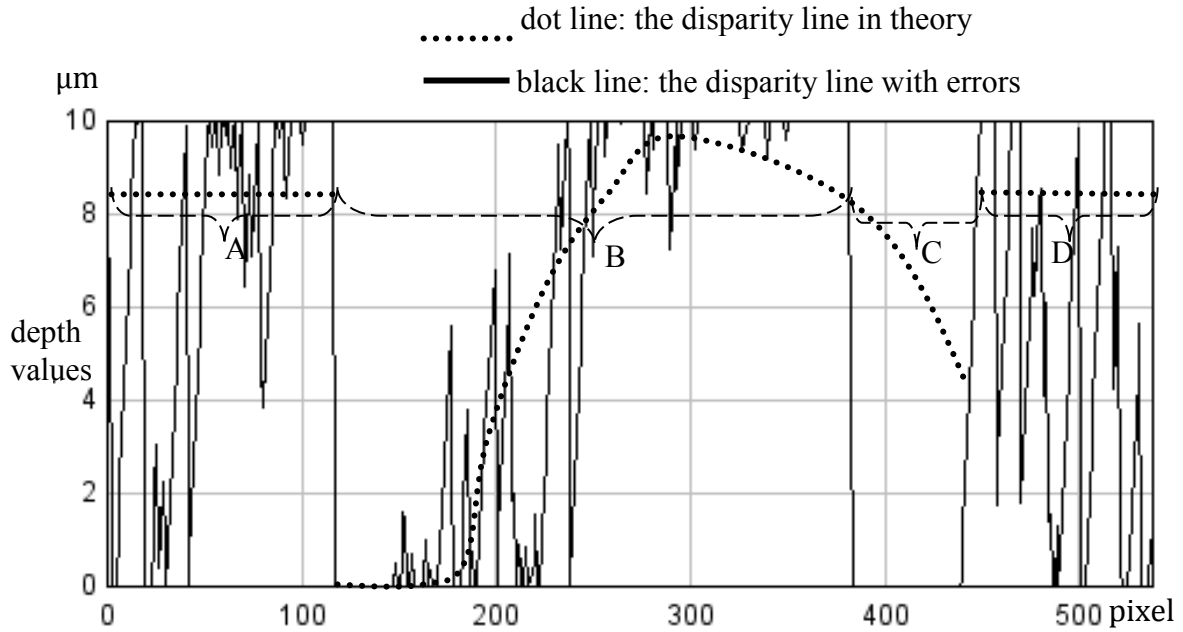


Figure 3-3: *The height value along the black line on the 3D SEM image.*

The dot line is the expectation of the height values, but the actual profile line (black line) is influenced by the errors. There are several kinds of errors influence the accuracy of the result which can be divided in two terms. One is due to the noise and is divided by the $2\sin\left(\frac{\Delta\theta}{2}\right)$ coefficient, and the other one is independent of $2\sin\left(\frac{\Delta\theta}{2}\right)$. In other words, the first part of the error is smaller with large stereoscopic angles, which is caused by the noise such as what is shown on region B, but the second part is independent of the angle which is result from the non-textured (region A and D) and occlusions regions (region C) [127] [128].

For the noise errors there a conclusion has been approved by Julie and Bernard [] : the more constant the image, the more influential the noise. For example region A and D will face more noise influence than that of region B. The influence from the noise is shown as below:

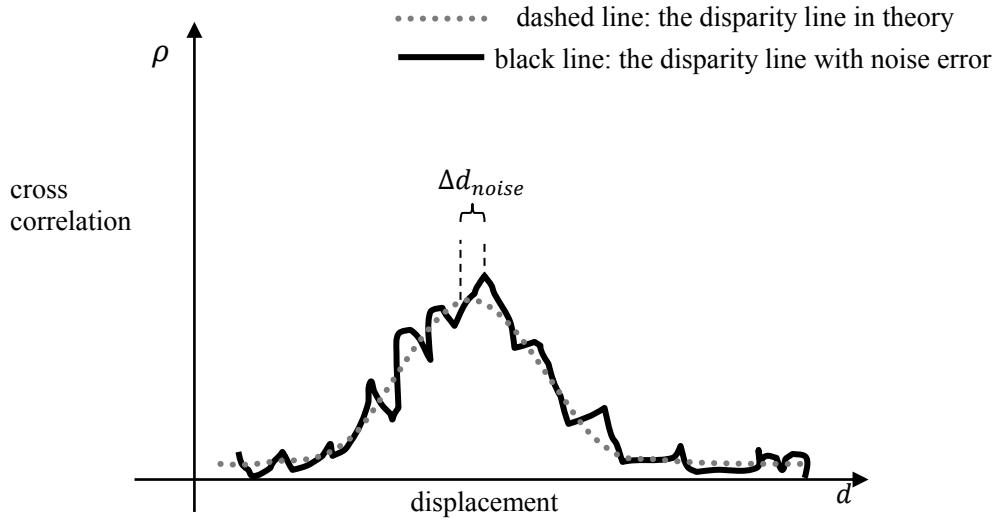


Figure 3-4: *The noise influence on the disparity searching*

The occlusions region can create points that do not belong to any matching pairs. For example in fig. 3-1 point B is shown in the image obtained before tilting however after tilt the sample the point B cannot be detected.

To point out the occlusion regions, the key observation is that matching is not a symmetric process: the visible points in one image can be matched but when the role of two images is reversed, new pairs are found. More specifically consider for instance an occluded point, e.g., B, in the image (a) of fig. 3-1: although there is no corresponding point in the image (b), the normalized cross-correlating algorithm matches it to the point C', because the algorithm can find a disparity value to achieve a relatively high similarity, though it is not the appropriate one. However the latter point, in turn, will correspond to a different point C in the image (a) to which C' is more similar than to the point B. The so-called “left-right consistency constraint” states that feasible matching pairs are those found with both direct and reverse matching and occlusions are detected, suppressing unfeasible matches [129] [130].

For each point on the left image (u) the $d(x)$ is computed as described in equation (3-1). The process is repeated after reversing the two images. If $d_u(x) = -d_{\bar{u}}(x + d_u(x))$ the

point keeps its computed disparity, otherwise it is marked as occluded. In our algorithm if the occlusions are determined, the value of the related points will be set as 0 during the reconstruction such as region C in the fig. 3-3 [129].

In addition, in dense stereo matching, the ambiguity arising from large regions of constant intensity makes it impossible in general to identify all locations in the two images with certainty which will introduce the matching errors. According to equation (3-1), the correlation will be null if the intensity on the two images are constant, where no reliable disparity can be recovered. This confirms the intuition that correlation needs texture information in order to succeed. For example the intensity value of the SE image depends on the slope of the sample surface, so the high curvature of the sample can produce the sharp intensity changes in the corresponding area in the SE image which produce sharp edges and distinct features. However, areas of low curvature of the sample produce relatively uniform intensities in the SE images, resulting in highly erratic disparity estimates [121] [131].

The flat regions such as A and D shown in fig.3-3 have constant intensity, because of the reason discussed above the algorithm cannot successfully identify all locations in the two images, causing the matching errors.

The profile line of the rectangle region is shown as below. According to the morphology of the substrate holding the particle, the profile line should be flat, however the actual values are influenced by the errors discussed above which make the profile line be fluctuating. According to the declaration of the software normally the maximum disparity cannot be more than 15, so that we use different maximum disparity settings (5 pixels, 10 pixels and 15pixels) respectively. The average intensity along the rectangle region is shown:

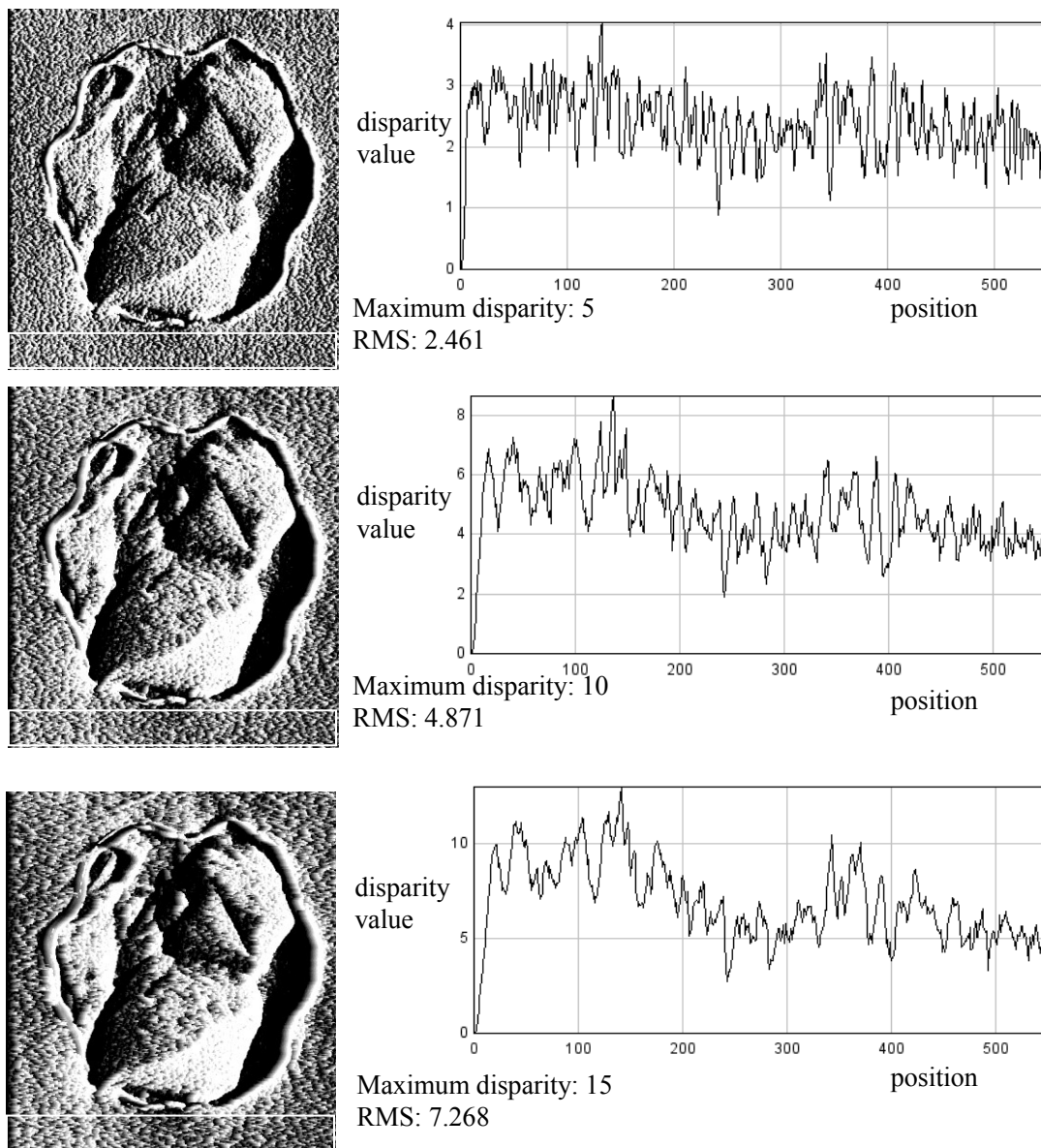


Figure 3-5: *The disparity matching results and the related profile lines of the non-textured region at different max disparity settings (5 pixels, 10 pixels and 15 pixels)*

From the profile it can be found that during the region the disparity value is nearly randomly chosen so that the RMS value is around half of the maximum disparity, so that for non-textured regions the algorithm cannot find reasonable disparity values.

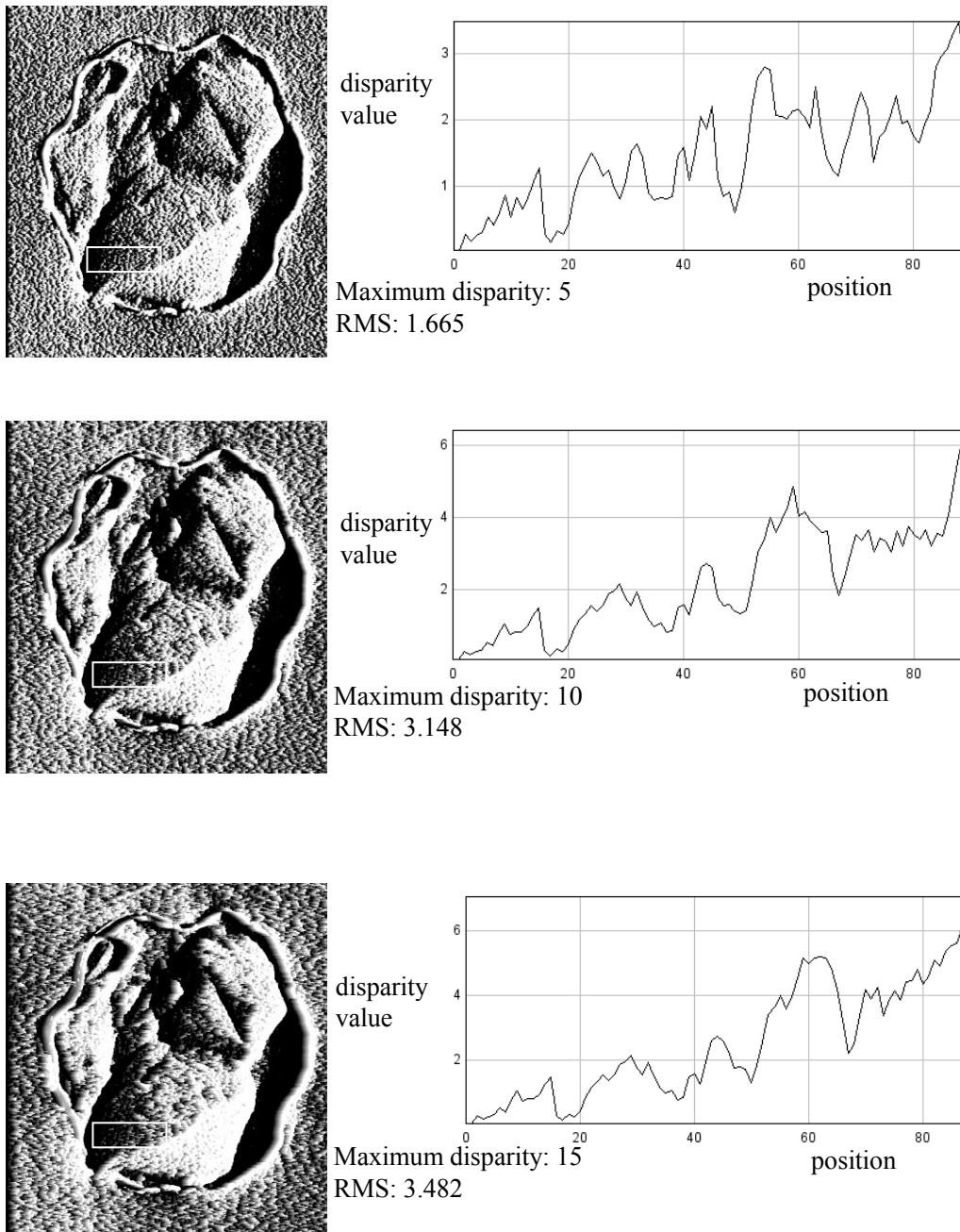


Figure 3-6: *The disparity matching results and the related profile lines of the textured region at different max disparity settings (5 pixels, 10 pixels and 15 pixels)*

Let us come to the textured region and still 3 maximum disparity values are used. Intuition tells us that if the maximum disparity is set as 10 or 15, the reconstruction is almost the

same. Also the RMS value shows similar values between 10 and 15 maximum disparity settings, which means that for the textured region if the maximum disparity is reasonably chosen, the algorithm can find meaningful disparities for final reconstruction, but for the non-textured region it will introduce errors and influence the final reconstruction.

The AFM image is also taken as a comparison. It can be found that the depth accuracy of AFM image is better than that of SEM stereoscopy.

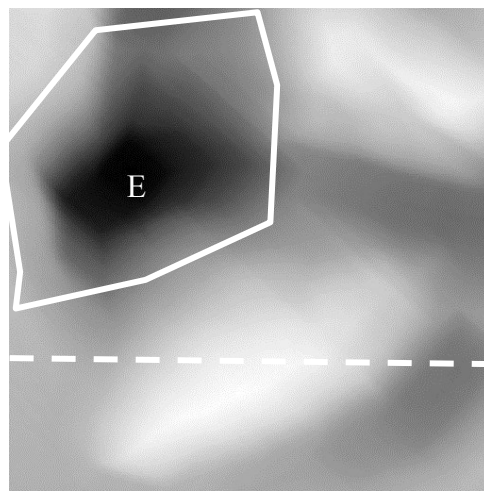


Figure 3-7: *The 3D height image obtained by AFM*

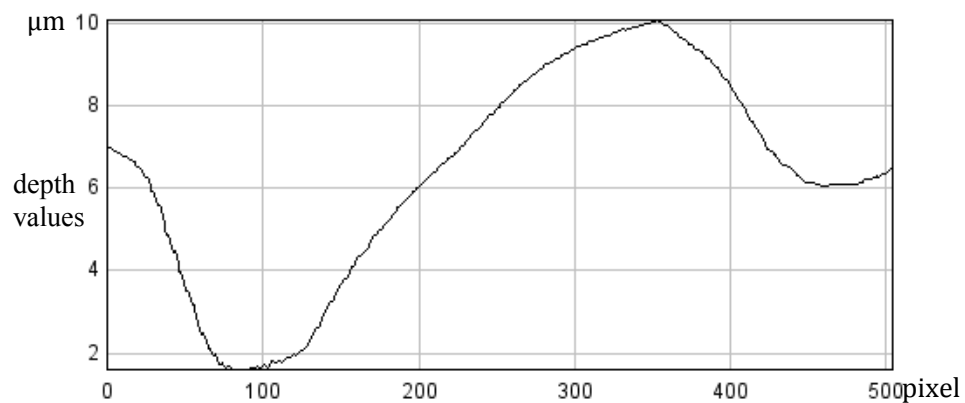


Figure 3-8: *The height value along the dashed line on the 3D AFM image.*

By comparing the profiles of the same region between AFM and stereoscopy it is evident that the stereo method is much noisier. However zone E shown in the SEM stereoscopy image (fig. 3-2) cannot be found in the AFM image (fig. 3-7) because the height of the zone was too low for the tip to touch. Hence there is complimentary information from both techniques.

The figures and discussions illuminate the information leakage of the AFM image which is limited by the tip and the information leakage of SEM due to the noise and the non-textured and occlusions regions. The comparison illuminates the potential of cooperation between the two height data sets, if a suitable way of combining the dataset can be found. We now turn to investigating such an approach.

3.1.2 Combining AFM with stereo SEM

A feasible method to complement each other is the iterative closest point (ICP) algorithm which can be used to describe the qualitative similarity between 3D images and then minimise the differences between them [132] [133].

The ICP algorithm is employed to minimise the difference between two digital images by aligning a ‘source’ shape with a ‘reference’ shape. In our experiments, the source and model shapes were represented by an AFM image and a 3D SEM image, respectively [134] [135], so that the stereoscopic SEM image can be used to position the distinct features and the adjusted AFM can give more depth resolution and less depth error in the first instance the datasets have to be aligned as accurately as possible.

In the algorithm the reference data set is kept fixed, while the other one is transformed to best match the reference data set. The algorithm iteratively revises the transformation (translation and rotation) needed to minimize the distance from the source to the reference point cloud. For each point in the source data set, find the closest point in the reference point cloud. Given two points s_1 and r_1 , the distance is

$$d(s_1, r_1) = \|s_1 - r_1\| = \sqrt{(x_{s1} - x_{r1})^2 + (y_{s1} - y_{r1})^2 + (z_{s1} - z_{r1})^2} \quad (3-5)$$

Given a point $s_1 \in$ source data set S and a reference data set R, the distance is

$$d(s_1, R) = \min_{i \in 1 \dots n} d(s_1, r_i) \quad (3-6)$$

Then estimate the combination of rotation and translation using a mean squared error cost function that will best align each source point to its match obtained in the previous step.

$$\text{Mean squared error} = \sum_{s \in S} \|\text{match}_R(s) - (\text{rot} \times s + \text{trans})\| \quad (3-7)$$

Where $\text{match}_R(s) \in$ reference data set R, $\text{rot} = \{r_x, r_y, r_z\}$ are the 3D rotation parameters for x, y and z directions and $\text{trans} = \{t_x, t_y, t_z\}$ are the translation parameters. To obtain the values of “rot” and “trans” the Newton’s minimization approach can be used [136].

The Newton method in one variable is implemented as follows: Given a function f defined over the x , and its derivative is f' , we begin with a first guess x_0 for a root of the function f . Provided the function satisfies all the assumptions made in the derivation of the formula, it has been proved that a better approximation is [137] [138].

$$x_1 = x_0 - \frac{f(x_0)}{f'(x_0)} \quad (3-8)$$

The process is repeated as

$$x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)} \quad (3-9)$$

until a sufficiently accurate value is reached.

Extend this to data fitting, where the goal is to find the parameters $\boldsymbol{\beta} = (\beta_1, \dots, \beta_n)$ such that a given model function $y = f(x, \boldsymbol{\beta})$ best fits some data points $(x_1 \text{ to } m)$ and $(y_1 \text{ to } m)$ with $m \geq n$, Newton algorithm iteratively finds the minimum of the sum of squares

$$s(\boldsymbol{\beta}) = \sum_{i=1}^m [y_i - f(x_i, \boldsymbol{\beta})]^2 \quad (3-10)$$

Starting with an initial guess $\boldsymbol{\beta}^{(0)}$ for the minimum, the method proceeds by the iterations

$$\boldsymbol{\beta}^{(s+1)} = \boldsymbol{\beta}^{(s)} - (J^T J)^{-1} J^T (\mathbf{y}_{1 \text{ to } m} - f(\mathbf{x}_{1 \text{ to } m}, \boldsymbol{\beta}^{(s)})) \quad (3-11)$$

Where J is a Jacobian matrix and $J_{ij} = \frac{\partial f(x_i, \beta_j)}{\partial \beta_j}$, $i \in m$ and $j \in n$.

For our application $\boldsymbol{\beta} = (r_x, r_y, r_z, t_x, t_y, t_z)$, $\mathbf{y}_{1 \text{ to } m}$ = the reference data set and $\mathbf{x}_{1 \text{ to } m}$ = the source data set. [136] By setting the initial guess to (1,0,0,0,0,0), $\boldsymbol{\beta}$ will be obtained by the Newton algorithm and will then transform the source points using the obtained transformation including rotation and translation. Iterate the steps until the threshold, normally the mean squared error, is achieved. The schematic of the method presented in chapter 3.1 is shown as below:

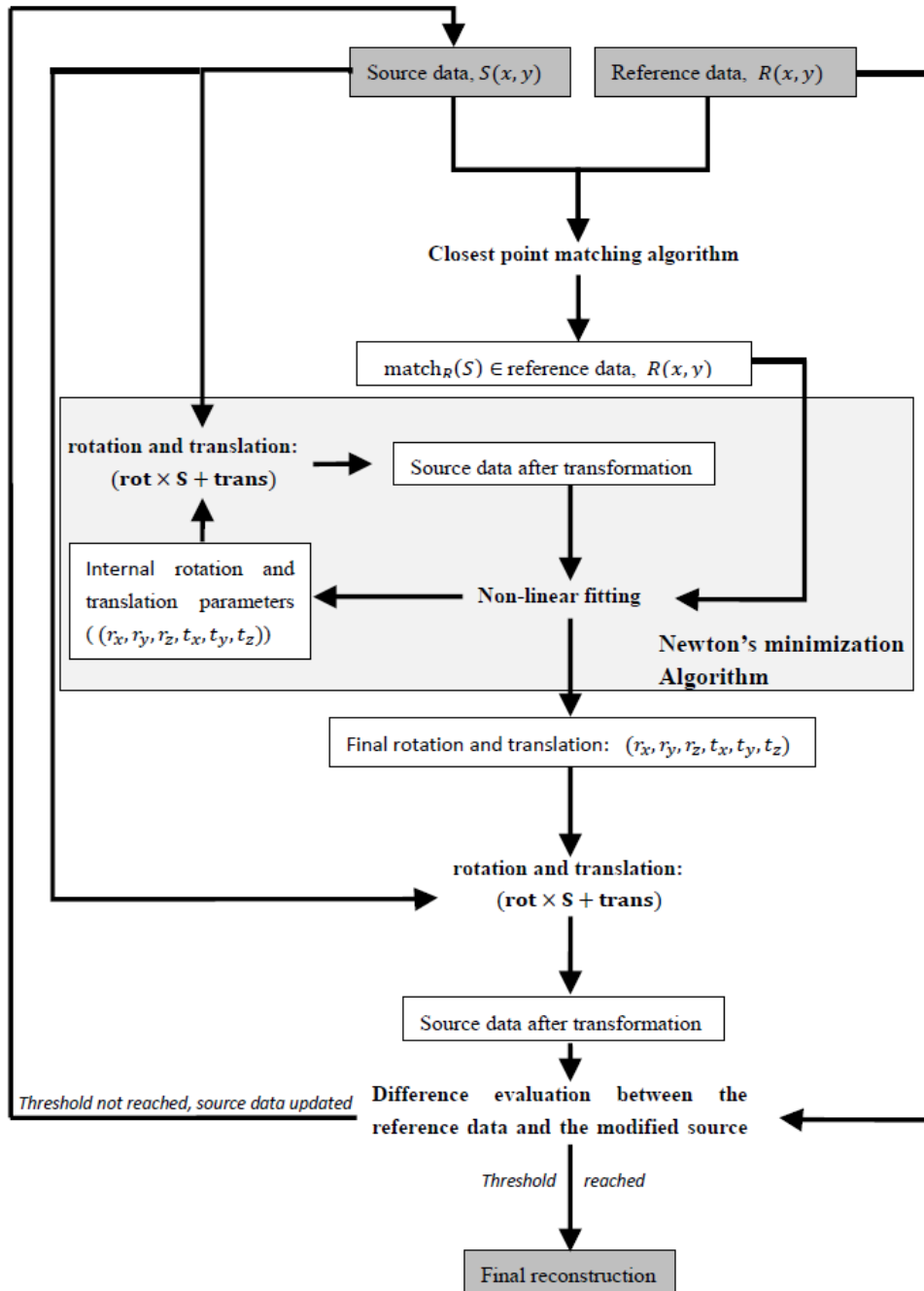
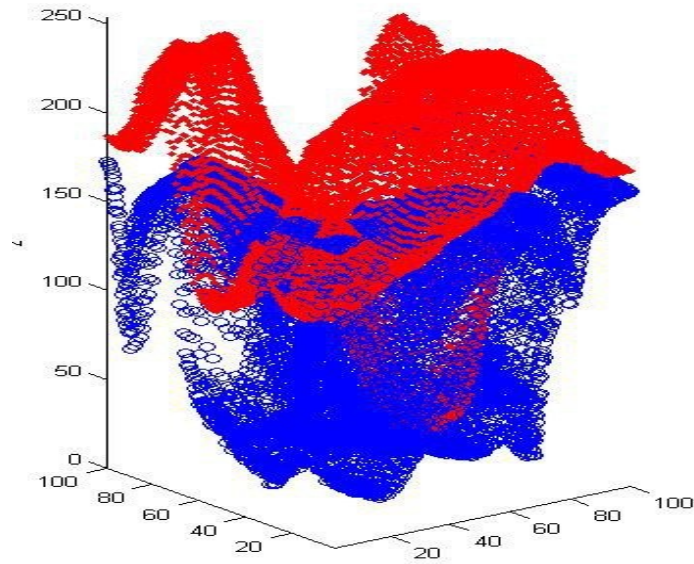


Figure 3-9: *The schematic of the ICP algorithm.*

The AFM image and the 3D SEM image are used as the source shape and reference shape respectively, and the number of iterations is 30. The results are shown in fig. 3-10 and 3-11.

Red: AFM Blue: SEM



ICP result

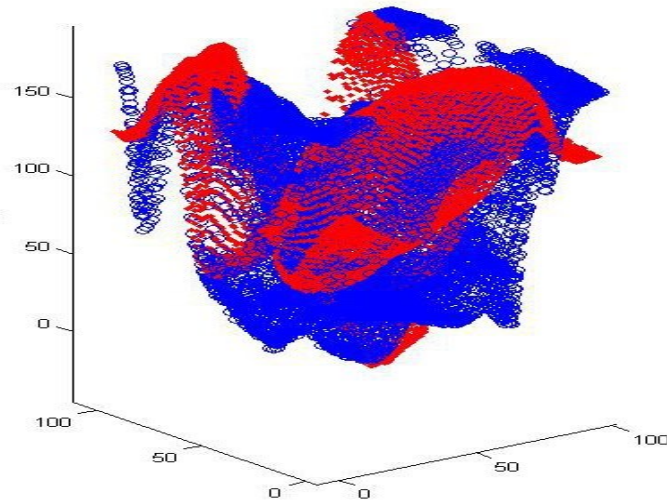


Figure 3-10: *Left: before ICP algorithm was applied to AFM and SEM images; Right: after ICP algorithm was applied to AFM and SEM images.*

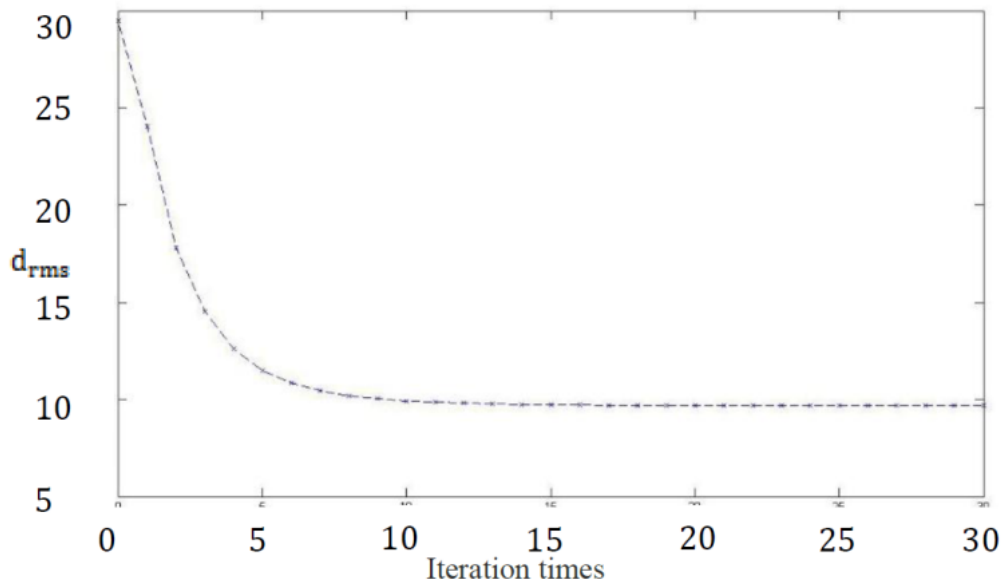


Figure 3-11: *Progress of the iterations*

The results showed that the mean squared error remained unchanged after ten iterations. Fig. 3-10 shows that after the ICP algorithm is applied, the transformed AFM image resembles the 3D SEM image much more closely than before. However, this method is not perfect for modifying an AFM image; there are still some limitations. Firstly it is difficult for SEM stereoscopy to provide a satisfactory 3D SEM image, which means that the details on a 3D SEM image used as a reference are quite blurry, especially for the constant intensity parts and occlusion parts on the SEM image. Also the tip-sample convolution of the AFM image cannot be removed by this kind of algorithm, so that even though the RMS error becomes stable after ten iterations, the algorithm cannot return a convincing result. Although ICP has found the best alignment, the difference between the two sets are too great to add further information. Given the large insignificant errors that stereomicroscopy produces, there appears to be little advantage in combining these datasets.

3.2 AFM and shape from shading (SFS) SEM

The next algorithm we applied is a form of minimisation SFS method that uses the AFM image as an initial height image for the shape information from SEM SFS which has been discussed in chapter one. The procedure can be described like this: produce a simulated SEM image from the AFM image and then compare the simulated SEM image with the real SEM image; depending on the results, modify the AFM image to minimize the difference between the simulated and real SEM and finally obtain a new 3D image.

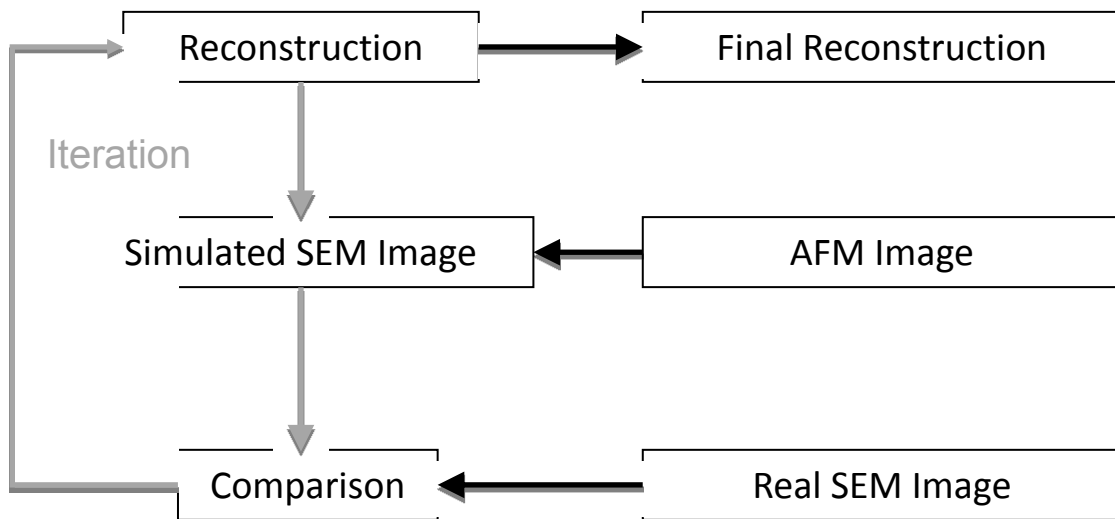


Figure 3-12: *The schematic of the SFS algorithm.*

3.2.1 Simulated SEM algorithm for shape from shading

To implement this algorithm, the first step for producing an elevation map is to create a simulated SEM image using a AFM image (height image). There are two basic methods to achieve this simulation.

3.2.1.1 The Monte Carlo Method

The MC method is a widely used technique for finding an approximate solution by using a computer to perform many randomised experiments [139]. To estimate an SEM signal,

the computer simulates many scattering electrons and computes quantity and trajectory of electrons that escape the specimen.

Although MC simulation is the most physically accurate model for SEM, it is too slow for AFM-based SEM simulation. In addition, it is difficult to reconstruct the AFM sample in the software due to the complexity of the surface in the AFM image, so the method has not been adopted by our algorithm.

3.2.1.2 Surface Slope- and Curvature-based simulation method

To overcome the impracticalities of MC simulation, the slope and curvature-based models of SEM intensity are introduced. There are two advantages of this: (1) it can provide more satisfying outputs; and (2) the speed of the algorithm will be fast enough to be part of iterative algorithm.

The model of slope- and curvature-based SEM simulation was first developed by Seeger [140] and contains a function that maps the slope and the curvature values to SEM intensity.

The flow graph of how to obtain the slope- and curvature-based simulation is shown as below:

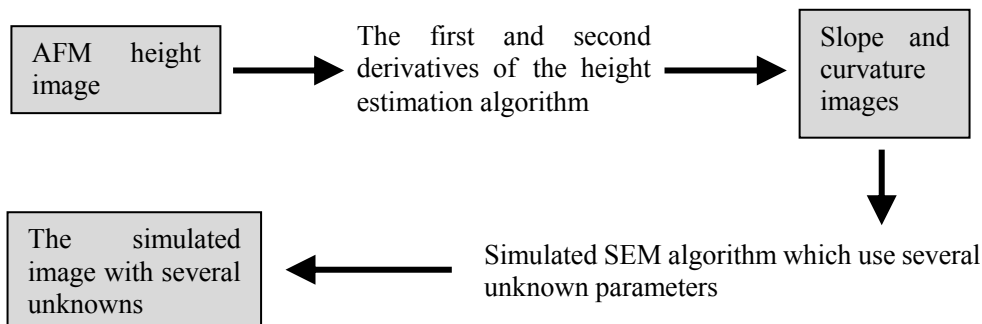


Figure 3-13: *The schematic of the surface slope- and curvature-based simulation method.*

The model developed by Haralick is used to estimate the first and second derivatives [141] to produce the slope and the curvature values which will be discussed in Appendix A in

details. In this model, the slope and curvature can be produced based on the first and second derivatives of the height image which is calculated out based on a height value window (5 by 5 pixels) centred at each point on the AFM image.

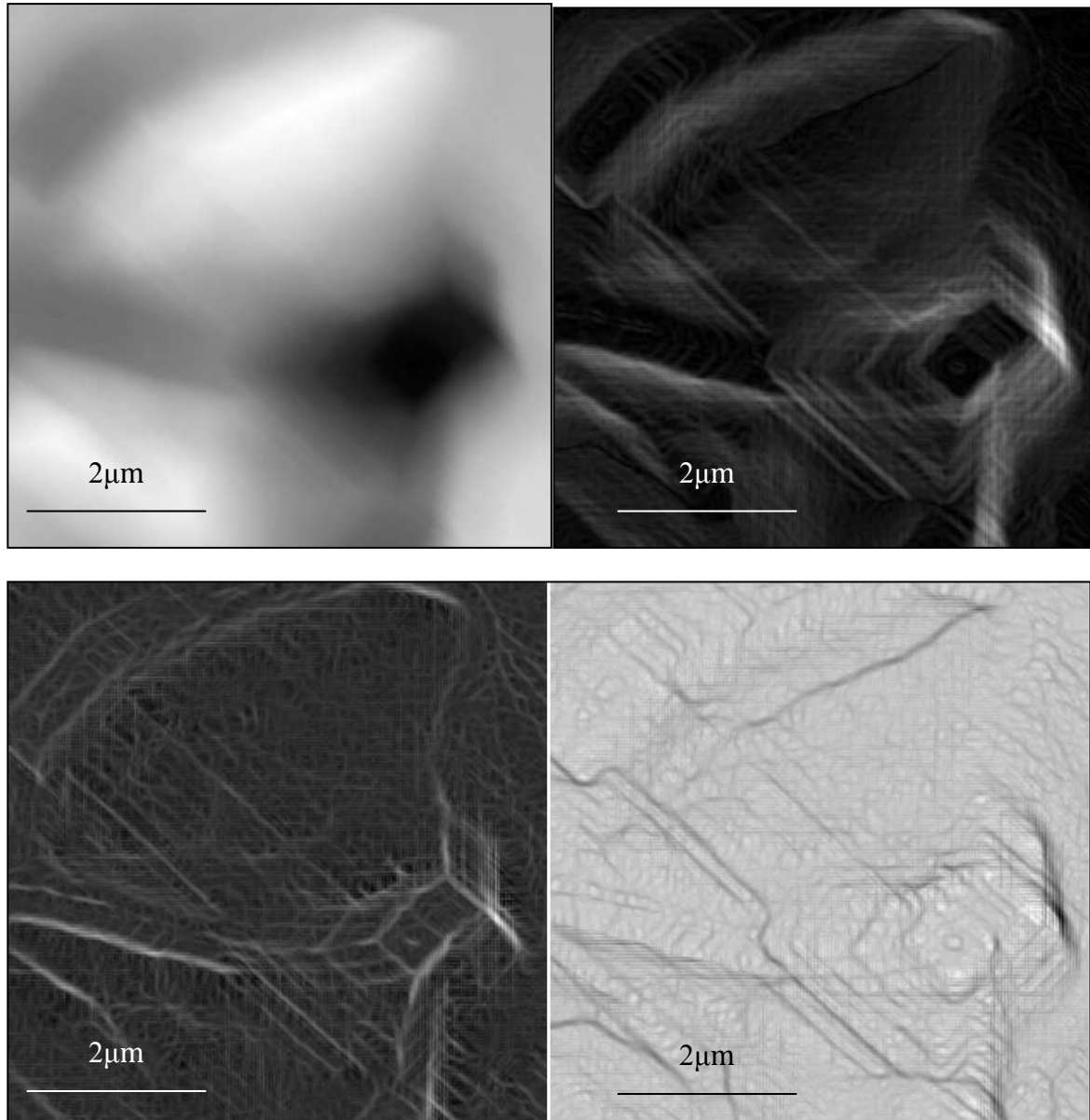


Figure 3-14: *The original AFM image (upper left), the gradient magnitude image (upper right), the maximum principal curvatures (lower left), and the minimum principal curvatures (lower right).*

In Seeger's model, the linear function is chosen to combine the gradient and curvature into the simulated SEM result.

$$FB = d + \sum_{n=1 \dots N} a \times G_n(x,y) + b \times K_{+n}(x,y) + c \times K_{-n}(x,y) \quad (3-12)$$

where N is the number of neighbourhood sizes and $G_n(x,y)$, $K_{+n}(x,y)$, and $K_{-n}(x,y)$ are the gradient magnitude, maximum, and minimum principal curvature, respectively obtained by the Haralick model (see Appendix A). The parameters a, b, c and d will be determined by fitting the simulated SEM image to the real SEM image, which will be introduced in the next subchapter together with modifying height values on the AFM image.

3.2.2 Combining AFM with SFS SEM

For the next step, comparisons between the real and simulated SEM images should be made. Then, based on the comparison results, the AFM image can be modified.

To explain the principle behind the automatic modification, we can look at a one-dimensional situation as an example.

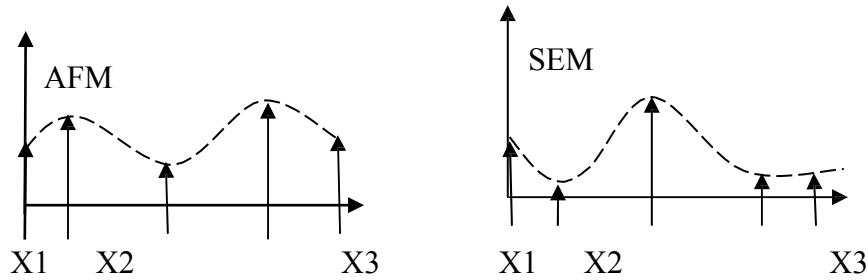


Figure 3-15: *The schematic diagram for the 1D situation*

Given there is a function that can map three AFM values to one SEM value; this can be called the 1-D simulated SEM function [142]:

$$SEM_{X_K} = F_{simulated\ SEM}(AFM_{X_{K-1}}, AFM_{X_K}, AFM_{X_{K+1}}) \quad (3-13)$$

Therefore, if we know all five SEM values $SEM_{X_1}SEM_{X_2}SEM_{X_3}SEM_{X_4}SEM_{X_5}$ and two AFM values AFM_{X_1}, AFM_{X_2} , according to the simulated SEM, we can obtain the remaining AFM values ($AFM_{X_3}, AFM_{X_4}, AFM_{X_5}$) from the following equations:

$$SEM_{X_2} = F_{simulated\ SEM}(AFM_{X_1}, AFM_{X_2}, AFM_{X_3}) \quad (3-14)$$

$$SEM_{X_3} = F_{simulated\ SEM}(AFM_{X_2}, AFM_{X_3}, AFM_{X_4}) \quad (3-15)$$

$$SEM_{X_4} = F_{simulated\ SEM}(AFM_{X_3}, AFM_{X_4}, AFM_{X_5}) \quad (3-16)$$

The modification method used has the similar calculation principles as the 1D situation. The new AFM image can be solved using the SEM image as a reference. We solved a system of nonlinear equations using the least squares method, in which the AFM image was used to provide the starting values during the computational process by modifying height values to minimise the difference between the simulated and real SEM images so that the new height image could be obtained.

There are two normal methods can be used for minimising differences. The first algorithm is based on the Newton method which has been described above in equation. [143]

The second algorithm is the Levenberg-Marquardt algorithm, also called the damped least-squares method, which generally provides the solution to the problem of the nonlinear function.

When the Levenberg–Marquardt algorithm is applied, the problem to be solved can be describe like this: given a set of m pairs of variables, ($\mathbf{x}_1$ to $\mathbf{m}$ and $\mathbf{y}_1$ to $\mathbf{m}$), optimize the parameters $\boldsymbol{\beta} = (\beta_1, \dots, \beta_n)$ of the model $f(x, \boldsymbol{\beta})$ so that the sum of the squares of the deviations becomes minimal. [143]

$$s(\boldsymbol{\beta}) = \sum_{i=1}^m [y_i - f(x_i, \boldsymbol{\beta})]^2 \quad (3-17)$$

Like the Newton algorithms, the LM algorithm is an iterative procedure. To start a minimization, the user has to provide an initial guess for the parameter vector, $\boldsymbol{\beta}$. In each iteration step, the parameter vector, $\boldsymbol{\beta}$, is replaced by a new estimate, $\boldsymbol{\beta} + \boldsymbol{\delta}$. To determine $\boldsymbol{\delta}$, the functions $f(x_i, \boldsymbol{\beta} + \boldsymbol{\delta})$ are approximated by their linearization $f(x_i, \boldsymbol{\beta} + \boldsymbol{\delta}) \approx f(x_i, \boldsymbol{\beta}) + J\boldsymbol{\delta}$ where $J_{ij} = \frac{\partial f(x_i, \beta_j)}{\partial \beta_j}$, $i \in m$ and $j \in n$. At the minimum of the sum of squares, $s(\boldsymbol{\beta})$, the gradient of s with respect to $\boldsymbol{\delta}$ will be zero. The above first-order approximation of $f(x_i, \boldsymbol{\beta} + \boldsymbol{\delta})$ gives

$$s(\boldsymbol{\beta} + \boldsymbol{\delta}) \approx \sum_{i=1}^m (y_i - f(x_i, \boldsymbol{\beta}) - J\boldsymbol{\delta})^2 \quad (3-18)$$

Taking the derivative with respect to $\boldsymbol{\delta}$ and setting the result to zero gives:

$$(J^T J)\boldsymbol{\delta} = J^T [\mathbf{y} - f(\boldsymbol{\beta})] \quad (3-19)$$

This is a set of linear equations which can be solved for $\boldsymbol{\delta}$.

If either the length of the calculated step, $\boldsymbol{\delta}$, or the reduction of sum of squares from the latest parameter vector, $\boldsymbol{\beta} + \boldsymbol{\delta}$, fall below predefined limits, iteration stops and the last parameter vector, $\boldsymbol{\beta}$, is considered to be the solution [144] [145].

In many cases, it finds a solution even if it starts far from the final minimum; however, the Levenberg–Marquardt algorithm tends to be slower than the Newton algorithm [146].

To choose a suitable method for this simulation, both of the two methods (Newton algorithm and Levenber-Marquardt algorithm) were tested. The results of the Newton method and the Levenberg-Marquardt method for modifying the AFM images are shown in fig. 3-16.

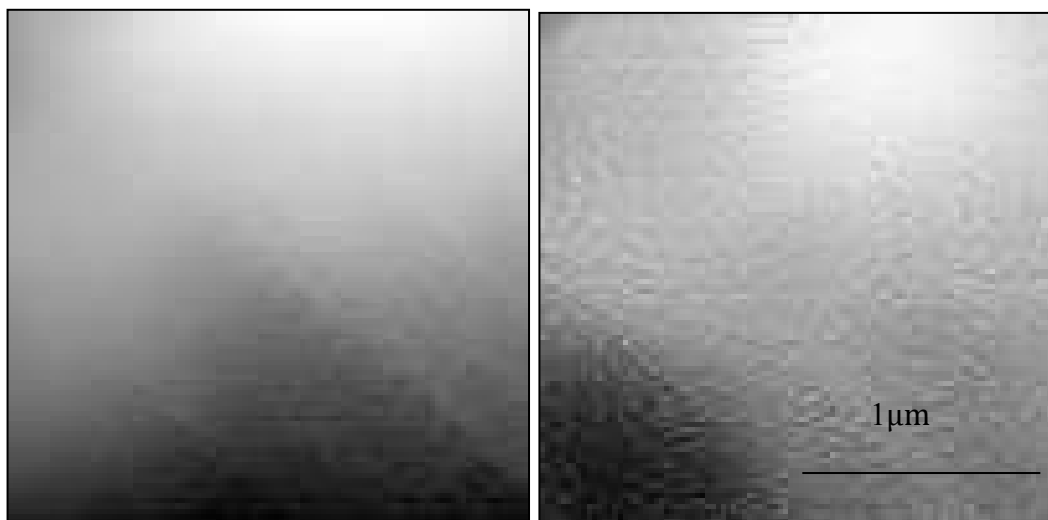


Figure 3-16: *The modified AFM images after the Newton method and the Levenberg-Marquardt method applied to the initial AFM image (from left to right).*

By comparing the two simulated SEM images based on the modified AFM image shown in fig. 3-16 with the initial SEM image, we found that the SEM image from the Levenberg-Marquardt method was a better match to the originals, which are shown in fig. 3-17. They have the same shape, and surface texture also looks similar.

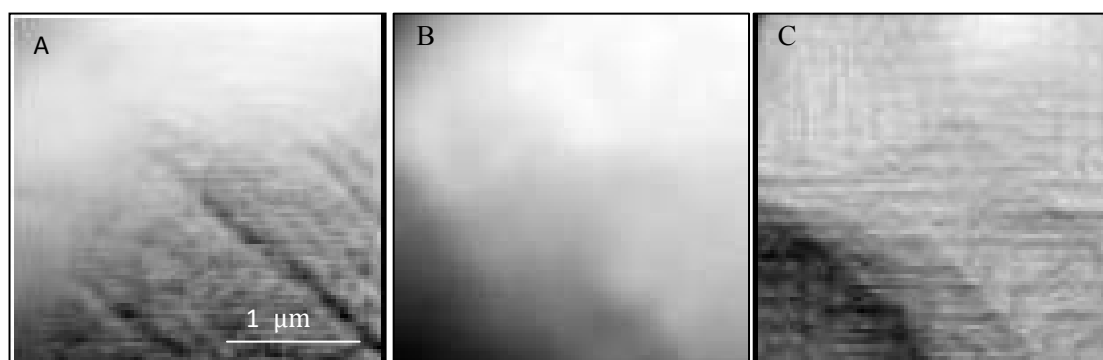


Figure 3-17: *The corresponding simulated SEM images based on the two modified AFM images shown in figure 3-16 (the Newton method based is (A), and the Levenberg-Marquardt method based is (B)); the real SEM image (C).*

The time and the memory required for obtaining the modified AFM images via different methods are listed in Table 3.

Method Used	Time Required (s/iteration)	Memory Required
Newton Method	938	1GB
Levenberg-Marquardt Method	9000	1GB

Table 3: *the differences between the two nonlinear least square algorithms*

Base on the data in Table 1 and the images we examined, we found that although the Levenberg-Marquardt method was the slowest method for AFM modification, the memory required for both methods was nearly the same, and the result of Levenberg-Marquardt was the best; therefore, the Levenberg-Marquardt method was the most suitable method for image processing.

The method is applied to 100×100 pixel images, and the result is depicted in fig 3-18.

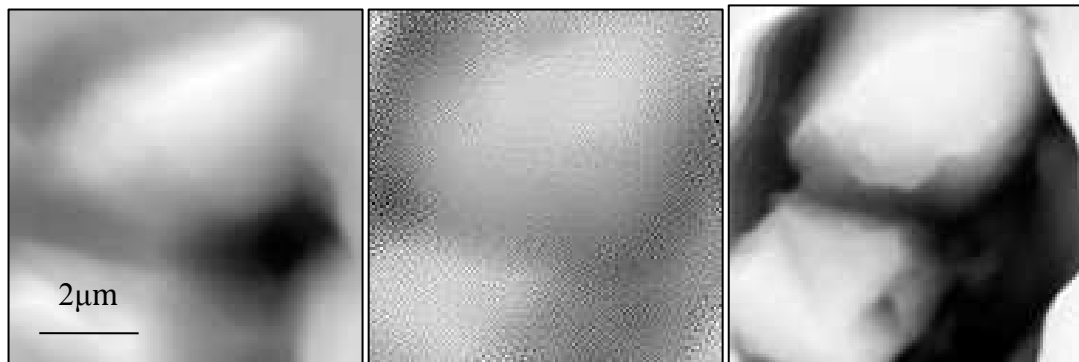


Figure 3-18: *AFM image, the corresponding modified AFM image, and SEM image.*

A comparison of the three images reveals that high noise is seen in the modified AFM image. The noise results from the over-fitting effect. This is because the AFM points chosen cannot be identical to the ideal points representing the real SEM intensity values on the corresponding points, so some ‘new’ AFM points must be very high or low to make the simulated SEM result resemble the real SEM image. To reduce the noise, median filtering was added to this algorithm.

Median filtering is a nonlinear operation often used for reducing ‘salt and pepper’ noise [147]. Median filtering contains a 2D matrix $[m, n]$. Each output pixel contains the median value in the $m \times n$ neighbourhood around the corresponding pixel in the input image, which is suitable for reducing the noise simultaneously.

The result of the filtering is depicted in fig 3-19.

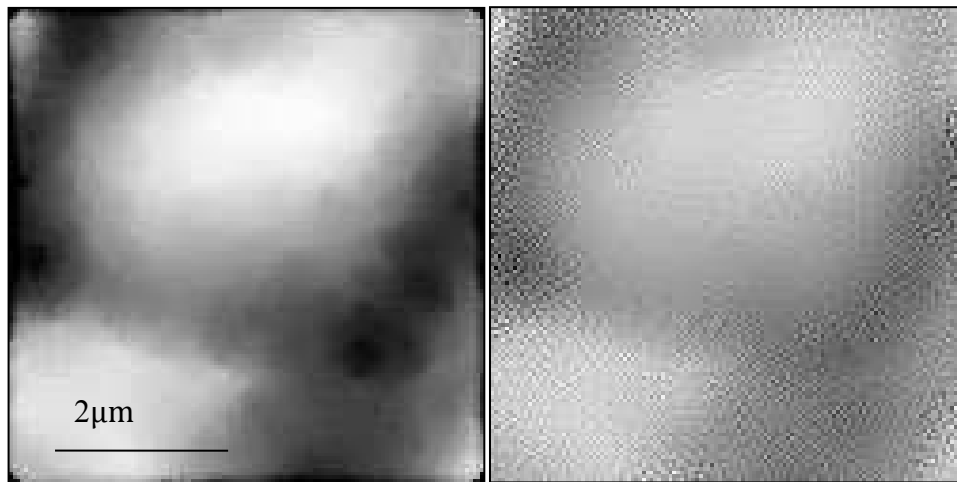


Figure 3-19: *The created AFM image after the filter was applied and the created AFM image before the filter was applied.*

From the image, we can see that although the median filter can reduce the noise, it will also reduce the resolution of the image.

3.3 Conclusion

We have demonstrated that SEM images can be used as a reference to modify AFM images to provide a more complete understanding of the sample elevation map. We proved that this modification can combine the ability of SEMs to image through the samples with little distortion and the 3D characteristics of AFM images.

There are two basic methods for this modification. The first is to use SEM stereoscopy. After taking several images from the same sample with different detecting angles, a 3D

SEM image was created. The corresponding AFM image could be adjusted by applying the ICP algorithm to minimise the difference between the two images. With the aid of Matlab, we obtained the ICP-based modified AFM results.

By considering the reverse process, the SFS method is used, in which the AFM image could also be transformed into a simulated SEM image; then, by minimising the difference between the simulated and real SEM images, we could modify the AFM image. This process contained several steps. First, we applied the simulated SEM image algorithm to the AFM image. Then the Levenberg-Marquardt algorithm was used to modify the AFM image, resulting in a high degree of similarity between the simulated and real SEM images. This method needs improvement in the speed limitation. To combine a 100×100 pixel image, the method discussed above needed approximately 36 hours, which is too long to be acceptable.

According to our discussion, there are three general disadvantages of this algorithm. The first is that the simulation function is too complicated, which will influence the reconstruction speed and increase the calculation time. The second is that the simulation function, which contains gradient magnitude, maximum principal curvatures, and minimum principal curvatures, is based on experimentation rather than theory and therefore is not supported by a solid theoretical framework. In addition, the reconstruction presented above is a variant of the SFS minimisation approach, which includes the brightness constraint and additional height information that can be enhanced if the smoothness constraint is also used. These are the three points that will be improved in the next stage discussed in the following chapters.

Chapter 4: A new approach for combining SEM and height data with minimal information leakage

This chapter presents a new approach that seeks to combine the advantages of the previous methods and avoid the weaknesses. The method maintains the maximum information content from the individual images, three SEM images and one additional height image, in a final product that can be readily computed.

To do this we have separated the problem into two parts. The first is a forward calculation that uses an improved BSE photometric stereo method to provide lower resolution information on the images while avoiding shadowing effects and reconstructs an initial elevation map. The method is then followed by a SFS algorithm that uses only the highest resolution data (SE image) to drive towards a final reconstruction.

More specifically, with help of the secondary electron image, the surface normal images can be obtained from the two BSE images from a detector pair in a suitable opposed configuration to avoid the shadowing effect. Then the surface-normal image is integrated line by line along the detector-pair axis to reconstruct the surface $Z(x,y)$, using profilometer data from the sample for calibration

The second part of the algorithm refines the estimates of the sample surface made in the first part. This is achieved through iterative matching of real and simulated secondary electron images. The SE image which gives information on the slope of the surface is used as a reference to modify the surface produced by the first part of the algorithm. The iteration is taken to convergence to reduce the influence of noise and restore details

The whole algorithm will involve four different images, profilometer image $z_h(x, y)$, BSE image A $I_{BSE1}(x, y)$, BSE image B $I_{BSE2}(x, y)$ and SE image $I_{SE}(x, y)$, to reconstruct a height estimate based on all the most reliable information in each of the images

4.1 General description of the algorithm

As we have discussed in Chapter 1, height measurement instruments such as the AFM and OP, are common techniques to study the structure of specimens at the micro scale. The SEM images are complementary to the height information because it is very good at detecting sharp changes, while both the AFM and OP are not. Table 4 shows the characteristics of the image taken by the microscopes.

	output	advantage	disadvantage
SEM with E-T detector	SEM image forming by both secondary electrons and backscattered electrons	high resolution	unquantifiable
SEM with E-T detector and collimator	secondary electron image	high resolution; quantifiable	cannot be used for reconstruction alone
SEM with quadrant backscattered detector (QBSD)	backscattered electron image	quantifiable; can be used for reconstruction alone	shadowing effect; relatively low resolution
Optical Profiler	height image	relatively large detecting range	low resolution; difficult to measure high slope parts on the surface
AFM	height image	high resolution	small detecting range; untrusted measurement for high slope parts; tip convolution

Table 4: comparison between the different microscope images

The established approach to reconstruct a height image from SEM images is usually based on the SFS, photometric stereo or stereoscopy. The method presented in this

chapter introduces a novel detector filtering geometry which ensures the image is formed only by the secondary electrons. Hence, the sample slope alone should determine the image contrast at the finest scale. As a result the simulated calculation is greatly simplified as there quantified starting point for subsequent simulation. More specifically we use the 3D reconstruction obtained by the improved BSE reconstruction method (BSE photometric stereo) as the initial input for the SFS method. The SE image which can be described by the slope of the surface is used as a reference to incrementally modify the input height image, iteration by iteration, to reduce the influence of noise and restore details, because the SE image has the better resolution. The whole algorithm will involve four different images to reconstruct a new height image and only the trustworthy parts of the images are used. The definition of trustworthiness in our work and how the relevant image parts are selected will be described further below in the following subchapters.

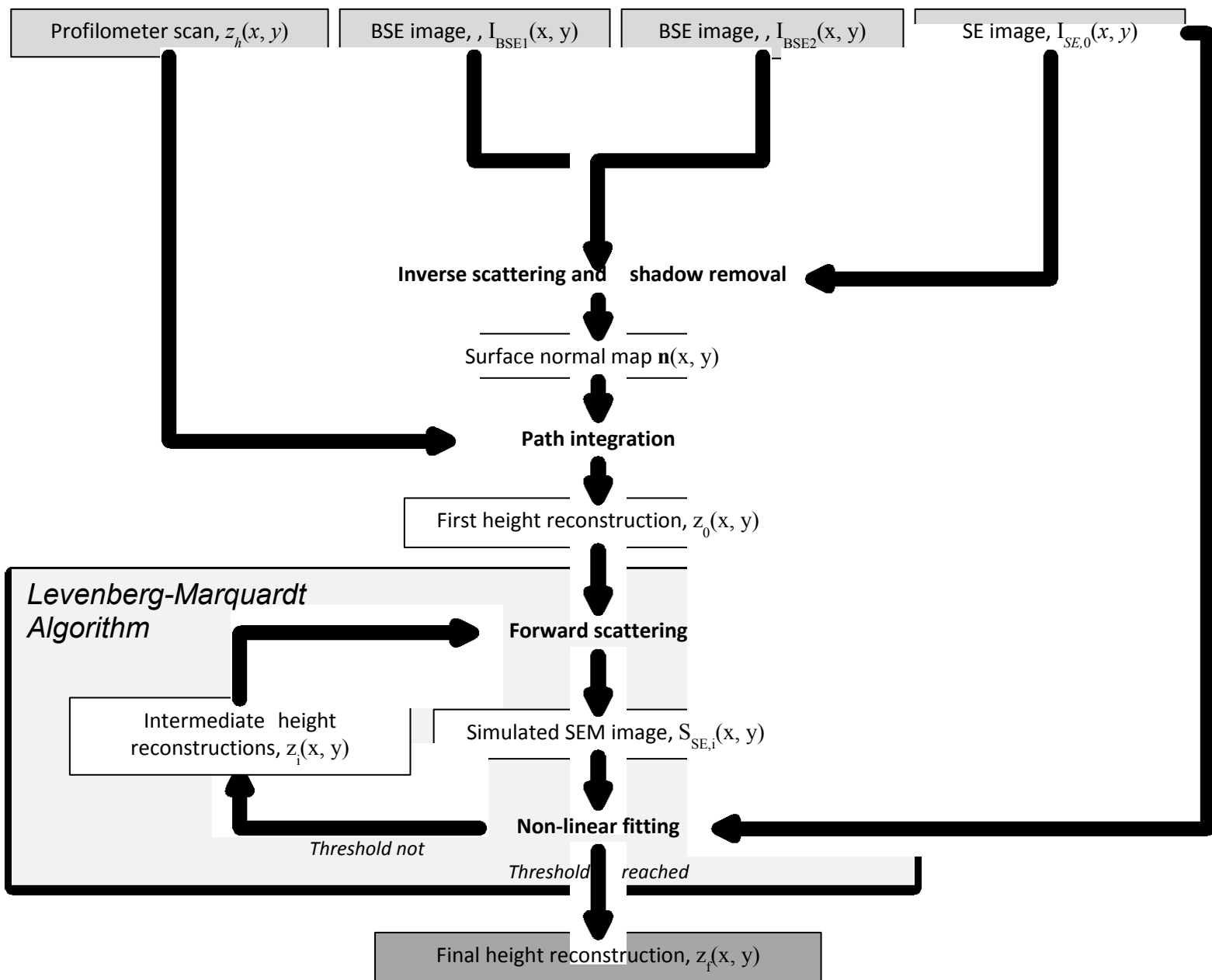


Figure 4-1: the schematic of our reconstruction algorithm

To further clarify the approach, an algorithm is shown schematically in fig. 4-1, and can be separated into two main parts. In the first part, a height image is obtained by combining three SEM images, two backscattered electron images and one secondary electron image.

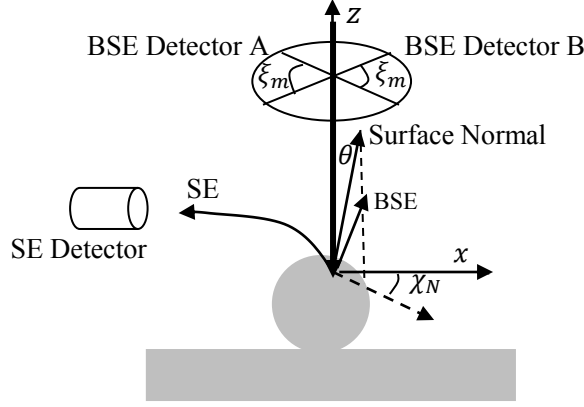


Figure 4-2: *The geometry used for imaging in the electron microscope.*

From fig.4-2 and equation (1-2) introduced and discussed earlier in Chapter 1, if the material contrast is neglected (the sample surface is coated by a gold layer), the signal of the SE detector, S_{SE} , is geometrically dependent on just the tilt of the surface normal θ (if the sample is coated with a gold layer):

$$S_{SE}(\theta) = S_0 \sec \theta + S_1 \quad (4-1)$$

where the S_0 and S_1 are constants depending on measurements conditions.

The signal of the BSE detectors, S_A and S_B depends on both the tilt and the azimuth χ_N of the surface normal with respect to the detector pair orientation, such that

$$S_{A,B} = S_2(\cos \theta \pm \sin \theta \cos \chi_N) + S_3 \quad (4-2)$$

where the S_2 and S_3 are the constants depending on measurement conditions. $\frac{dz}{dx} = \tan \theta \cos \chi_N$ is the slope of the sample in the detector-pair axis direction.

Although only the two BSE images obtained by the BSE detector pair would appear to be necessary to solve for slope of the sample in the detector direction ($\frac{S_A - S_B}{S_A + S_B} =$

$\frac{S_A - S_B}{S_A + S_B} = \tan \theta \cos \chi_N$), the secondary electron image allows the slope to be determined.

By substituting into the equation $S_{A,B} = \frac{\eta}{2}(\cos \theta \pm \sin \theta \cos \chi_N)$ the slope azimuth $\chi_N(x, y)$ can be obtained from the BSE detector A image and BSE detector B image

respectively. By combining the two $\cos\chi_N$ images to suppress the shadowing effect, it is possible to reconstruct the surface $Z(x,y)$, through integration line by line along the detector-pair axis and minimise the shadowing effect. The method of combining the two $\cos\chi_N$ images will be discussed in Subchapter 4.7

In the second part of the algorithm, the estimates of the sample surface made in the first part are refined. This is achieved through iteratively matching the acquired with the simulated secondary electron images. From equation (4-1), we can see that simulation of an SE image requires the slope of the surface. The slope can be extracted from the height data using a 5×5 pixel facet model (see Appendix A) [148] [149] which provides a robust point-by-point slope estimate, so that the slope image based on the height image can be obtained to simulate the SE image.

The iteration uses a Levenberg-Marquardt approach to minimise the least squares difference between the simulated and acquired SEM by adjusting the height values.

To suppress the noise artefacts such as over-fitting that are commonly injected into an LM iteration and eventually achieve the smoothness constraint, we use the standard approach of introducing a median filter. In our case, usage of a 5×5 pixels window is used to match the facet model, and has the advantage of not being computationally intensive. The iteration continues until the reduction in the residual falls below a predefined threshold level. For the 100×100 pixel image the residual threshold is normally set as 10000 meaning that the average error for each pixel between the simulated and acquired images is less than 1.

Seeger and Haussecker [150] present a method that combines the SEM and AFM image using the SFS method, which is similar to the second part of our method but differs in that they use an AFM as the initial input. In addition, they also use an E-T detector to collect electrons scattered from specimens which contains both backscattered electrons and emitted secondary electrons in unknown proportions. Hence, they are able to prevent the

simple extraction of topographic information, because a theoretical expression of the SEM intensity without knowledge about the proportion between SE and BSE cannot be easily obtained. For the SEM simulation algorithm, Seeger and Haussecker take into account both the slope and curvature of the surface to simulate the intensity of the SEM image. However, the coefficients of curvature and the slope used for the simulation are experimentally based rather than theoretically based. There is no sound theory to support their approach. In our method, we have introduced a novel detector filtering geometry which ensures the image is formed only by the secondary electrons. Hence, the sample slope alone should determine the image contrast at the finest scale, so curvature is not used. As a result, the simulated calculation is greatly simplified and there is a widely validated theoretical guidance for the simulation.

4.2 Description of the sample from validation

An ideal test sample shown such as fig. 4-3 should have a well-defined surface profile over a variety of scales. We used silicon micromachining to produce the sample, namely through-wafer deep reactive ion etching (DRIE) [151]. This sample represents an extrusion of a 1-D profile of protruding and re-entrant semicircles of pre-arranged diameters from $x \text{ } \mu\text{m}$ to $y \text{ } \mu\text{m}$. The sample can provide a stable and regular shape which is beneficial in verifying the qualification of the reconstruction.

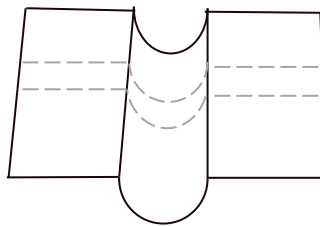


Figure 4-3: *the schematic of the sample which is obtained by the DRIE*

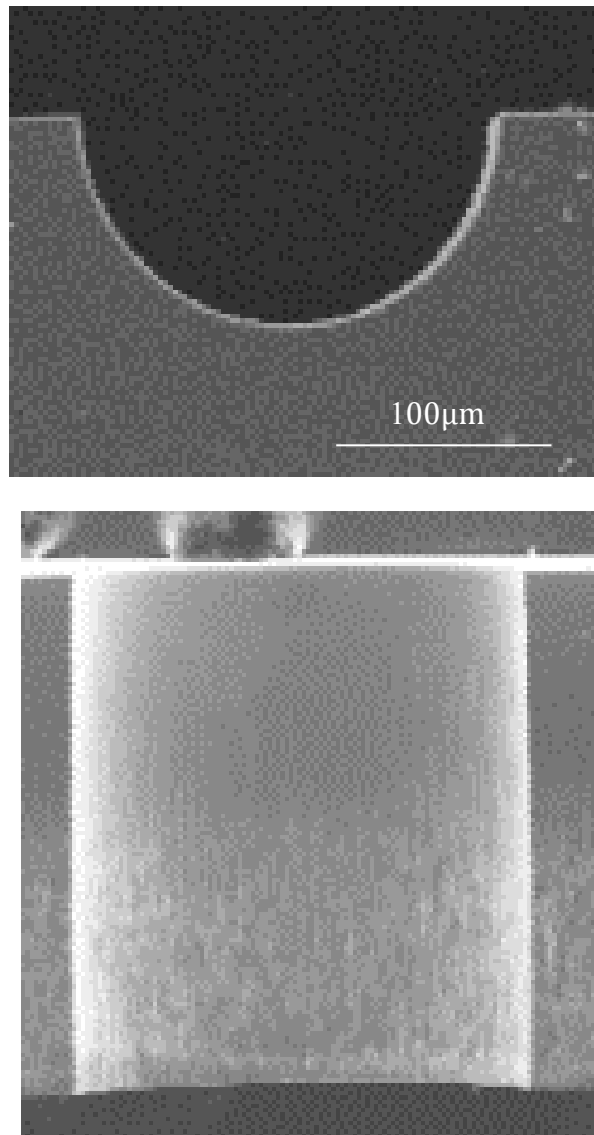


Figure 4-4: *the side view and top view of the sample*

4.3 Acquisition of the images

4.3.1 SE imaging

The SEM used is the LEO 1455 VP which contains a side-mounted Everhart-Thornley (E-T) detector and a 4-quadrant solid-state backscattered detector.

The images collected by the E-T detector are formed by a mixture of both BSE and SE in unknown proportions, which is not only dependent on the topography of the sample surface, but also on the geometry between the sample and the detector, and the parameters of the detector such as the voltage, the size of receiver and so on. This mixing prevents any quantification using the relationships we have previously outlined, and so the first step of the approach is to remove the BSE component from the E-T detected signal. A relatively simple approach was used by placing a conductive collimator above the sample surface, allowing only small scattering angles to be detected, which in our case was up to approximately 30 degrees (see fig. 4-5 for the schematic). The E-T detector is placed outside of the line of sight to the sample through the collimator, ensuring that while low energy secondaries are detected, there is no achievable trajectory for the back-scattered electrons from the sample to the detector. This approach is geometrically equivalent to the in-lens detector configuration available in some SEMs [152].

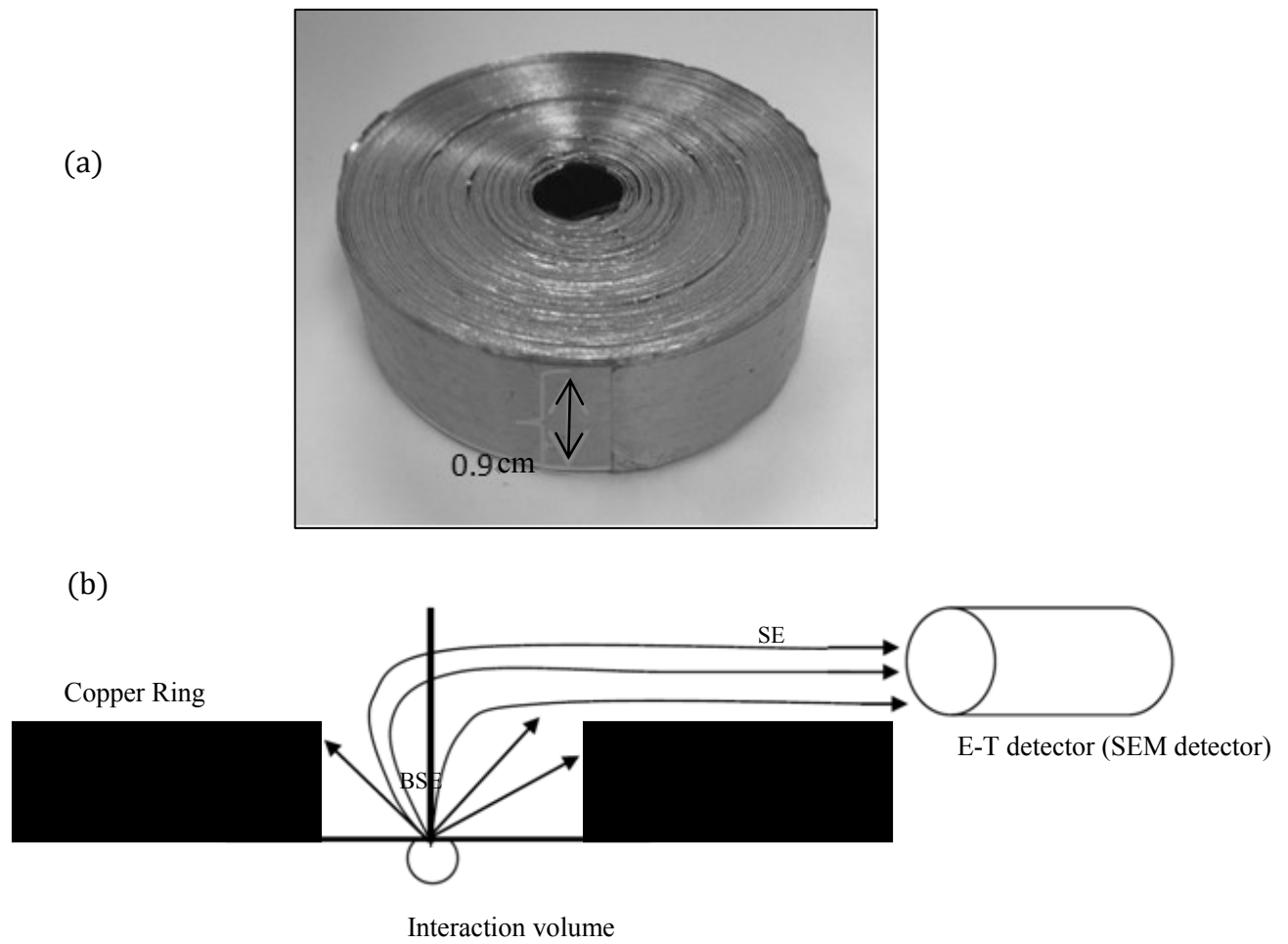


Figure 4-5: (a) the dimension of the “ring wall”, which can eliminate the effect of the BSE. (b) The schematic of the geometry of the SEM set-up

For a clear comparison, the sample image is taken with and without the metal ring respectively and shown in figure 4-6:

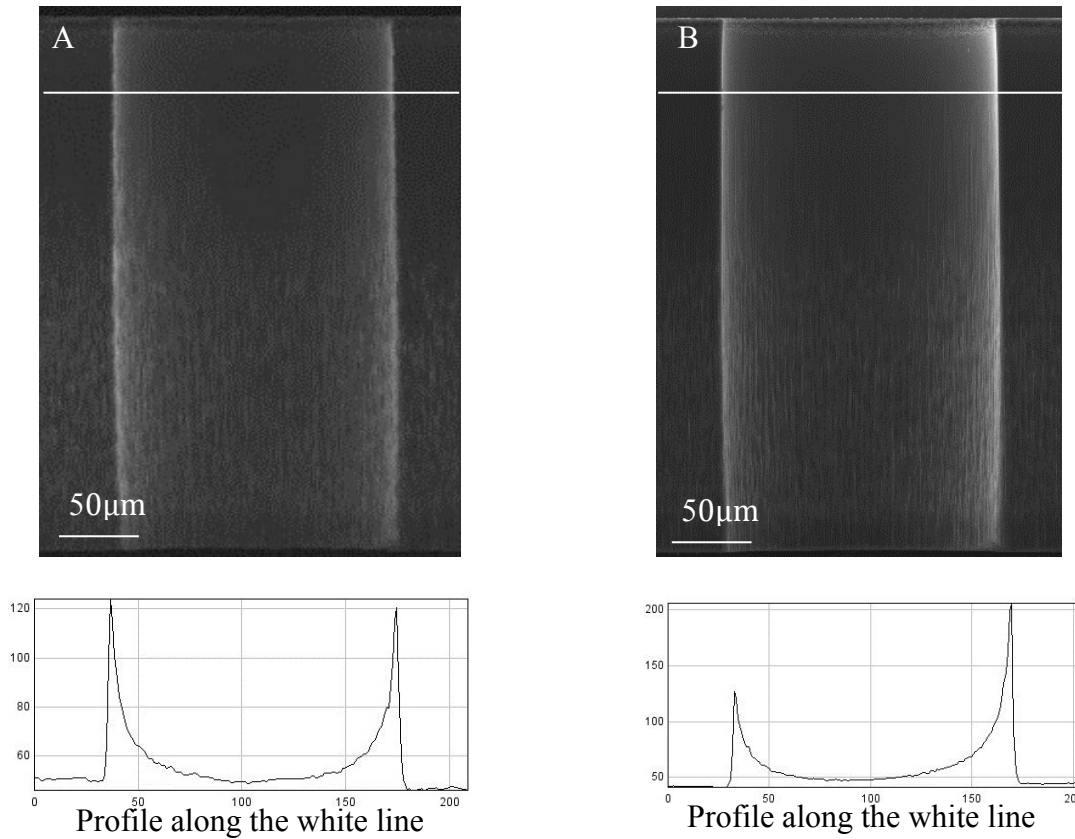


Figure 4-6: *Left: The image obtained with the help of the protection metal ring. Right: The image obtained without the help of the protection metal ring*

From the comparison of the results above, it is easy to find the difference. In image B, it is easy to observe the brightness difference for the parts which have the same tilt angle, but in image A the brightness of those parts is almost that same. The metal ring is thus worthwhile to be placed around the sample to block the BSE signal.

To confirm the SE selectivity of the collimator, we took a series of images from our calibration standard rotated from the nominal scan direction. This varies the azimuth of the slope, χ_N , in fig. 4-2 and hence any BSE component will cause a divergence of the E-T signal from linearity with $\sec\theta$.

Fig. 4-7(a) shows the sample aligned to the nominal scan direction with fig. 4-7(b) the corresponding column average plot of the highlighted region. fig. 4-7(c) shows for three rotation directions ($0^\circ, 7^\circ, 45^\circ$) the variation of image intensity against $\sec\theta$ for three sample rotations, with the column average calculated equivalently. All three are highly linear, confirming that with the collimator we are able to isolate the SE component.

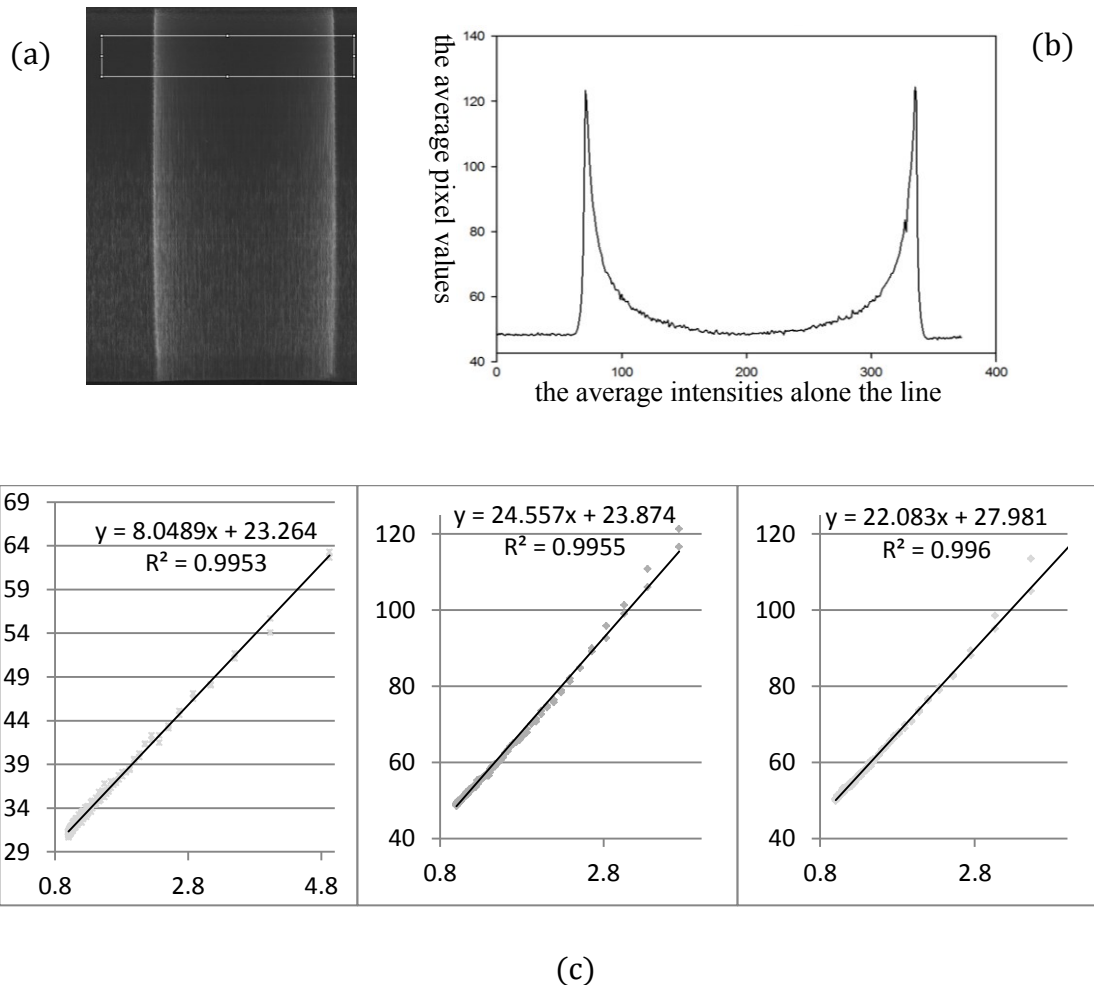


Figure 4-7: (a) the image taken with help of copper ring wall. (b) the average intensities along the line. (c) plot the acquired SE intensities (y axis) against the simulated SE intensities (x axis).

4.3.2 BSE imaging

To confirm quantification of the BSE image, the same sample was imaged using a quadrant BSE detector and the intensity compared to the predictions of equation (4-2).

Fig. 4-8 shows that this sample geometry exhibits shadowing, with BSE from part of the sample unable to be detected. Fig. 4-8(a) quantifies this with a plot of the simulated intensities from equation 4-2 plotted against the column-averaged data from the indicated region of the sample. There is good linearity between the simulated and acquired data outside of the shadow region in fig. 4-8(b). In the shadowed region, no surface determination is possible with the BSE image.

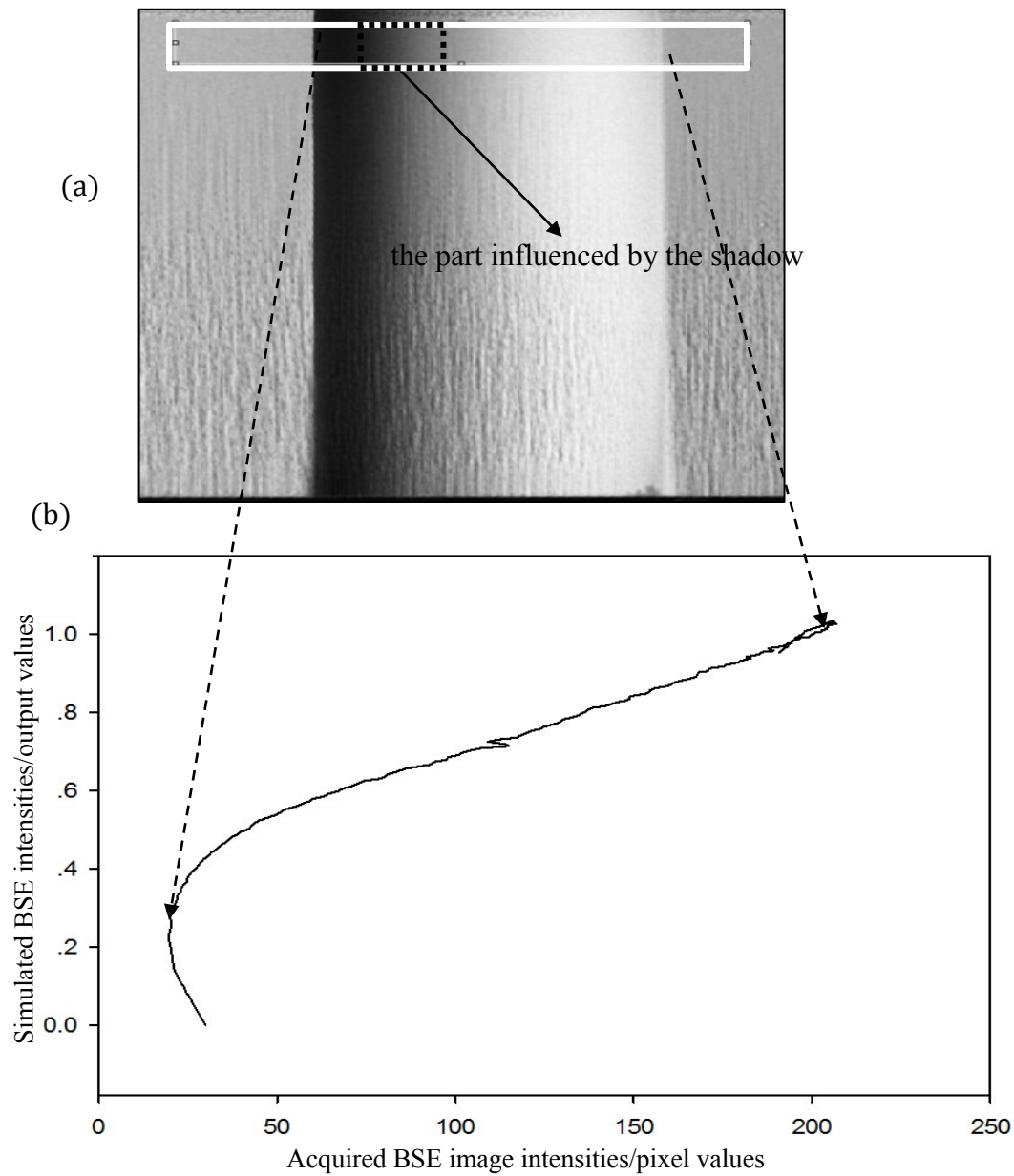


Figure 4-8: *a: the QBSD image b: plot the related average intensity profile along the rectangle against the simulated BSE intensity*

4.3.3 Height acquisition

The height image is taken by using the Veeco NT9100S Optical Profiler (OP) which is a 3D surface measurement interferometer. The reason why we use an interferometer rather

than an AFM is that the interferometer can provide a much larger X - Y - Z scanning region and a quicker measurement. Although the AFM can provide a high a resolution image, the maximum scanning X - Y region is around $75\text{ }\mu\text{m} \times 75\text{ }\mu\text{m}$ which is not suitable for our sample, which is around $200\text{ }\mu\text{m} \times 200\text{ }\mu\text{m}$. In this thesis, all the 3D images are taken by the Wyko NT9300, and using this the sample roughness can then be measured along any line in the x or y axis of the resultant image. The results are limited by the vertical resolution of the Wyko, which is $<0.1\text{ nm}$, and the optical (lateral) resolution of $0.55\text{ }\mu\text{m}$. [153] [154]

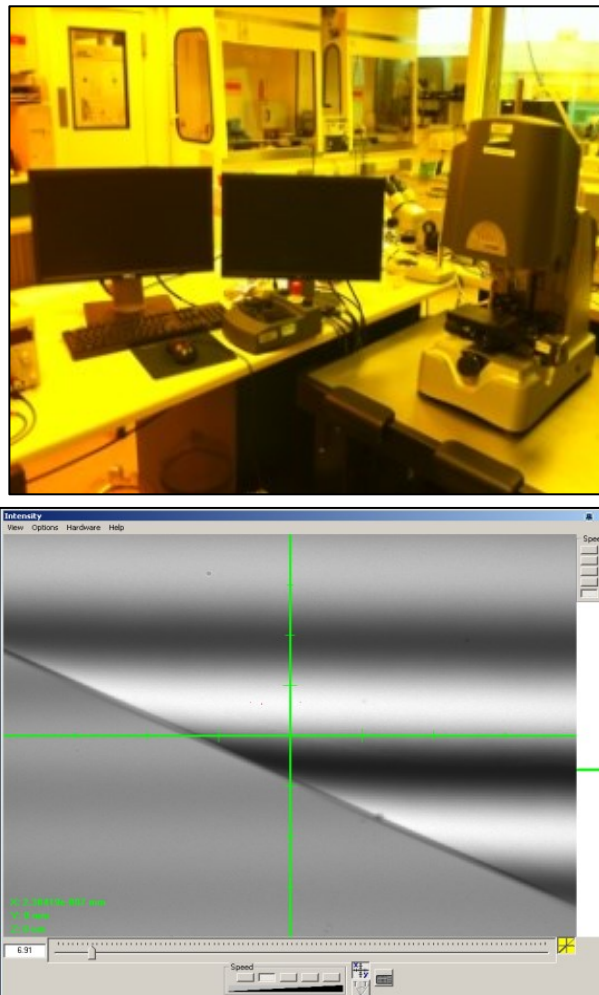


Figure 4-9:A: *The Wyko NT9300*(up) B: *The interference pattern obtained from the Wyko NT9300*(down)

This technique has a limited ability to determine the height of highly sloped regions, as is evident in the artifacts of fig. 4-10 at the borders of the cylindrical section. For low-angle portions of the surface, the interferometer produces a slope calibration standard that can be used to quantify the SEM images.

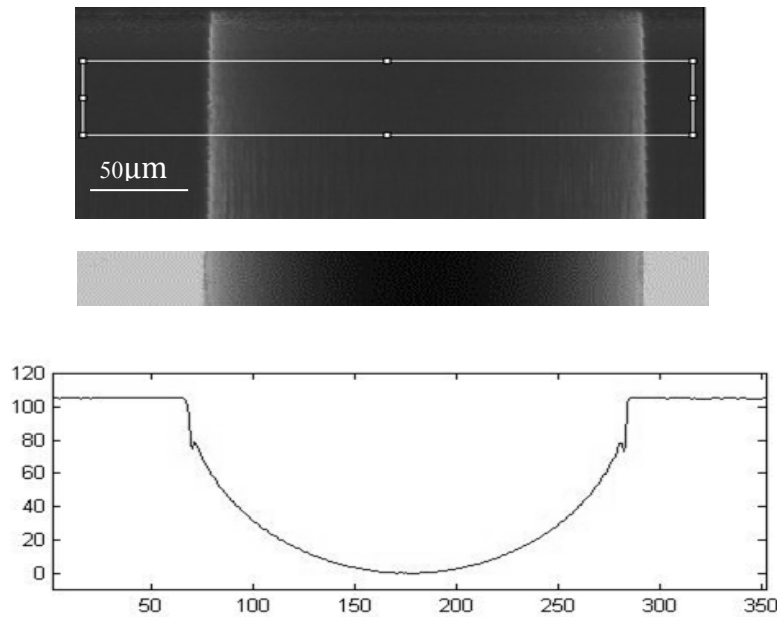


Figure 4-10: *The Veeco optical profiler image and the related average intensity profile along the white rectangle*

4.4 Calibration of the SEM image

The first step in the data fusion is to use the preselected height data to determine the constants needed for simulation of the SE and BSE images, which can be referred to the calibration of the SEM image. As the algorithm uses the difference between the intensity values of the actual and simulated images to produce the most accurate fusion of the data, it is important that the simulated images are accurately calibrated so as to be directly comparable.

To perform this calibration, areas of the profilometer image with low slopes (normally the parts with less than 45 degree slope can avoid profile artifacts in the optical profiler images as aforementioned) are first selected. These areas are then used to produce uncalibrated simulations which are compared to the acquired SEM images of the same areas to obtain S_0 to S_3 in equations (4-1) and (4-2) which are the slope coefficients and constants of the equation, in effect setting the end points of the subsequent stages of the algorithm. From fig.4-11 to fig.4-13 it shows the calibrations of the SE and BSE images.

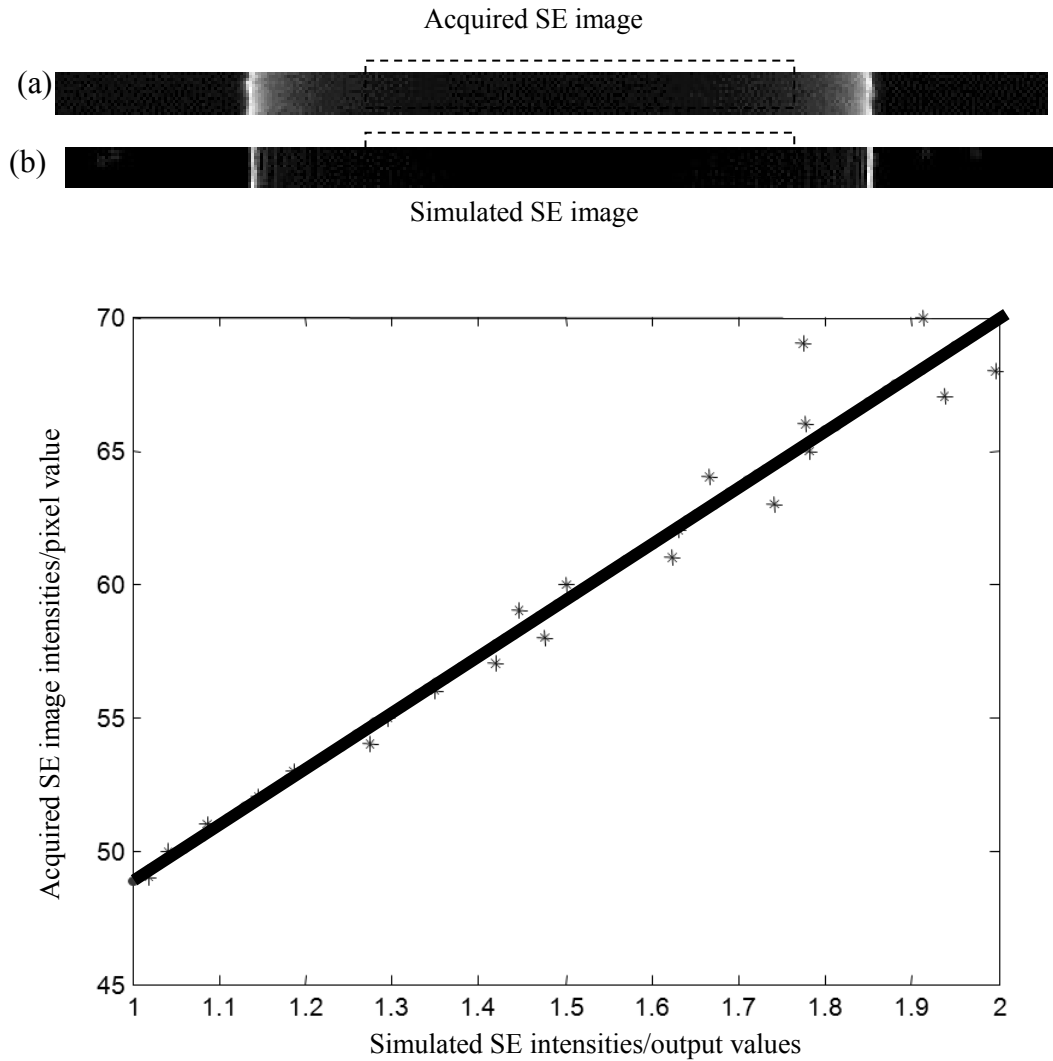


Figure 4-11: (a) a portion of the acquired SE image of the calibration standard (b) a corresponding simulated SE image (c) a plot of the pixel values of these images used to calibrate the simulated output. The regions used for the comparison, with low slope are indicated in (a) and (b) (inside the dashed box)

If the values of the azimuth for the BSE image obtained by detector A are positive, the corresponding points are then considered to be trustworthy. This, in effect, means the parts are not influenced by shadowing. Additionally, the azimuth values for the BSE image obtained by detector B should be confirmed as negative.

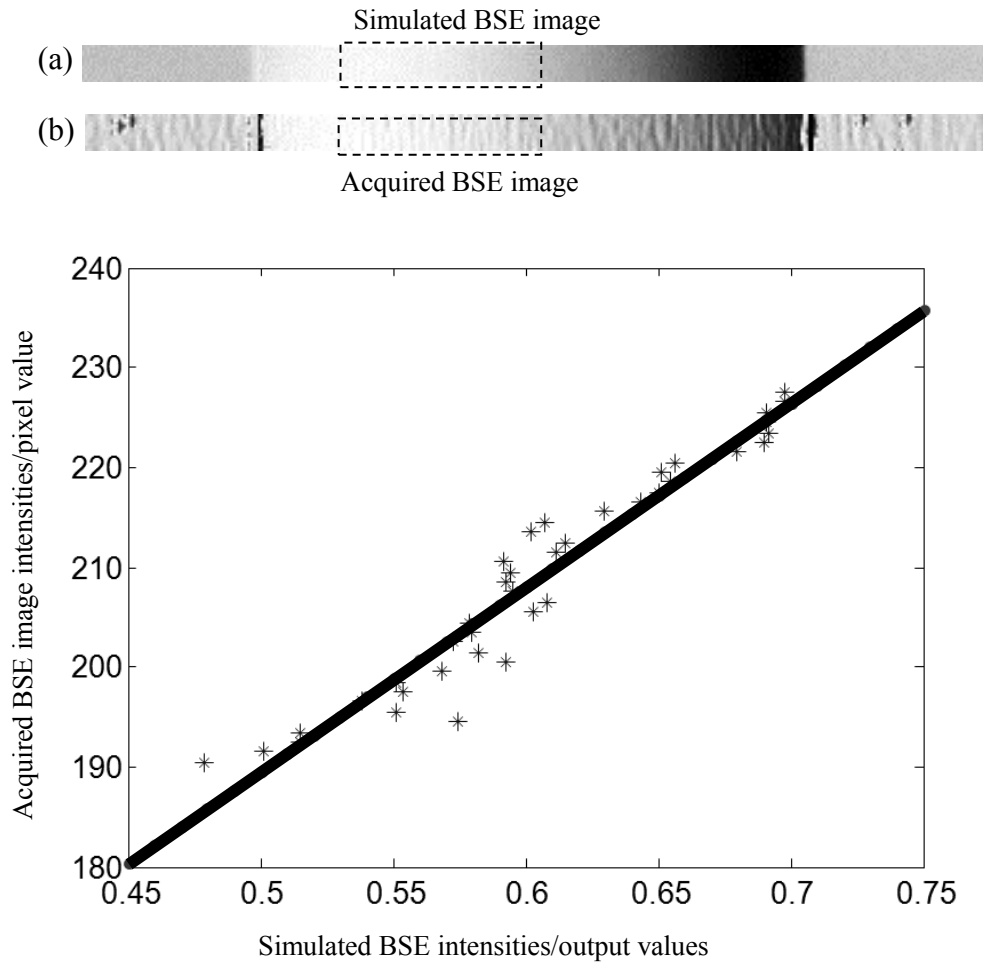


Figure 4-12: (a) a portion of the acquired detector A BSE image of the calibration standard (b) a corresponding simulated detector A SE image (c) a plot of the pixel values of these images used to calibrate the simulated output. The regions used for the comparison, with low slope and of which the angle between the normal of the surface at that point and the direction of the detector is less than 90 degree are indicated in (a) and (b) (inside the dashed box)

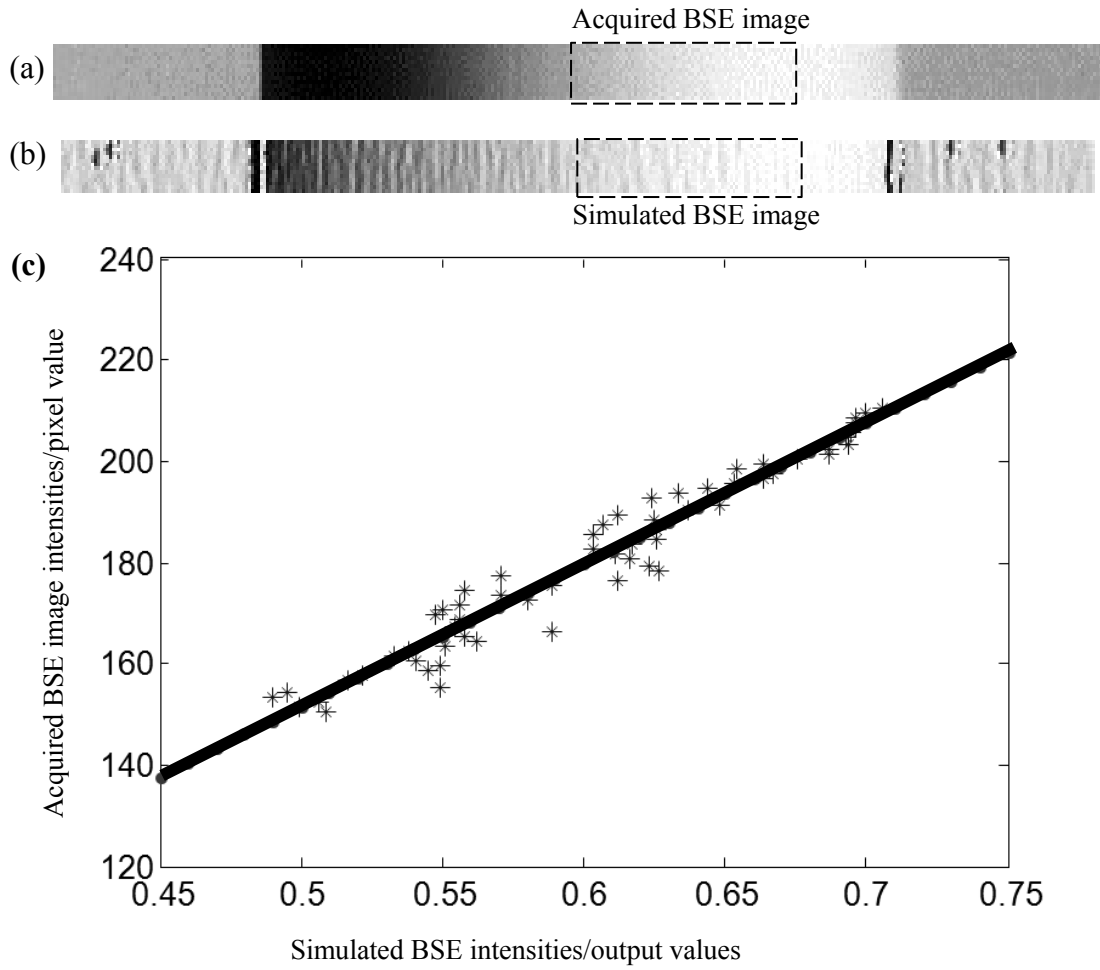


Figure 4-13: (a) a portion of the acquired detector B BSE image of the calibration standard (b) a corresponding simulated detector B BSE image (c) a plot of the pixel values of these images used to calibrate the simulated output. The regions used for the comparison, with low slope and of which the angle between the normal of the surface at that point and the direction of the detector is less than 90 degree are indicated in (a) and (b) (inside the dashed box)

4.5 Initial data fusion of the SE and BSE images

Once the constants S_0 to S_3 are obtained, the slope of the surface, $\theta(x,y)$, can be calculated from the acquired SE image via equation (4-1). The azimuth of the slope,

$\chi_N(x, y)$, can be obtained from the QBS detectors using equation (4-2). However, any shadowing will invalidate the relationship required to determine the slope azimuth. To avoid this limitation the algorithm uses images from the opposed pair of QBS detectors to eliminate any shadowing effects: if the image of one detector is shadowed, the other detector will be unaffected. Fig. 4-14 shows the approach applied to the calibration sample. The derived azimuth from the calibrated signal from both detectors is shown.

In the shadowed regions the derived azimuth is outside of the mathematical range for the detector without a line of sight to the surface. For the $\cos(\chi_N)$ image derived from the BSE image taken by the Detector B, if the value of $\cos(\chi_N)$ is negative which means the angle between the line of sight of detector B and the surface normal is smaller than that of detector A, then the value of the $\cos(\chi_N)$ will be adopted as the final $\cos(\chi_N)$ value. Similarly, for the Detector A the positive $\cos(\chi_N)$ value will be adopted for the final one. Hence, the final azimuth value is selected from the detector with a smaller angle between the line of sight and the surface normal, $\theta(x, y)$. By this way, azimuth values obtained from both Detector A image and Detector B image are thus able to be fused. There is a central transition region where the local roughness of the surface determines which detector is used, though the lack of shadowing in this region ensures that both detectors give identical azimuth information. In fig. 4-14, the final azimuth information is also shown, selected from the most appropriate detector signal.

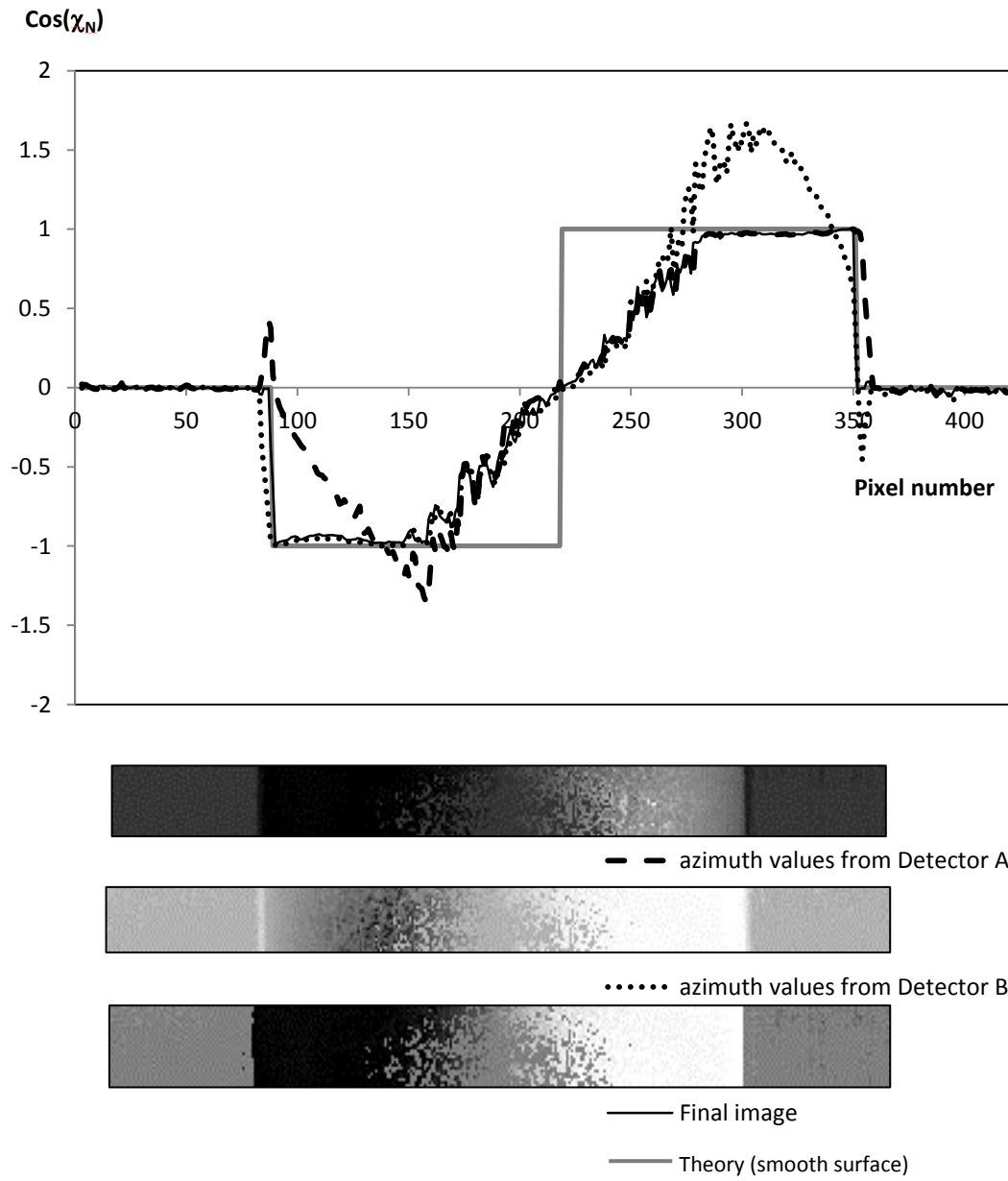


Figure 4-14: *Fusion of the azimuth values obtained from both Detector A image (negative parts) and Detector B image (positive parts).*

Fig. 4-15 shows the values of $\theta(x, y)$ from the SE image and $\chi_N(x, y)$ from the BSE pair of images that are combined to give the component of the slope in the image scan direction x . Finally in fig. 4-16, this slope is integrated along x to determine $Z(x, y)$,

with the starting point provided by the profilometer image. This can be mathematically expressed as below:

$$\cos(\chi N) \times \tan(\theta) = \frac{\partial z}{\partial x} \quad (4-3)$$

so that

$$Z(x, y) = \int \frac{\partial z}{\partial x} dx = \int (\cos(\chi N) \times \tan(\theta)) dx \quad (4-4)$$

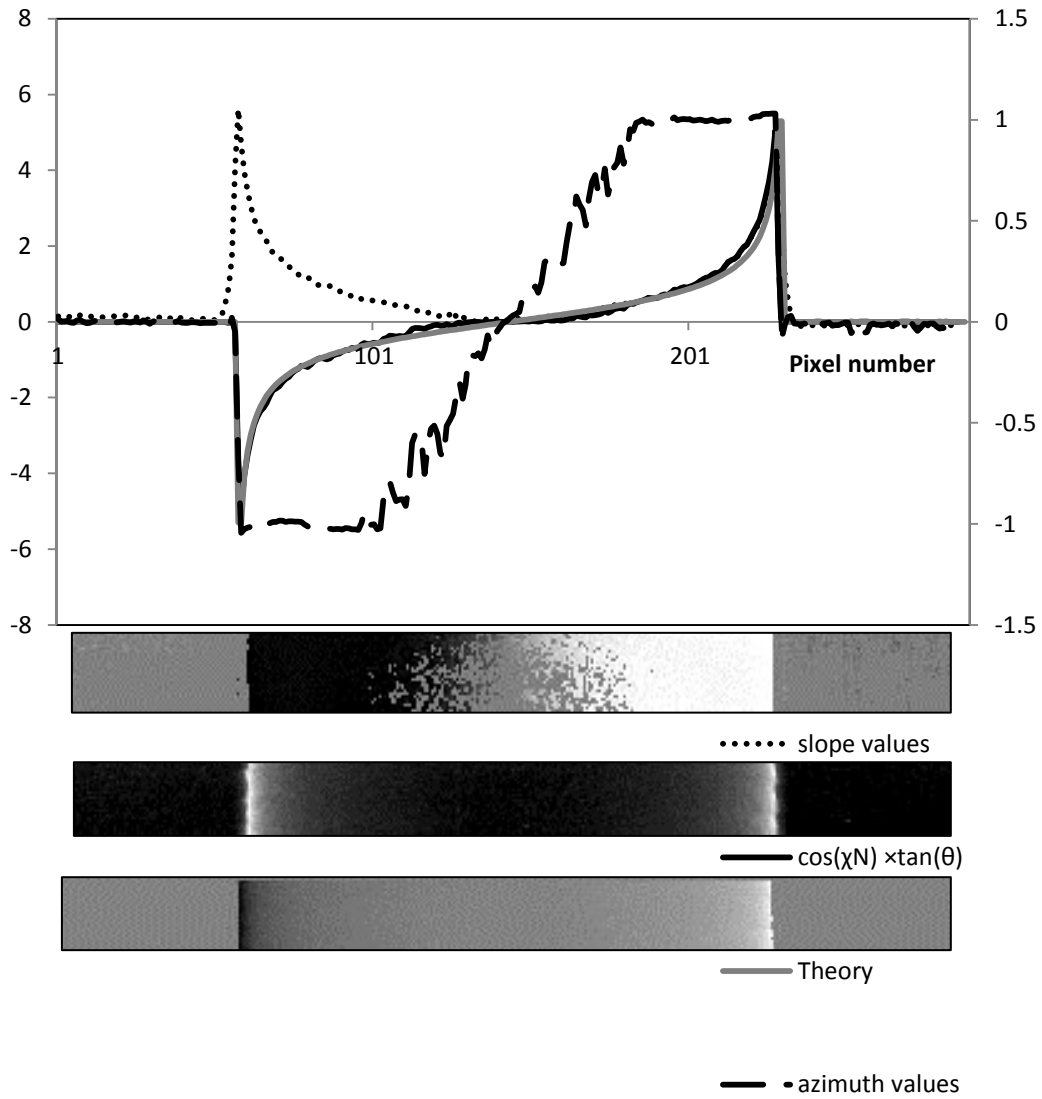


Figure 4-15: Extraction of the $\cos(\chi N) \times \tan(\theta)$ values

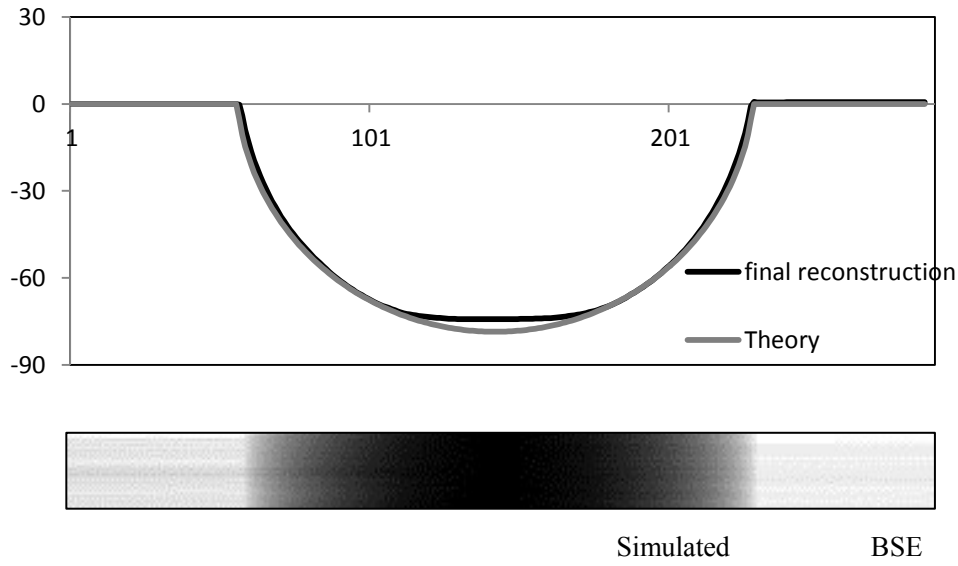


Figure 4-16: *Integrating to produce the height image.*

From the result it can be found that for the high slope part the reconstruction matches the theory shape very well, but for the low slope part there is information distortion. This is caused by the original BSE image. For the low slope part the measurement intensity is relatively low and sensitive to the noise, which cause the distortion of the $\cos(\chi_N)$ and finally influence the reconstruction.

4.6 Refinement through iteration matching of simulated images

The result of the path integration is limited by the resolution of the lowest imaging mode used to produce the resulting height image. The BSE image pair in this case limits the resolution, while the SE imaging is capable of achieving a better resolution. Hence, while path integration is used for larger image scales to provide the overall profile, further refinement is achieved by incorporating information of just the SE images using a SFS approach. This is the most computationally intensive portion of the algorithm, but has as

its initial input the path integration image which is an optimum estimate at reduced resolution.

Unlike in the previous step of path integration, where the height could be directly mapped from the SE and BSE images, using the SE image alone requires handling the non-linear relationships between the SE intensity and height. The SFS algorithm uses a brightness constraint that drives the iteration to minimising the image irradiance difference between the real and the reconstructed images by nonlinear fitting of the height image via the Levenverg-Marquardt method which has been discussed in Chapter 3.2 and Chapter 4.1. The initial height image obtained from the first stage is used as input for the simulated SE algorithm, which is discussed in Appendix A.

In addition, a smoothness constraint is required in order to preserve the accurate information of the lower resolution path integration image, and also prevent over fitting to the highest resolution noise elements. To achieve both of these requirements the smoothness constraint in our case implements a median filter which has been discussed in Chapter 3.2, based on a 5×5 kernel in this work. Hence, compared to the more commonly used application of the SFS algorithm, the initial image in our method is a better estimate of the surface of the object and the algorithm is used to improve the details, allowing a much faster convergence for large images. The procedure of our SFS method is shown in figure 4-17.

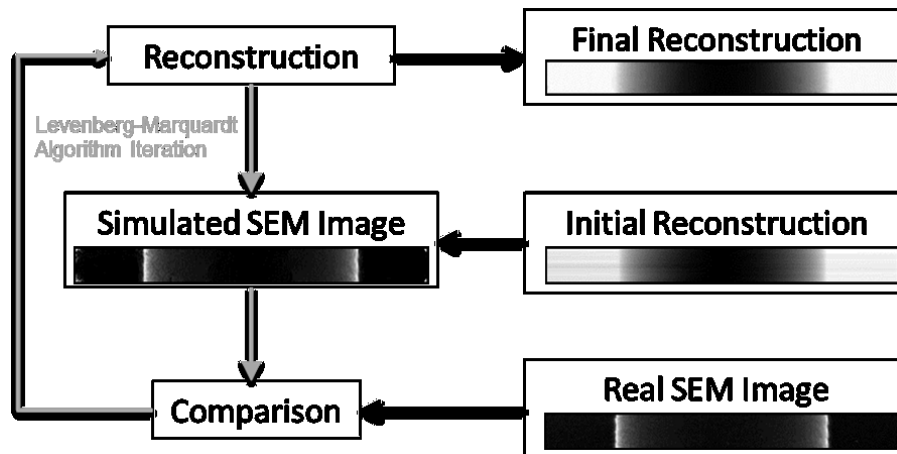


Figure 4-17: The schematic of the “SFS” algorithm

The following results (fig. 4-18) shows the residual (Root-Mean-Square errors between the simulated and acquired images) changes during the iterations.

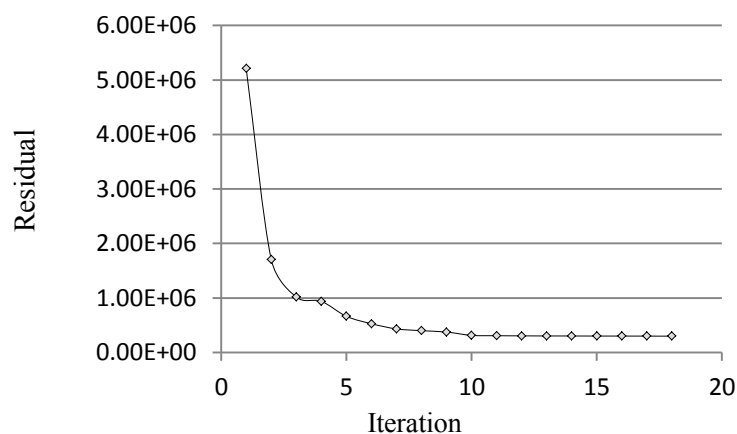


Figure 4-18: convergence of L-M algorithm

From this image we can find that the first 5 iterations change dramatically after 10 which is a suitable iteration time and be used as the threshold, because after 10 iteration times the algorithm cannot provide a substantially better result.

4.7 Comparison to the existing BSE reconstruction method

The classic BSE detector pair method uses the whole information from two BSE images measured by the detector pair:

$$S_A + S_B \propto \cos(\theta) \quad (4-5)$$

$$S_A - S_B \propto \sin(\theta) \times \cos(\chi_N) \quad (4-6)$$

$$(S_A - S_B)/(S_A + S_B) \propto \tan(\theta) \times \cos(\chi_N) \propto -\partial z / \partial x \quad (4-7)$$

Then, integration of $\partial z / \partial x$ along the x axis, to reconstruct the height image is performed. In this method, the whole image is used, including the shadowing part. Application of this method to the same sample as what we used above and the result is shown in fig 4-19.

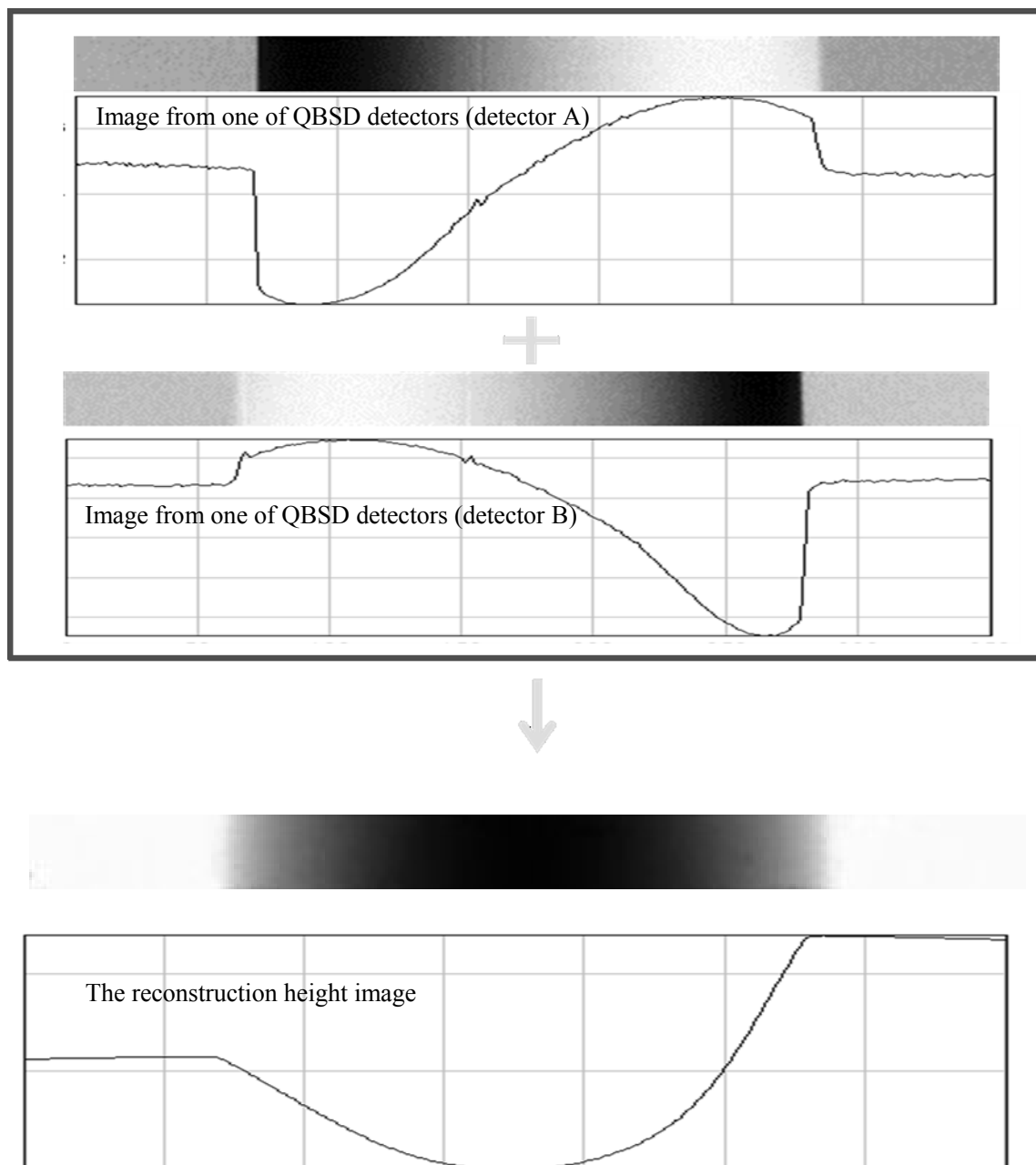


Figure 4-19: *The result obtained by the classic BSE reconstruction algorithm.*

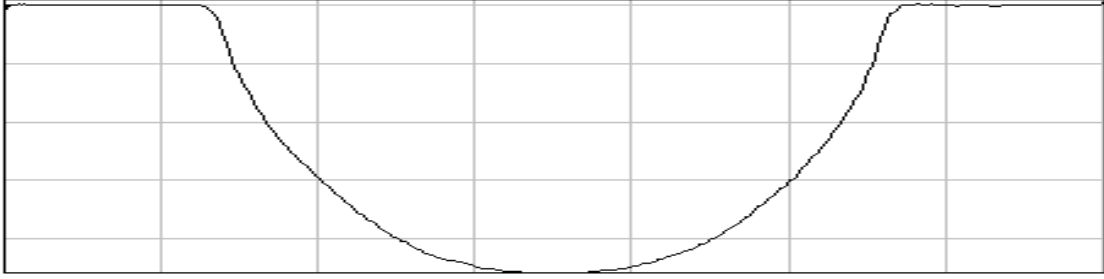


Figure 4-20: *The result obtained by our algorithm.*

For the LEO 1455VP SEM, the images from detectors A and B can be fused directly during the measurements, so that according to (4-5), (4-6) and (4-7), the images $(S_A + S_B)$ and $(S_A - S_B)$ can be outputted directly and by integrating $(S_A - S_B)/(S_A + S_B)$ the reconstruction of the surface is obtained shown in fig. 4-19 (c).

Comparing with the result obtained from our algorithm (fig.4-20), it can be seen from fig. 4-19 that along the cross section, the height of two sides is not the same. This is because both images are used as a whole and the final result will be changed depending on the shadowing influence on the two images, so that it may be deemed not trustworthy.

Comparing the previous method with our algorithm shows that the $\tan(\theta)$ information is provided by the SE image. The two images from QBSD are combined together to provide the trustworthy azimuth, χ_N , information. Because the two detectors are placed against each other, they are complementary by suppressing shadowed points of view, so that the reconstruction result is more trustworthy.

4.8 Conclusion

We have demonstrated an algorithm to construct a sample surface using data fusion of SEM and profilometer data. The algorithm takes account of the strengths and weaknesses of each data set by using a series of successive iterations which retain the most reliable

information from the previous steps while improving the accuracy and resolution. Such an approach also allows the data fusion to be achieved in short time scales.

The algorithm uses four different images to reconstruct a new height image by two steps: the “Path Integration method” stage to obtain the initial height image and the “SFS method” stage to modify the height image. Comparing to the pervious method, only the trustworthy parts of the four images are used in our method to achieve a better result. Also the main limitation is the distortion around the low angle area which is caused by the noise sensitivity around the area.

Chapter 5: Application of algorithm for minimising information leakage

Although the algorithm can maintain the trustworthy part of the images by two steps, some disadvantages need to be further suppressed, especially for the edge effect. This effect occurs at the edges of an object and always contributes to a loss of accuracy in the final reconstruction.

To illuminate this weakness, a more regular and standard sample is used – the polystyrene bead. The bead has a diameter of $5\mu\text{m}$ and can be used as a stand-alone particle to evaluate the quality of reconstruction. By modifying the residual equation which is used in the SFS algorithm, the edge effect is reduced and the reconstruction is improved. This is demonstrated quantitatively using the correlation coefficient method. The algorithm is thus applied to an real particle and the result is discussed.

5.1 Sample and preparation

A 5 micron diameter polystyrene bead is used for this improvement fig. 5-1.

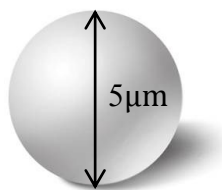


Figure 5-1: the schematic of the sample, the 5 micro polystyrene bead (Sigma-Aldrich).

The properties of the 5 micro polystyrene bead are shown in Table 5: [155]

Crosslinking	0% cross-linked
Concentration	10% (solids)
Particle size	5um std dev<0.1um, coeff var <2%
Density	1.05 g/cm ³
Storage temp.	2-8°c

Table 5: *The properties of the 5 micro polystyrene bead*

The polystyrene bead cannot be detected by the SEM directly. A 50nm gold layer is deposited by sputtering to make the surface of the sample conductive. The E-T detector is then used to take the SEM image and the result is shown in figure 5-2

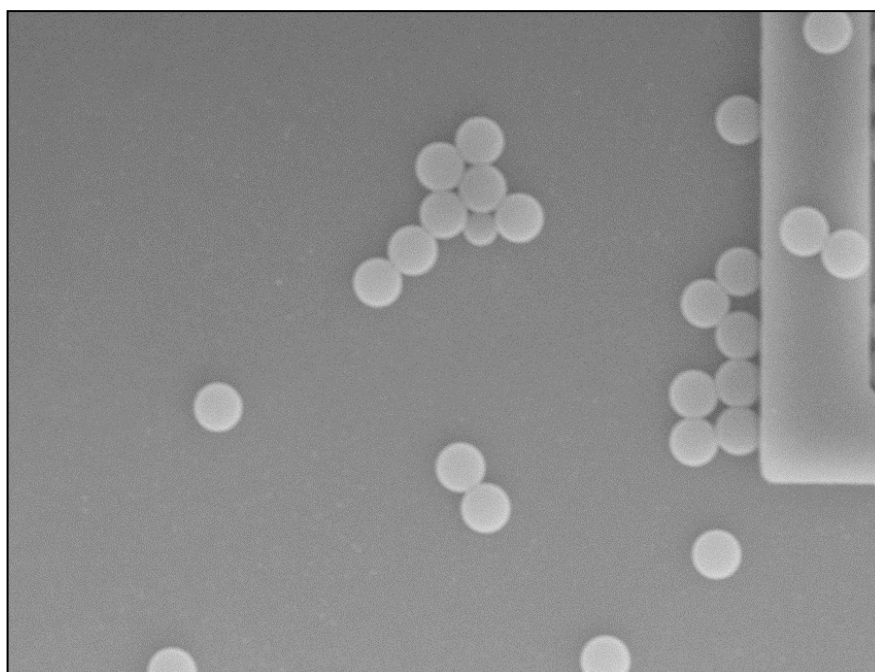


Figure 5-2: *The SEM image of beads imaged by the E-T detector.*

As the dimension of the bead is known, it can be used to test the precision of the result obtained. We can create synthetic images as a reference by synthesising in Matlab a hemisphere on top of a cylinder of which the diameter and height are the same.

The SE image and an ideal synthetic height image are shown in fig. 5-3. The ideal image corresponds to the case where the algorithm performs perfectly and the reconstructed height image should exactly confirm to the original sample, within the limitations of the approach. The image below shows a perfect upper half of the sphere where the lower half of the ball is draped vertically as even a perfect AFM or any other height measurement, can only obtain the highest Z value of the X-Y points on the surface.

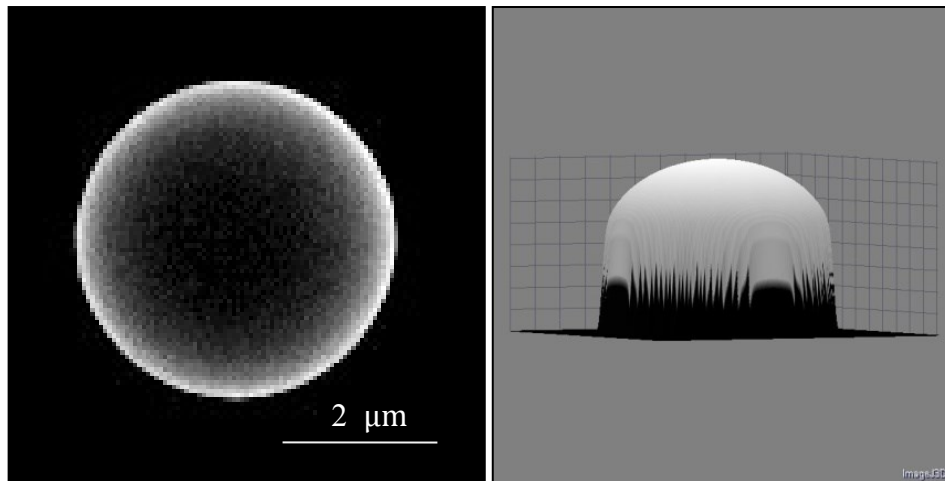


Figure 5-3: *the SE image and ideal height image which is synthesised by the Matlab.*

5.2 Modification of the algorithm

The relationship between the SEM intensity and the simulated SEM intensity from the synthetic ideal height image can be obtained by using the facet method discussed before in Chapter 4. This relationship is shown below in fig.5-4:

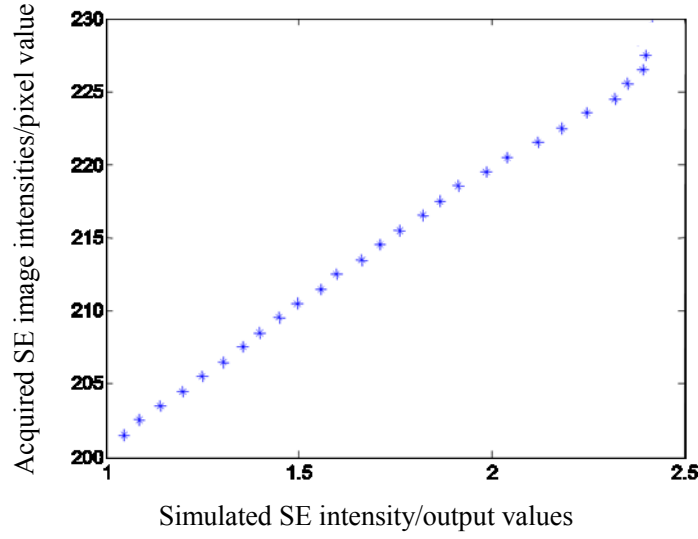


Figure 5-4: *The relationship between the SEM intensity and the corresponding secant values*

It can be found that where the angle is high, the relationship is not perfectly linear, which is caused by the SE image. For the high slopes, there will be some errors for the electron collection and the edge effect, which means for the high slope the intensity of SE image will not obey the mathematic description of equation 4-1. Although other parts match the linear relationship very well, we have modified the implementation of the SFS brightness constraint to take into account the observed divergence for the highest slopes.

Because the reliability of the mathematic description on the high slope portion is lower, less weight should be used for these areas in calculating the final image difference. We therefore weight the difference by dividing by the slope-dependent magnitude of the initial image:

$$R = \left(\left(\frac{I_{SEM} - I'_{SEM}}{Sec(\theta)} \right)^{0.5} \right)^2 \quad (5-1)$$

Where I_{SE} is the SEM intensity matrix, I'_{SE} is the simulated SEM intensity matrix, $Sec(\theta)$ is the corresponding secant value of the slope angle, and R is the residual. The above equation is equivalent to minimising the sum of the squares of the relative differences between the images, rather than the sum of the squares of just the difference.

5.3 Assessment of the reconstruction

The reconstruction technique was applied to the spherical Sigma-Aldrich particle. Fig 5-5 shows both the top and the side view of the final images derived using two different weightings in our method. The image obtained by the previous method is shown in fig. 5-5 A and B. For the previous method discussed in Chapter 4 the minimisation was driven by the mean square of the intensity differences between successive iterations of the algorithm. This causes the low-reliability sides of the sphere to dominate the minimisation, producing an apparent deformation of the top of the sphere. In the second (see fig. 5-5 C and D), the relative changes were used and the iteration converges to match the known spherical profile.

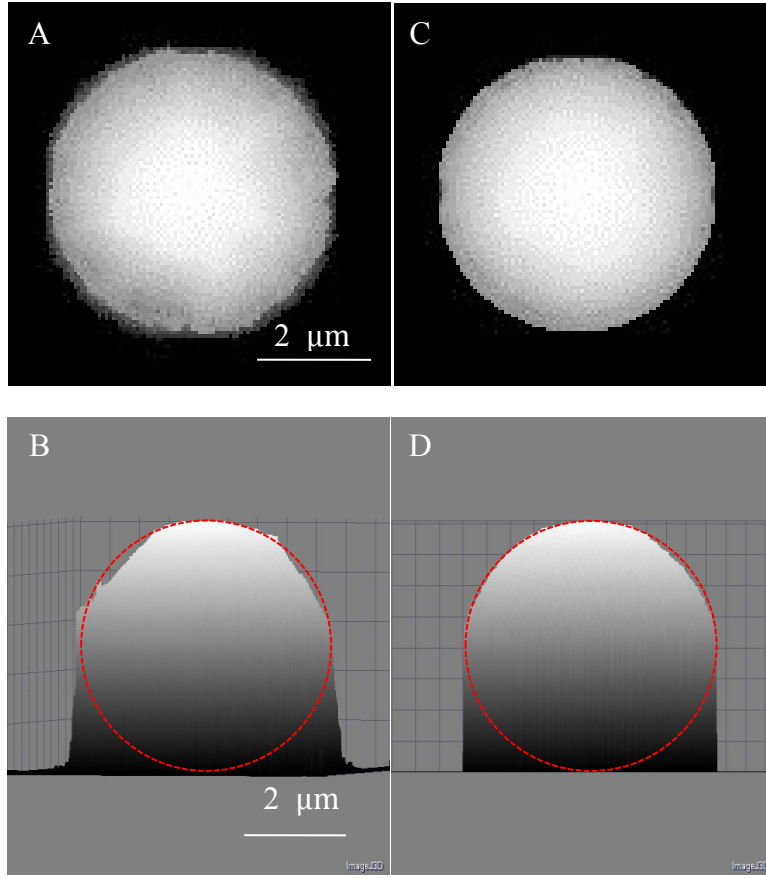


Figure 5-5: the comparison between the results which are obtained by the previous method (A,B) and the improved method (C,D) respectively.

For a quantitative comparison of the two images and to emphasise the improvement, the following function is used to quantify the similarity between the ideal synthetic images and the two reconstruction images respectively [156]:

$$cor = \frac{\sum_m \sum_n (A_{mn} - \bar{A})(B_{mn} - \bar{B})}{\sqrt{(\sum_m \sum_n (A_{mn} - \bar{A})^2)(\sum_m \sum_n (B_{mn} - \bar{B})^2)}} \quad (5-2)$$

where cor is the correlation coefficient, $\bar{A}$ is the mean value of A with respect to the ideal synthetic images, $\bar{B}$ is the mean value of B with respect to the reconstructed image and the closer to 1 the correlation coefficient is, the higher the similarity between A and B is.

Comparing the ideal image with the improved and original result, the correlation coefficients are 0.9557 and 0.9048 respectively. Since closer to 1 the higher the similarity is, the improvement can be quantified.

In summary, the 5 micron polystyrene bead is used to quantify the improvement in our algorithm. By weighting the linear relationship between the actual and simulated intensity to de-emphasize the less reliable values, the algorithm has been improved and the result is closer to the ideal one as indicated by the correlation coefficient.

5.4 Application to real particles

The reconstruction algorithm is applied to the real particles introduced in Chapter 2. The images were acquired by the LEO 1455VP and Veeco NT9100S Optical Profiler which has also been introduced in Chapter 2 and 4. This specimen was coated by a gold layer, the thickness of which was around 50 nanometres to improve the conductivity and without influencing the texture on the surface. The major and minor axis of the particle is around 5 and 2 micrometre respectively. The related images and the result are shown in fig.5-6.

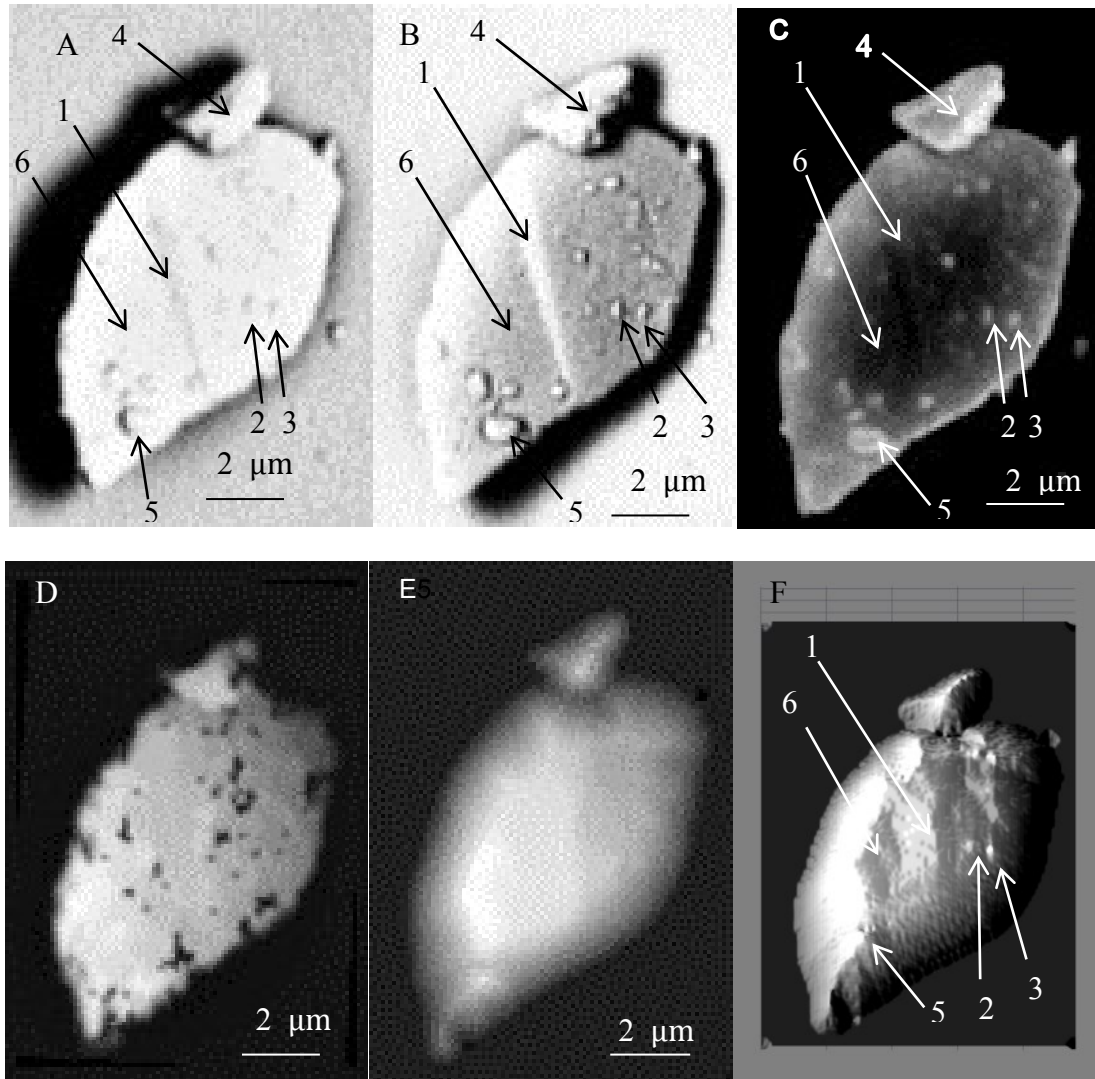


Figure 5-6: *A and B: Images from QBSD detectors. C: the SE image. D: the Optical Profiler image. E and F: the final reconstruction and the corresponding 3D image*

For image A the detector is placed on the right side, which causes the shadowing shown on the left side of the particle. For image B the detector is placed on the left side which cause the shadowing shown on the right side of the particle. For region 1 there is a gently spindly rectangle slope which can be obviously observed on BSE images (A and B). From the two BSE images it can be found that the surface of the slope is towards to the left down side. Because the detector is placed on the left side in image B, the part is brighter. For the image A the part is darker because of the right-side placed detector. For

image C the intensity is dependent on the slope of the surface. We can find that for the slope area the intensity is nearly constant which proof the existence of the slope because for the SE image the intensity is dependent on the degree of the slope. If the intensity is constant, it means that for this area the slope degree is constant which is consistent with the conclusion obtained from image A and B. For the final reconstruction (image F) the slope area towards to the left down side, which can be observed obviously and matches the conclusion obtained from the BSE and SE images (images A, B and C). Also for the region 6 it can be found that this region is towards to the up-right side. Contrary to region 1 in image A the region 6 is brighter and in image B it is darker which proof that the region 1 and region 6 is towards to the opposite sides. From image F it can be found that the slope is really towards to the right-up-side which matches the conclusion obtained from the BSE and SE images.

In addition for points 2 and 3, which can be recognized in all three SEM images (images A, B, C), they can be reconstructed in the final height image (image F), but these two points cannot be recognized in optical profiler image (image D). This is the benefit of the algorithm: it can reconstruct the details shown on the SEM image which cannot be provided by the original (input) height image. Comparing the reconstruction of the height image with the height image obtained by the Veeco (image D) we can find that indeed more details come out. The details on the SE can be restored on the new height image. In addition the holes (defects) on the Veeco image are eliminated on the final reconstruction.

However this algorithm also has the disadvantages, for the small particle 4 it can be found in images C that one side of the small particle is on the main particle and the opposite side of the small particle is on the ground. From the image A and B the situation of the particle 4 can also be proved, but the reconstruction (image F) does not reflect the situation of the two particles. In image E and F the corner of particle 4 is not on the main particle. It shows that the particle 4 and the main particle are next to each other. Also for point 5 it can be clearly recognized in images A, B and C, but in the reconstruction image F point 5 cannot be clearly recognized. It can be found that both of

the distortions discussed above happen around the edge region and actually the distortions are caused by the edge effect which means that if the slope of the surface is close to 90 degree the algorithm cannot reconstruct the fact of the surface very well. Because the situation that the corner of particle 4 is on the main particle makes the slope of the junction part close to 90° , the algorithm cannot restore this kind of situation because of the edge effect and can only reconstruct relatively smooth slope which makes the two particles be next to each other rather than “overlap”. For the point 5 because it happens to be inside the edge region, so the reconstruction will be distorted because of the edge effect will influence the reconstruction inside the edge region.

This edge effect is caused by four reasons: the first reason is from the SE image which has the highest resolution among all the SEM images and is used as the “reference” of the SFS step. Normally the intensity of the SE image is dependent on the slope (equation 4-1), but for the high slope part it cannot match the equation very well as shown in fig. 5-4. This is caused by the spot size of the electron beam. For the step part the intensity must be proportional to the average slope value inside the spot size, so that the intensity of the transition part of the edge region must be influenced by the spot size of the electron beam. Because the SE image is used in the SFS step the final reconstruction of the edge region will be influenced.

In addition charging effects will influence the SE image. Typically the gold layer will not be coated very well in the edge regions because of the high slope and complex structures. It will cause the charging effects in the bad coating region around the edge region resulting in electric fields. The electric fields will modify the trajectories of electrons and can create complicated variations in intensity, so that the intensity of the SE image around the edge region will be influenced resulting in the final reconstruction distorted.

Further, the reconstructed surface must be representable as a height field which means that surfaces with undercuts cannot be reconstructed, but the SEM can detect the hidden

surface of a specimen such as the overlap situation. Because electrons can penetrate some distance before escaping, electrons escaping from the hidden surface may interact with the up surface. Thus the information in an SEM image may contain the information from such hidden surfaces and influence the intensity of the edge regions.

The fourth reason is that the simulated SE algorithm uses 5 by 5 height values to simulate one SE intensity value. As a reverse processing when we use the simulated algorithm in the SFS step, the inaccurate intensity value of the SE image can influence its 5 by 5 neighbour reconstruction height values. This will broaden the distortions caused by the reasons discussed above, which means that it will amplify the distortions. Combining the four influences together the high slope part cannot be reconstructed very well and can only be reconstructed as a relatively gentle slope.

The algorithm has been applied to both model and natural samples, revealing microstructural information which is not reliably exhibited in any of the raw datasets (input height image) which demonstrates the accuracy of the approach. Also because the edge effect the reconstruction will be influenced in the edge regions. The edge effect can be found in the reconstruction. For example some of the small particles such as particle 5 cannot be found around the particle edge, although it is shown on the BSE images. This effect is unavoidable because of the inherent edge effect on the SE image.

Chapter 6: Conclusion

In this thesis, several microscope data fusion methods to reconstruct surface topography are discussed and finally, a novel method to reconstruct the height image in the micro-scale is developed and implemented.

Before we combine the datasets from different microscope images, it is necessary to evaluate the ability and the characteristics of the related microscopes. A real particle is used as the sample. The experiments show that although an AFM can provide 3D surface topography, it is influenced by tip convolution which will cause information leakage. The SEM can image the sample with high resolution and without defects caused by dilation, but this technique can only provide 2D images. This means that the two techniques are complimentary in the information they can provide. Initial experiments suggested a combination of SEM images with additional height information could reproduce a better reconstruction of the sample.

Some existing methods for this combination are explored (Chapter 3). The first is stereoscopy, using SEM images taken from different angles to extract 3D information. An integrative algorithm (ICP) is used to fuse AFM and SEM datasets. However this method is shown to provide a limited reconstruction with serious information leakage because of the combination algorithm itself. The second approach considered is the SFS method using an AFM image as an initial input to minimise the difference between the simulated and real SEM images. Though the simulated method introduced in Chapter 3 has the advantage over Monte Carlo simulation (widely used method) of being faster, the major disadvantage of this SFS algorithm is the computationally intensive simulation calculation which is necessary for each iteration. Also the mode of electron production that contributes to the image is difficult to be determined, which is necessary for simulating the SEM image.

A new way that combines the trustworthy parts of each microscope image with minimum information leakage has been developed and introduced in Chapter 4. A range of samples both micro-fabricated and natural irregular one have been examined and used to validate the method. The results demonstrate that the new algorithm can provide a reliable reconstruction of the sample surface. Examples in chapter 5 show how the reconstruction can be achieved using the method. This method could be applied to either model or natural samples. The new method provides a more comprehensive understanding of the surface topography compared to existing techniques.

Comparing this new technique to the previous method there are two significant advantages:

- (1) By comparing SEM and optical interferometer images, the most reliable portions in the data are identified. This takes advantage of the strengths of each imaging modality to suppress the less trustworthy information in each image.
- (2) The second advantage is that, as shown in fig. 4-1, after the reconstruction from the integration method, we use the SE image which has high resolution and little noise, to refine the result. This restores more details on the sample and the new method has been demonstrated to produce an improved surface reconstruction.

However, at present the algorithm has only been demonstrated for surface coated samples to eliminate the effect of materials contrast to the images. This limitation simplifies the problem to simulate the SEM images because different materials will in general influence the intensity of the SEM image. Further work is needed to explore how best to extend this algorithm to samples containing multiple materials. It could be extended to simulate the specimens composed of multiple materials by using X-ray detector to provide material map and modify the simulating algorithm to respond differently to different material types.

Also the algorithm is limited by the edge effect. It causes the reconstruction of the sample to be distorted in the edge region which has been discussed in Chapter 5.

In addition the minimization method used for every iteration is achieved by the smoothness constraint. In the future it is worthwhile to try other methods which are more mathematical such as:

Minimising the surface normal:

$$\iint \left(\|\vec{N_x}\|^2 + \|\vec{N_y}\|^2 \right) dx dy \quad (6-1)$$

Where $\|\vec{N_x}\|$ and $\|\vec{N_y}\|$ are the surface normal modulus along the x and y directions. This means that the surface normal should change gradually. This is the normal way to improve the SFS iteration, however this may not be better than what we have used, i.e. a median filter, for two reasons: the first is that the median filter is easy for calculation but this method is not, which will take more time to achieve one iteration. The second is that the median filter can best match the useful information that we try to maintain and the noise we try to remove, which means that the method is going to minimise information leakage.

In addition, the reconstruction relies on alignment of all the images. Currently the alignment is achieved manually. Errors in registering the images will introduce errors in the surface reconstruction. In the future, fiducials can be added to a substrate, for example by micromachining, to allow automatic alignment between the datasets

Although the approach has been validated against a model sample, the full capability of the technique has not been investigated at a wide range of magnifications. Further work could determine the high resolution limits of this approach.

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Appendix A: Cubic Facet Coefficients

The cubic facet model treats each surface facet as a two-dimensional cubic form:

$$f = K_1 + K_2 r + K_3 c + K_4 r^2 + K_5 r c + K_6 c^2 + K_7 r^3 + K_8 r^2 c + K_9 r c^2 + K_{10} c^3 \quad (\text{A-1})$$

where the K coefficients can be estimated using a least-square-error surface fit. More specifically we assume the rectangular-shaped neighbourhood with centre at $(0,0)$ and row-column indices are taken to be $r \in R$ and $c \in C$. The square error is given by

$$e^2 = \sum_{r \in R} \sum_{c \in C} ((K_1 + K_2 r + K_3 c + K_4 r^2 + K_5 r c + K_6 c^2 + K_7 r^3 + K_8 r^2 c + K_9 r c^2 + K_{10} c^3 - f(r, c))^2 \quad (\text{A-2})$$

Take partial derivatives for each K :

$$\begin{aligned}
& \begin{bmatrix} \frac{\partial e^2}{\partial K_1} \\ \frac{\partial e^2}{\partial K_2} \\ \frac{\partial e^2}{\partial K_3} \\ \frac{\partial e^2}{\partial K_4} \\ \frac{\partial e^2}{\partial K_5} \\ \frac{\partial e^2}{\partial K_6} \\ \frac{\partial e^2}{\partial K_7} \\ \frac{\partial e^2}{\partial K_8} \\ \frac{\partial e^2}{\partial K_9} \\ \frac{\partial e^2}{\partial K_{10}} \end{bmatrix} = 2 \sum_{r \in R} \sum_{c \in C} (K_1 + K_2 r + K_3 c + K_4 r^2 + K_5 r c + K_6 c^2 + K_7 r^3 + K_8 r^2 c + \\
& K_9 r c^2 + K_{10} c^3 - f(r, c)) \begin{bmatrix} 1 \\ r \\ c \\ r^2 \\ r c \\ c^2 \\ r^3 \\ r^2 c \\ r c^2 \\ c^3 \end{bmatrix}
\end{aligned} \tag{A-3}$$

Because of the symmetric region $[R, C]$ the system can be reduced to

$$\begin{bmatrix} \frac{\partial e^2}{\partial K_1} \\ \frac{\partial e^2}{\partial K_2} \\ \frac{\partial e^2}{\partial K_3} \\ \frac{\partial e^2}{\partial K_4} \\ \frac{\partial e^2}{\partial K_5} \\ \frac{\partial e^2}{\partial K_6} \\ \frac{\partial e^2}{\partial K_7} \\ \frac{\partial e^2}{\partial K_8} \\ \frac{\partial e^2}{\partial K_9} \\ \frac{\partial e^2}{\partial K_{10}} \end{bmatrix} = 2 \sum_{r \in R} \sum_{c \in C} \begin{bmatrix} K_1 + K_4 r^2 + K_6 c^2 - f(r, c) \\ K_2 r^2 + K_7 r^4 + K_9 r^2 c^2 - r f(r, c) \\ K_3 c^2 + K_{10} c^4 + K_8 r^2 c^2 - c f(r, c) \\ K_1 r^2 + K_4 r^4 + K_6 r^2 c^2 - r^2 f(r, c) \\ K_5 r^2 c^2 - r c f(r, c) \\ K_1 c^2 + K_6 c^4 + K_4 r^2 c^2 - c^2 f(r, c) \\ K_2 r^4 + K_7 r^6 + K_9 r^4 c^2 - r^3 f(r, c) \\ K_3 r^2 c^2 + K_8 c^2 r^4 + K_{10} r^4 c^2 - r^2 c f(r, c) \\ K_2 r^2 c^2 + K_7 c^2 r^4 + K_9 r^2 c^2 - c^2 r f(r, c) \\ K_3 c^4 + K_{10} c^6 + K_8 c^4 r^2 - c^3 f(r, c) \end{bmatrix} \quad (A-4)$$

By setting the system to zero, K_5 can be expressed as the following:

$$K_5 = \frac{\sum_{r \in R} \sum_{c \in C} r c f(r, c)}{\sum_{r \in R} \sum_{c \in C} r^2 c^2} \quad (A-5)$$

According to the following systems of equations, the rest K can be obtained:

$$\begin{bmatrix} \sum_{r \in R} \sum_{c \in C} 1 & \sum_{r \in R} \sum_{c \in C} r^2 & \sum_{r \in R} \sum_{c \in C} c^2 \\ \sum_{r \in R} \sum_{c \in C} r^2 & \sum_{r \in R} \sum_{c \in C} r^4 & \sum_{r \in R} \sum_{c \in C} r^2 c^2 \\ \sum_{r \in R} \sum_{c \in C} c^2 & \sum_{r \in R} \sum_{c \in C} r^2 c^2 & \sum_{r \in R} \sum_{c \in C} r^4 \end{bmatrix} \begin{bmatrix} K1 \\ K4 \\ K6 \end{bmatrix} = \begin{bmatrix} \sum_{r \in R} \sum_{c \in C} f(r, c) \\ \sum_{r \in R} \sum_{c \in C} r^2 f(r, c) \\ \sum_{r \in R} \sum_{c \in C} c^2 f(r, c) \end{bmatrix} \quad (A-6)$$

$$\begin{aligned}
& \begin{bmatrix} \sum_{r \in R} \sum_{c \in C} r^2 & \sum_{r \in R} \sum_{c \in C} r^4 & \sum_{r \in R} \sum_{c \in C} r^2 c^2 \\ \sum_{r \in R} \sum_{c \in C} r^4 & \sum_{r \in R} \sum_{c \in C} r^6 & \sum_{r \in R} \sum_{c \in C} r^4 c^2 \\ \sum_{r \in R} \sum_{c \in C} c^2 r^2 & \sum_{r \in R} \sum_{c \in C} r^4 c^2 & \sum_{r \in R} \sum_{c \in C} c^4 r^2 \end{bmatrix} \begin{bmatrix} K1 \\ K7 \\ K9 \end{bmatrix} = \\
& \begin{bmatrix} \sum_{r \in R} \sum_{c \in C} r f(r, c) \\ \sum_{r \in R} \sum_{c \in C} r^3 f(r, c) \\ \sum_{r \in R} \sum_{c \in C} c^2 r f(r, c) \end{bmatrix} \tag{A-7}
\end{aligned}$$

$$\begin{aligned}
& \begin{bmatrix} \sum_{r \in R} \sum_{c \in C} c^2 & \sum_{r \in R} \sum_{c \in C} r^2 c^2 & \sum_{r \in R} \sum_{c \in C} c^4 \\ \sum_{r \in R} \sum_{c \in C} r^2 c^2 & \sum_{r \in R} \sum_{c \in C} r^4 c^2 & \sum_{r \in R} \sum_{c \in C} r^2 c^4 \\ \sum_{r \in R} \sum_{c \in C} c^4 & \sum_{r \in R} \sum_{c \in C} r^2 c^4 & \sum_{r \in R} \sum_{c \in C} c^6 \end{bmatrix} \begin{bmatrix} K_3 \\ K_8 \\ K_{10} \end{bmatrix} = \\
& \begin{bmatrix} \sum_{r \in R} \sum_{c \in C} c f(r, c) \\ \sum_{r \in R} \sum_{c \in C} r^2 c f(r, c) \\ \sum_{r \in R} \sum_{c \in C} c^3 f(r, c) \end{bmatrix} \tag{A-8}
\end{aligned}$$

Denote $R_n = \sum r \in R r^{2n}$ and $C_n = \sum c \in C c^{2n}$ for $n = 0, 1, 2, 3$. Define also:

$$G = R_0 R_2 C_0 C_2 - R_1^2 C_1^2 \quad (\text{A-9})$$

$$A = R_1 R_3 C_0 C_2 - R_2^2 C_1^2 \quad (\text{A-10})$$

$$B = R_1 R_3 C_0 C_2 - R_2^2 C_1^2 \quad (\text{A-11})$$

$$Q = C_0 (R_0 R_2 - R_1^2) \quad (\text{A-12})$$

$$T = R_0 (C_0 C_2 - C_1^2) \quad (\text{A-13})$$

$$U = C_0 (R_1 R_3 - R_2^2) \quad (\text{A-14})$$

$$V = C_1 (R_0 R_2 - R_1^2) \quad (\text{A-15})$$

$$W = R_1 (C_0 C_2 - C_1^2) \quad (\text{A-16})$$

$$Z = R_0 (C_1 C_3 - C_2^2) \quad (\text{A-17})$$

Using this notation the solution of the system becomes:

$$K_1 = \frac{1}{QT} \sum_r \sum_c (G - T R_1 r^2 - Q C_1 c^2) f(r, c) \quad (\text{A-18})$$

$$K_2 = \frac{1}{UW} \sum_r \sum_c (A - W R_2 r^2 - U C_1 c^2) r f(r, c) \quad (\text{A-19})$$

$$K_3 = \frac{1}{VZ} \sum_r \sum_c (B - Z R_1 r^2 - V C_2 c^2) c f(r, c) \quad (\text{A-20})$$

$$K_4 = \frac{1}{Q} \sum_r \sum_c (R_0 r^2 - R_1) f(r, c) \quad (\text{A-21})$$

$$K_6 = \frac{1}{T} \sum_r \sum_c (R_0 r^2 - R_1) f(r, c) \quad (\text{A-22})$$

$$K_7 = \frac{1}{U} \sum_r \sum_c (R_1 r^2 - R_2) f(r, c) \quad (\text{A-23})$$

$$K_8 = \frac{1}{V} \sum_r \sum_c (R_0 r^2 - R_1) c f(r, c) \quad (\text{A-24})$$

$$K_9 = \frac{1}{W} \sum_r \sum_c (C_0 c^2 - C_1) r f(r, c) \quad (\text{A-25})$$

$$K_{10} = \frac{1}{Z} \sum_r \sum_c (C_1 c^2 - C_2) c f(r, c) \quad (\text{A-26})$$

The following figure is used to help understand the geometrical relationship.

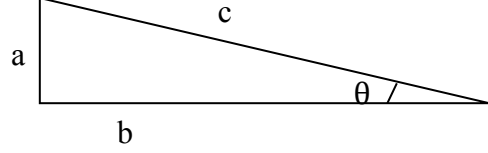


Figure A-1: *the schematic diagram to help understand the expressions of sin, cos, tan and secant*

$$\text{The slope of the surface is equal to } a/b = ((K_2)^2 + (K_3)^2)^{0.5} \quad (\text{A-27})$$

so the secant of the surface is equal to

$$c/b = ((a^2 + b^2)^{0.5})/b = (1 + (K_2)^2 + (K_3)^2)^{0.5} \quad (\text{A-28})$$

$$\sin(\theta) = ((KRC_1)^2 + (KRC_3)^2)^{0.5} / ((KRC_2)^2 + (KRC_3)^2 + 1)^{0.5}; \quad (\text{A-29})$$

$$\cos(\theta) = (1 / ((KRC_2)^2 + (KRC_3)^2 + 1)^{0.5}); \quad (\text{A-30})$$

$$\tan(\theta) = ((KRC_2)^2 + (KRC_3)^2)^{0.5}; \quad (\text{A-31})$$

$$\cos(\chi_N) = -KRC_3 / ((KRC_2)^2 + (KRC_3)^2 + 1)^{0.5}; \quad (\text{A-32})$$

$$\text{maximum principal curvatures} = KRC_6 + KRC_4 + ((KRC_6 - KRC_4)^2 + KRC_5^2)^{0.5} \quad (\text{A-33})$$

$$\text{minimum principal curvatures} = KRC_6 + KRC_4 - ((KRC_6 - KRC_4)^2 + KRC_5^2)^{0.5} \quad (\text{A-34})$$

% The function to obtain the equations of the slope from the Facet model

clc;

clear;

for i=1:85% create a virtual matrix 85 by 85

for ii=1:85

zzz(ii,i)=sym(strcat('R',num2str(ii),'C',num2str(i)));

end

end

SCALENO=1;% the conditions are the same as the discussion above

syms a b c;

CONSTANT=1;

POINTS=85;

N=5;

N1=-(N-1)/2;

N2=(N-1)/2;

M=POINTS-((N-1)/2);

M1=(POINTS+1-M);

R0=0;

for r=N1:N2

```
R0=r^0+R0; % obtain Rn and Cn for n=0,1,2,3.
```

```
end;
```

```
R1=0;
```

```
for r=N1:N2
```

```
R1=r^2+R1;
```

```
end;
```

```
R2=0;
```

```
for r=N1:N2
```

```
R2=r^4+R2;
```

```
end;
```

```
R3=0;
```

```
for r=N1:N2
```

```
R3=r^6+R3;
```

```
end;
```

```
C0=R0;
```

```
C1=R1;
```

```
C2=R2;
```

```

C3=R3;

G=R0*R2*C0*C2-((R1)^2)*((C1)^2); % obtain  $G=R_0R_2C_0C_2 - R_1^2C_1^2$ 

A=R1*R3*C0*C2-(R2^2)*(C1^2); % obtain  $A=R_1R_3C_0C_2 - R_2^2C_1^2$ 

B=R0*R2*C1*C3-(R1^2)*(C2^2); % obtain  $B=R_1R_3C_0C_2 - R_2^2C_1^2$ 

Q=C0*(R0*R2-(R1^2)); % obtain  $Q=C_0(R_0R_2 - R_1^2)$ 

TT=R0*(C0*C2-(C1^2)); % obtain  $T=R_0(C_0C_2 - C_1^2)$ 

U=C0*(R1*R3-(R2^2)); % obtain  $U=C_0(R_1R_3 - R_2^2)$ 

V=C1*(R0*R2-(R1^2)); % obtain  $V=C_1(R_0R_2 - R_1^2)$ 

W=R1*(C0*C2-(C1^2)); % obtain  $W=R_1(C_0C_2 - C_1^2)$ 

Z=R0*(C1*C3-(C2^2)); % obtain  $Z=R_0(C_1C_3 - C_2^2)$ 

XX=zzz;

for S=M1:M

for T=M1:M

X=SCALENO*XX(S-((N-1)/2):S+((N-1)/2),T-((N-1)/2):T+((N-1)/2));

KRC2=0;

for R=N1:N2

KC=0;

for C=N1:N2

```

```
KC=KC+(A-W*R2*R^2-U*C1*C^2)*R*X(R+N2+1,C+N2+1);
```

```
end
```

```
KRC2=(CONSTANT/(U*W))*KC+KRC2; % obtain  $K_2 = \frac{1}{UW} \sum_r \sum_c (A -$   

 $WR_2r^2 - UC_1c^2)rf(r, c)$ 
```

```
end
```

```
KRC3=0;
```

```
for R=N1:N2
```

```
KC=0;
```

```
for C=N1:N2
```

```
KC=KC+(B-Z*R1*R^2-V*C2*C^2)*C*X(R+N2+1,C+N2+1);
```

```
end
```

```
KRC3=(CONSTANT/(V*Z))*KC+KRC3; % obtain  $K_3 = \frac{1}{VZ} \sum_r \sum_c (B -$   

 $ZR_1r^2 - VC_2c^2)cf(r, c)$ 
```

```
End
```

```
KRC4=0;
```

```
for R=N1:N2
```

```
KC=0;
```

```
for C=N1:N2
```

```
KC=KC+(R0*R^2-R1)*X(R+N2+1,C+N2+1);
```

end

KRC4=(CONSTANT/Q)*KC+KRC4; % obtain $K_4 = \frac{1}{Q} \sum_r \sum_c (R_0 r^2 - R_1) f(r, c)$

end

KRC51=0;

for R=N1:N2

KC=0;

for C=N1:N2

KC=KC+C*R*X(R+N2+1,C+N2+1);

end

KRC51=CONSTANT*KC+KRC51;

end

KRC52=0;

for R=N1:N2

KC=0;

for C=N1:N2

KC=KC+C^2*R^2;

end

KRC52=CONSTANT*KC+KRC52;

end

KRC5=KRC51/KRC52;

KRC6=0;

for R=N1:N2

KC=0;

for C=N1:N2

KC=KC+(C0*C^2-C1)*X(R+N2+1,C+N2+1);% obtain $K_6 = \frac{1}{T} \sum_r \sum_c (R_0 r^2 - R_1) f(r, c)$

end

KRC6=(CONSTANT/TT)*KC+KRC6;

end

KAD=KRC6+KRC4+((KRC6-KRC4)^2+KRC5^2)^0.5; % obtain maximum principal curvatures =KRC6+KRC4+((KRC6-KRC4)^2+KRC5^2)^0.5

KMU=KRC6+KRC4-((KRC6-KRC4)^2+KRC5^2)^0.5; % obtain minimum principal curvatures =KRC6+KRC4-((KRC6-KRC4)^2+KRC5^2)^0.5

GRC=((KRC2)^2+(KRC3)^2)^0.5; % obtain the slope of the surface $=((K_2)^2 + (K_3)^2)^{0.5}$

GRCsin=((KRC2)^2+(KRC3)^2)^0.5./((KRC2)^2+(KRC3)^2+1)^0.5; % obtain $\sin(\theta) = ((K_2)^2 + (K_3)^2)^{0.5} / ((K_2)^2 + (K_3)^2 + 1)^{0.5}$;

```
GRCcos=1./((KRC2)^2+(KRC3)^2+1)^0.5; % obtain cos(θ)=1/((KRC2)  
2+(KRC3) 2+1) 0.5;
```

```
GRCtan=((KRC2)^2+(KRC3)^2).^0.5; % obtain tan(θ)=((KRC2) 2+(KRC3) 2)  
0.5;
```

```
GRCsecant=((KRC2)^2+(KRC3)^2+1)^0.5; % obtain the secant of the surface  
is equal to b/c=b/((a2+b2)0.5) = (1 + (K2)2 + (K3)2)0.5
```

```
FY=-KRC2;
```

```
FX=-KRC3;
```

```
FZ=1;
```

```
FFXX=FX./((FX.^2+FY.^2+FZ.^2).^0.5);
```

```
FFYY=FY./((FX.^2+FY.^2+FZ.^2).^0.5);
```

```
FFZZ=FZ./((FX.^2+FY.^2+FZ.^2).^0.5);
```

```
end
```

```
end
```

Finally the slope value can be obtained from the height image:

$R1C1$	.	.	.	.	$R1C5$
.					.
.					.
.					.
.					.
$R5C1$	.	.	.	.	$R5C5$

Figure A-2: the schematic diagram of the 5 by 5 matrix used in the Facet model.

Slope value at the point $R3C3$ =

$$0.002381 * ((31.0 * R1C1 - 44.0 * R1C2 + 44.0 * R1C4 - 31.0 * R1C5 - 5.0 * R2C1 - 62.0 * R2C2 + 62.0 * R2C4 + 5.0 * R2C5 - 17.0 * R3C1 - 68.0 * R3C2 + 68.0 * R3C4 + 17.0 * R3C5 - 5.0 * R4C1 - 62.0 * R4C2 + 62.0 * R4C4 + 5.0 * R4C5 + 31.0 * R5C1 - 44.0 * R5C2 + 44.0 * R5C4 - 31.0 * R5C5)^2 + (31.0 * R1C1 - 5.0 * R1C2 - 17.0 * R1C3 - 5.0 * R1C4 + 31.0 * R1C5 - 44.0 * R2C1 - 62.0 * R2C2 - 68.0 * R2C3 - 62.0 * R2C4 - 44.0 * R2C5 + 44.0 * R4C1 + 62.0 * R4C2 + 68.0 * R4C3 + 62.0 * R4C4 + 44.0 * R4C5 - 31.0 * R5C1 + 5.0 * R5C2 + 17.0 * R5C3 + 5.0 * R5C4 - 31.0 * R5C5)^2)^{(1/2)}$$

Appendix B: the algorithm used for the coefficients

%This algorithm is used to obtain the coefficients

clear

close all

global RZ CZ

RZ=18;

CZ=211;

SEM_se=textread('chaohou3_se.txt');% read the SE image

SEM_se_mu2=SEM_se(3:end-2,3:209);

vecco=textread('vecco_211_18.txt');% read the height image

Fsecantvecco=Fsecant(vecco);%input the height image to the simulated secant algorithm

SEM_se_coxfuzhu=Fsecantvecco;

mun=1;% this part is to find rough coefficients which are used to obtain a rough idea about the correspondence between slope and the SEM image.

for i=0:255 % All the SEM intensity values will be included to find the coefficients of the linear relationship between the secant values obtained from height image and the values of the SEM points. If several SEM intensity points have the same value then the mean of the corresponding secant values is used to reduce noise.

```

[Rrcom ,Cccom]= find(SEM_se_mu2==i);%find the positions of the SEM
points which values are equal to i.

sizeRrcom=size(Rrcom);

Fmeanfull=zeros(1,sizeRrcom(1));

Fmeanfull=Fsecantvecco(Rrcom+(Cccom-1)*(RZ-4));%find the
corresponding secant points which are calculated from the input height image

Fmean=trimmean(Fmeanfull,25);%exclude outliers and average the other
values to reduce the noise.

if ~isnan(Fmean)% From 0 to 255 sometimes we cannot find some values on
the SEM image. If it is not that case we will plot the value of the SEM (i) against
the corresponding mean secant value later for curve fitting.

SEM_mean_0(mun)=i;

Fmean_0(mun)=Fmean;

mun=mun+1;

end

end

SEM_X_seini= polyfit(Fmean_0,SEM_mean_0,1); %curve fitting is used to
obtain the coefficients

mun=1;% this part is to find coefficients obtained from the SEM values and the
corresponding height values of the low slope parts of the object.

for i=(0:(1.414*SEM_X_seini(1)+SEM_X_seini(2)));% In this time only
specified intensity values of the SEM will be included and this values
corresponding to the low slope part of the object. According to the coefficients

```

obtained from the last part on the SEM the points of which the value are $1.414 \cdot \text{SEM_X_seini}(1) + \text{SEM_X_seini}(2)$ corresponding to the points on the object of which the slope is around 45 degree.

```
[Rrcom ,Cccom]= find(SEM_se_mu2==i);%find the positions of the SEM  
points which values are equal to i. It is the same as that of the last part.
```

```
sizeRrcom=size(Rrcom);
```

```
Fmeanfull=zeros(1,sizeRrcom(1));
```

```
Fmeanfull=Fsecantvecco(Rrcom+(Cccom-1)*(RZ-4));%find the  
corresponding secant points which are calculated from the input height image. It  
is the same as that of the last part.
```

```
Fmean=trimmean(Fmeanfull,25);%exclude outliers and average the other  
values to reduce the noise. It is the same as that of the last part.
```

```
if ~isnan(Fmean)%plot the value of the SEM (i) against the corresponding mean  
secant value later for curve fitting.
```

```
SEM_mean_1(mun)=i;
```

```
Fmean_1(mun)=Fmean;
```

```
mun=mun+1;
```

```
end
```

```
end
```

```
figure(1);
```

```
SEM_X_se= polyfit(Fmean_1,SEM_mean_1,1);%curve fitting is used to  
obtain the coefficients. It is the same as that of the last part.
```

```
x=1:0.01:1.8;
```

```

y=SEM_X_se(1).*x+SEM_X_se(2);

plot(Fmean_1,SEM_mean_1,'*',x,y,'r');

save('SEM_X_se.txt','SEM_X_se','-ascii');

```

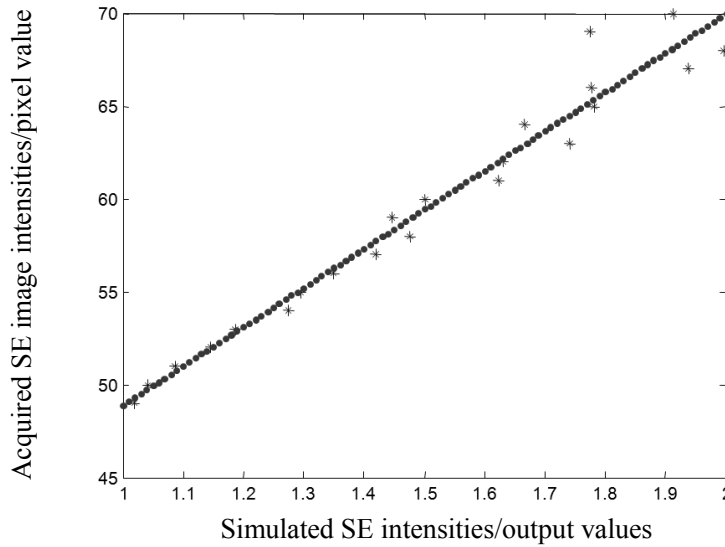


Figure B-1: *The liner relationship between the SEM values and the corresponding height values of the slope parts obtained by the upper code*

% This part is to find the coefficients for the Detector A image

```
SEM_back_08right=textread('08right_bse.txt');% read the QBSD image
```

```
SEM_back_08right_mu2=SEM_back_08right(3:end-2,3:209);
```

```
Fadvecco=FFcosquan_adNEW_halfpi(vecco);% obtain the simulated
0.5*COS(theta)+0.5*SIN(theta)*COS(XN) image from input height image
```

```
mun=1;
```

for i=190:255% To eliminate the influence from the shadow, we must use the parts of which the COS(XN) values are more than 0. 190 is the BSE mean value of the points on the flat surface. According to $(0.5 \cdot \cos(\theta) + 0.5 \cdot \sin(\theta) \cdot \cos(XN))$, the value of the points on the image will not be more than 190, only if $\cos(XN)$ is more than 0, so when the values of

the points on the QBSD image is more than 190, the $\cos(XN)$ values of the corresponding points are more than 0.

```
[Rrcom ,Cccom]=  
find(SEM_back_08right_mu2>=i&SEM_back_08right_mu2<i+1&SEM_se_  
mu2<=(1.414*SEM_X_seini(1)+SEM_X_seini(2)));%find the positions of the  
QBSD points of which values are between i and i+1 and the corresponding SE  
points must be lower than (1.414*SEM_X_seini(1)+SEM_X_seini(2)) (the  
slope is less than 45 degree).
```

```
sizeRrcom=size(Rrcom);
```

```
Fmeanfull=zeros(1,sizeRrcom(1));
```

```
Fmeanfull=Fadvecco(Rrcom+(Cccom-1)*(RZ-4));%find the corresponding  
0.5*cos( $\theta$ )+0.5*sin( $\theta$ )*cos(XN) points which are calculated from the input  
height image.It is the same as that of the last part.
```

```
Fmean=trimmean(Fmeanfull,25);%exclude outliers and average the other  
values to reduce the noise. It is the same as that of the last part.
```

```
if ~isnan(Fmean)%plot the value of the QBSD against the corresponding mean  
0.5*cos( $\theta$ )+0.5*sin( $\theta$ )*cos(XN) value later for curve fitting. It is the same  
as that of the last part.
```

```
SEM_mean_2(mun)=i+0.5;
```

```
Fmean_2(mun)=Fmean;
```

```
mun=mun+1;
```

```
end
```

```
end
```

```
figure(2);
```

SEM_X_08right = polyfit(Fmean_2,SEM_mean_2,1);%curve fitting is used to obtain the coefficients. It is the same as that of the last part.

x=0.45:0.01:0.75;

y=SEM_X_08right(1).*x+SEM_X_08right(2);

plot(Fmean_2,SEM_mean_2,'*',x,y,'r');

save('SEM_X_08right.txt','SEM_X_08right','-ascii');

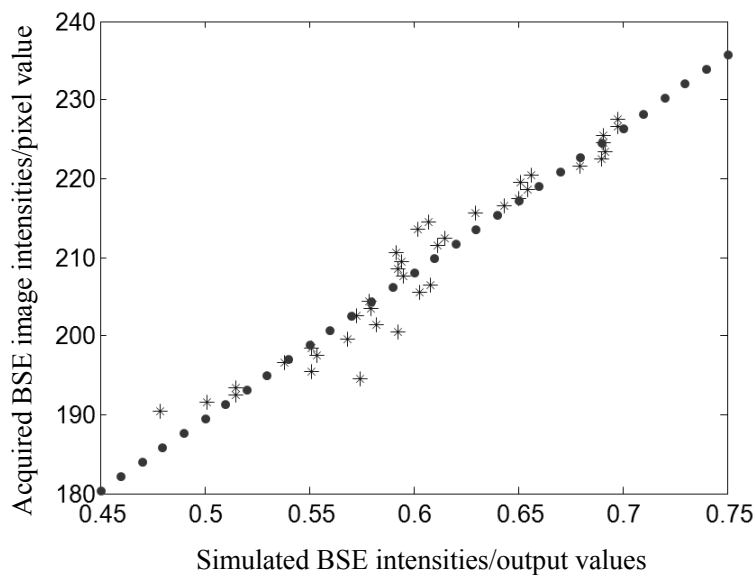


Figure B-2: *The liner relationship between the BSE values from the right detector and the corresponding height values of the slope parts*

% This part is to find the coefficients for the detector B image and all the steps is the

% similar to the last part.

SEM_back_82left=textread('82left_bse.txt');% read the QBSD image

SEM_back_82left_mu2=SEM_back_82left(3:end-2,3:209);

Fmuvecco=FFcosquan_muNEW_halfpi(vecco);% obtain the simulated
0.5*COS(θ)-0.5*SIN(θ)*COS(XN) image from input height image

mun=1;

for i=150:255% To eliminate the influence from the shadow, we must use the parts of which the $\cos(XN)$ values are less than 0. 150 is the value of points on the flat surface. According to $(0.5*\cos(\theta)-0.5*\sin(\theta)*\cos(XN))$, the value of the points on the image will not be more than 150, only if $\cos(XN)$ is less than 0, so when the values of the points on the QBSD image is more than 150, the $\cos(XN)$ values of the corresponding points are less than 0.

[Rrcom ,Cccom]=

find(SEM_back_82left_mu2>=i&SEM_back_82left_mu2<i+1&SEM_se_mu2<=(1.414*SEM_X_seini(1)+SEM_X_seini(2)));%find the positions of the QBSD points of which values are between i and i+1 and the corresponding SE points must be lower than $(1.414*SEM_X_seini(1)+SEM_X_seini(2))$ (the slope is less than 45 degree).

sizeRrcom=size(Rrcom);

Fmeanfull=zeros(1,sizeRrcom(1));

Fmeanfull=Fmuvecco(Rrcom+(Cccom-1)*(RZ-4));%find the corresponding $0.5*\cos(\theta)-0.5*\sin(\theta)*\cos(XN)$ points which are calculated from the input height image.

Fmean=trimmean(Fmeanfull,25);%exclude outliers and average the other values to reduce the noise.

if ~isnan(Fmean)%plot the value of the QBSD against the corresponding mean $0.5*\cos(\theta)-0.5*\sin(\theta)*\cos(XN)$ value later for curve fitting. It is the same as that of the last part.

SEM_mean_3(mun)=i+0.5;

Fmean_3(mun)=Fmean;

```

mun=mun+1;

end

end

figure(3);

SEM_X_82left = polyfit(Fmean_3,SEM_mean_3,1);%curve fitting is used to
obtain the coefficients. It is the same as that of the last part.

x=0.45:0.01:0.75;

y=SEM_X_82left(1).*x+SEM_X_82left(2);

plot(Fmean_3,SEM_mean_3,'*',x,y,'r');

save('SEM_X_82left.txt','SEM_X_82left','-ascii');

```

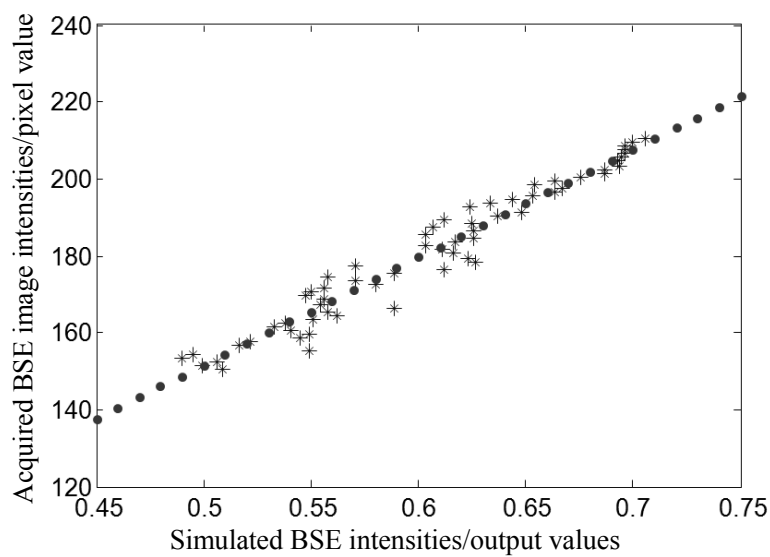


Figure B-3: *the liner relationship between the BSE values from the right detector and the corresponding height values of the slope parts*

Appendix C: the algorithm used to obtain the initial reconstruction

%This algorithm is a integration method to obtain the initial reconstruction
(height image)

clc

clear

close all

SEM_se=textread('chaohou3.txt');% Read the SE image

SEM_X_se=textread('SEM_X_se.txt');% Read the coefficients of SE image.

All the coefficients are obtained from another function of ours.

SEM_se=(SEM_se-SEM_X_se(2))./SEM_X_se(1);% convert the SE image to
the secant image

SEM_se(SEM_se<1)=1;% the lowest value for secant is 1; some values may be
a little bit lower than 1 caused by such as noise influence ; make these values be
equal to 1;

save('SEM_se.txt','SEM_se','-ascii');%save the image as txt file

SEM_back_q1=textread('08right.txt');% read BSE image (detector A)

SEM_X_08right=textread('SEM_X_08right.txt');% read the coefficients of
BSE image(detector A)

SEM_back_q1=(SEM_back_q1-SEM_X_08right(2))./SEM_X_08right(1);%

convert the BSE image to the $0.5 \cdot \cos(\theta) + 0.5 \cdot \sin(\theta) \cdot \cos(XN)$ image

```
COX_q1=(SEM_back_q1-0.5.*(1./SEM_se))./(1/pi.*(1-(1./SEM_se).^2).^0.5.  
*(0.5*pi));%convert the  $0.5 \cdot \cos(\theta) + 0.5 \cdot \sin(\theta) \cdot \cos(XN)$  image to the  
COS(XN) image with the help of the secant image
```

```
COX_q1(COX_q1==inf)=0;% eliminate some special values if it has.
```

```
COX_q1(COX_q1==-inf)=0;
```

```
COX_q1(isnan(COX_q1))=0;
```

```
COX_q1(COX_q1>=1)=1;% the highest value for COS(XN) is 1; make the  
values which are a little bit more than 1 be equal to 1
```

```
save('COX_q1.txt','COX_q1','-ascii');
```

SEM_back_q3=textread('82left.txt');% read BSE image (detector B) and the
following steps are similar to that of detector A

```
SEM_X_82left=textread('SEM_X_82left.txt');
```

```
SEM_back_q3=(SEM_back_q3-SEM_X_82left(2))./SEM_X_82left(1);
```

```
COX_q3=-(SEM_back_q3-0.5.*(1./SEM_se))./(1/pi.*(1-(1./SEM_se).^2).^0.5  
.*(0.5*pi));
```

```
COX_q3(COX_q3==inf)=0;
```

```
COX_q3(COX_q3==-inf)=0;
```

```
COX_q3(isnan(COX_q3))=0;
```

```
COX_q3(COX_q3<=-1)=-1;
```

```
save('COX_q3.txt','COX_q3','-ascii');
```

COX_q13=zeros(28,352);% COX_q13 is the final COS(XN) image which will combine both the information from detector A and detector B BSE images

COX_q13test=zeros(28,352);% COX_q13test is a testing image which will point out the positions the values of which are determined by both of detector A and detector B because they have very low slope and sensitive to the random errors.

[Rrcom ,Cccom]= find(COX_q3<0);% find the positions of the points on COX_q3 of which the values is less than 0 and can be used for the final COS(XN) image.

COX_q13(28*(Cccom-1)+Rrcom)=COX_q3(28*(Cccom-1)+Rrcom);%
Replace the corresponding points on the COX_q13 with the points on the COX_q3

COX_q13test(28*(Cccom-1)+Rrcom)=COX_q13test(28*(Cccom-1)+Rrcom)
+500;% mark the corresponding points using the value of 500

[Rrcom ,Cccom]= find(COX_q1>0);

COX_q13(28*(Cccom-1)+Rrcom)=COX_q1(28*(Cccom-1)+Rrcom);

COX_q13test(28*(Cccom-1)+Rrcom)=COX_q13test(28*(Cccom-1)+Rrcom)
+500;

[Rrcom ,Cccom]= find(COX_q13test==1000);% On the COX_q13test if the values of the points are 1000, both COX_q1 and COX_q3 values can be used in this points. These positions are around the zone of transition which mean the COS(XN) is around 0 and any little influence from the random errors will make the positive become negative or vice versa,so set the values of these points to 0.

COX_q13(28*(Cccom-1)+Rrcom)=0;

```
save('COX_q13.txt','COX_q13','-ascii');
```

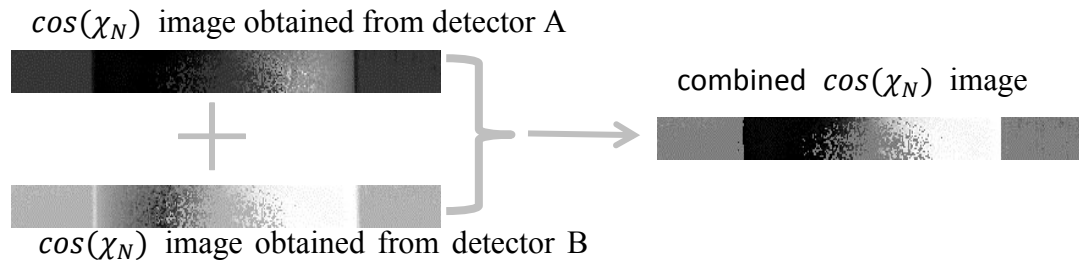


Figure C-1: The upper code is to combine the useful parts (trustworthy parts) of the two BSE image together.

```
tanZZ=((1-(1./SEM_se).^2).^0.5)./(1./SEM_se);%obtain the tan(θ) image from  
the sec(θ) image
```

```
save('tanZZ.txt','tanZZ','-ascii');
```

```
semtancos=-tanZZ.*COX_q13;%tan(θ)*cos (XN) =-∂z/ ∂x,so  
-tanZZ.*COX_q13 is equal to ∂z/ ∂x
```

```
save('semtancos.txt','semtancos','-ascii');
```

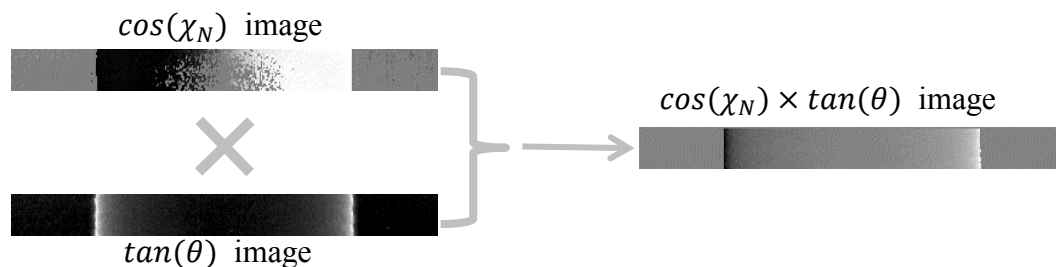


Figure C-2: The upper code is used to obtain the $\cos(\chi_N) \times \tan(\theta)$ image which will be integrated later

```
intsem_1=cumsum(semtancos(:,176:352),2);% integrate ∂z/ ∂x along X axis  
to reconstruct the height image; we integrate the from middle to the two  
sides to reduce the "build-in" error and this command integrate from middle to  
the right side.
```

```

begintsem_tancos=-1.*imrotate(sem_tancos(:,1:176),-180,'bilinear','loose'); %
The following three commands integrate from middle to the left side. Firstly we
rotate it 180°.

intsem_2=cumsum(begintsem_tancos,2);% Then integrate it along X axis from
left to right.

intsem_2=imrotate(intsem_2,180,'bilinear','loose');% Finally rotate it back.

intsem=zeros(28,352);% Finally combine these two parts together.

intsem(:,1:176)=intsem_2;

intsem(:,176:352)=intsem_1;

```

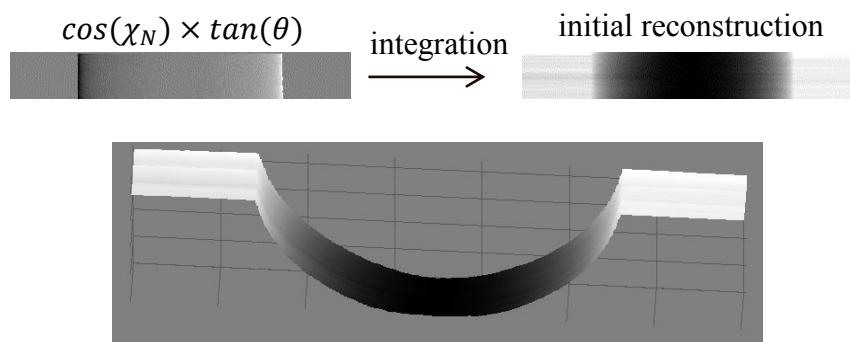


Figure C-3: *This result is the initial reconstruction*

```

save('intsemAFM.txt','intsem','-ascii');

plot(mean(intsem))

axis equal

```

Appendix D: the algorithm used to modify the height image

% This is the Reverse Simulated SEM Algorithm (minimization SFS method)
to modify the height image

% obtained from the integration method

clear

clear global

global Rrcom Cccom intsem SEMfunc Rrcom2 Cccom2

SEMimage=textread('chaohou3.txt');% read the SE image

SEMimage(SEMimage<38.356)=38.356;% According to the coefficients of the
SEM the lowest value of the SEM should be 38.356

(1.1975286e+01+2.6380721e+01).If the values are lower than that, they are
influenced by random errors, we set them to 38.356 to improve the final result.

intsem=zeros(28,352);

intsem_intsemAFM=textread('intsemAFM.txt');% read the height image
obtained from integration method.

[Rrcom_AFM ,Cccom_AFM]= find(SEMimage>=43.31);% According to the
SEM if the value is higher than 43.31 the corresponding slope is larger than
45°.If it is larger than 45°,we adopt the height image obtained from integration
method as initial input.

intsem(Rrcom_AFM+(Cccom_AFM-1)*28)=intsem_intsemAFM(Rrcom_AF
M+(Cccom_AFM-1)*28);

intsem_vecco=textread('vecco_352_28.txt');% read the height image obtained from optical profiler .

[Rrcom_AFM_2 ,Cccom_AFM_2]= find(SEMimage<43.31);%If the corresponding slope is lower than 45° , we adopt the height image obtained from optical profiler as initial input.

intsem(Rrcom_AFM_2+(Cccom_AFM_2-1)*28)=intsem_vecco(Rrcom_AFM_2+(Cccom_AFM_2-1)*28);

save('intsem_com.txt','intsem','-ascii');

FBSEMimage=Fsecant(intsem);% input the initial height image to the simulated secant algorithm

FBini= 1.1975286e+01.*FBSEMimage+ 2.6380721e+01;% Then it become the simulated SEM image, when the coefficients are added.

save('FBini.txt','FBini','-ascii');

SEMfunc=SEMimage(3:end-2,3:end-2);% the corresponding real SEM image

save('SEMfunc.txt','SEMfunc','-ascii');

pointtest=abs(FBini-SEMfunc);%Compare the simulated SEM with the real SEM image.

save('pointtest.txt','pointtest','-ascii');

[Rrcom_test ,Cccom_test]= find(pointtest>2);%check if the difference between the two values are more than 2 (the normal noise on the SEM is around 2)and record the corresponding Row and Column values.

Rrcom_test =Rrcom_test+2;

Cccom_test=Cccom_test+2;

```

test_zero=zeros(28,352);% this is a testing matrix

for i=-2:2

    for j=-2:2

test_zero(Rrcom_test+i+(Cccom_test+j-1)*28)=test_zero(Rrcom_test+i+(Cccom_test+j-1)*28)+1;%if the difference between the simulated and real SEM values are more than 2 then on the testing image the surrounding 5 by 5 points around that position will be added 1 to mark these positions which will be identified later and the corresponding input height points will be treated as unfixed points during the iteration.

    end

end% find the positions of the unfixed points

save('test_zero.txt','test_zero','-ascii');

[Rrcom ,Cccom]= find(test_zero==0);% if in testing matrix the points are equal to zero then the corresponding input height points will be treated as fixed points during the iteration. This command find the corresponding Row and Column values.

CZ_1=-1000*ones(28,352);

CZ_1(Rrcom+(Cccom-1)*28)=intsem(Rrcom+(Cccom-1)*28);

save('fixed_point.txt','CZ_1','-ascii');

[Rrcom2 ,Cccom2]= find(test_zero~=0); % For the others (not equal to zero) because they can result the difference between the simulated SEM and the real

```

SEM more than 2, the corresponding input height points will be treated as unfixed points. This command find the corresponding Row and Column values.

```
sizeRrcom2=size(Rrcom2);
```

```
sizeRC2=sizeRrcom2(1);% to obtain the number of the unfixed points.
```

```
CZ_2=-1000*ones(28,352);
```

```
CZ_2(Rrcom2+(Cccom2-1)*28)=intsem(Rrcom2+(Cccom2-1)*28);
```

```
save('chuzhi.txt','CZ_2','-ascii');
```

chuzhi=intsem(Rrcom2+(Cccom2-1)*28); % This is the initial values of the unfixed points which will be changed during iterations.

chuzhi=unifrnd(-0.5,0.5,sizeRC2,1)+chuzhi;% Based on the experience if the input values is smoothness then add a little bit random noise will improve the iteration speed if we use levenberg-marquardt algorithm.

```
parametersLM=optimset('Algorithm',  
'levenberg-marquardt','TolFun',1e-4,'Tolx',1e-4,'Display','iter','FunValCheck','on',  
'MaxFunEvals',900000000,'MaxIter',100);
```

beta=lsqnonlin(@(zzz) function_in(zzz),chuzhi,[],[],parametersLM);% using levenberg-marquardt algorithm to point out the final value of the unfixed points.

```
betaf=zeros(28,352);
```

betaf(Rrcom+(Cccom-1)*28)=intsem(Rrcom+(Cccom-1)*28);% For the final image the fixed points will not be changed

betaf(Rrcom2+(Cccom2-1)*28)=beta;% For the final image the result obtained from the iteration is used as the values of the unfixed points.

```
save('resultAFM_fsolve_185_1stepfinal.txt','betaf','-ascii');
```

```
betaf=medfilt2(betaf,[5 5]);% This is the filter to keep the image smoothness  
and this is a step to keep the image the same as the final integration result. The  
function_in.m provide more details
```

```
save('resultAFM_fsolve_185_2stepfinal.txt','betaf','-ascii');
```

```
clear global
```

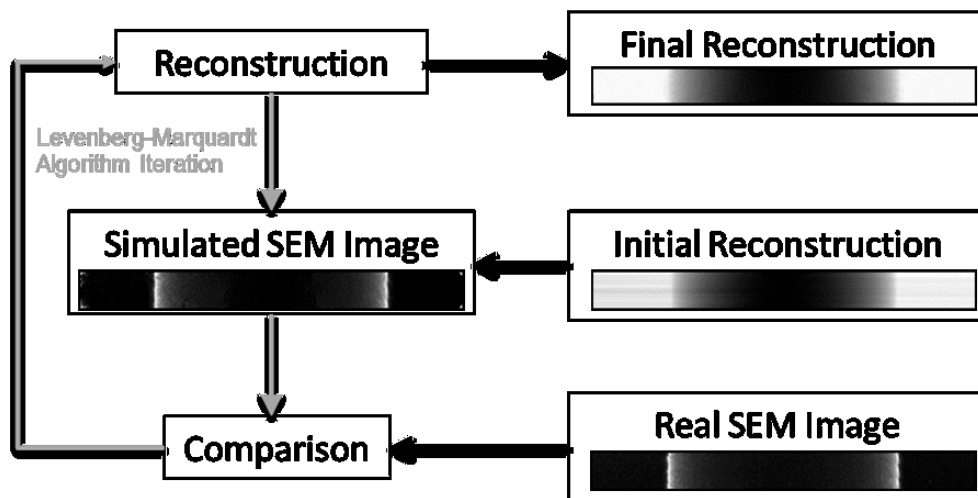


Figure D-1: The schematic diagram of the SFS algorithm

```
function Fyin=function_in(zzz)
```

```
global Rrcom Cccom SEMfunc Rrcom2 Cccom2 intsem
```

```
zzzz=zeros(28,352);
```

```
zzzz(Rrcom+(Cccom-1)*28)=intsem(Rrcom+(Cccom-1)*28);% the fixed  
points will not be changed during every iteration.
```

```
zzzz(Rrcom2+(Cccom2-1)*28)=zzzz;% the unfixed points will be changed  
during every iteration.
```

```
zzzz=medfilt2(zzzz,[5 5]);% the height image must meet the smoothness  
constraint.
```

```
FB=Fsecant(zzzz);% the height image is converted to the secant image to  
simulate the SEM image
```

```
Fyin= 1.1975286e+01 .*FB+ 2.6380721e+01-SEMfunc;% the direction to  
change the unfixed points is to minimize the difference between the simulated  
and real SEM.
```

```
end
```

```
% This is the modified function used for the Reverse Simulated SEM  
Algorithm which is applied on the 5 Micro Polystyrene Bead
```

```
function Fyin=function_in(zzz)
```

```
global Rrcom Cccom SEMfunc Rrcom2 Cccom2 intsem RZ CZ SEM_X_se  
Fyin_2
```

```
zzzz=zeros(RZ,CZ);
```

```
zzzz(Rrcom+(Cccom-1)*RZ)=intsem(Rrcom+(Cccom-1)*RZ);% the fixed  
points will not be changed during every iteration.
```

```
zzzz(Rrcom2+(Cccom2-1)*RZ)=zzz;% the unfixed points will be changed  
during every iteration.
```

```
zzzz=medfilt2(zzzz,[5 5]);% the height image must meet the smoothness  
constraint.
```

```
FB=Fsecant(zzzz);% the height image is converted to the secant image to  
simulate the SEM image
```

```
Fyin=(abs((SEM_X_se(1).*FB+SEM_X_se(2)-SEMfunc))./Fyin_2).^0.5;%  
the direction to change the unfixed points is to reduce the difference between  
the simulated and real SEM.
```

```
end
```

Appendix E: The algorithm obtain the relationship between the SEM intensity and the slope

%This algorithm is used to obtain the relationship between the SEM intensity and the corresponding secant values of the slope which are simulated from the ideal height image

close all

global RZ CZ

RZ=111;

CZ=111;

SEM_se=textread('SE_1.txt');% read the SE image

SEM_se_mu2=SEM_se(3:end-2,3:end-2);

vecco=textread('Ve.txt');% read the height image

Fsecantvecco=Fsecant(vecco);%input the height image to the simulated secant algorithm

SEM_se_coxfuzhu=Fsecantvecco;

save('Fsecantveccotest.txt','SEM_se_coxfuzhu','-ascii');

mun=1;% this part is to find coefficients obtained from the SEM values and the corresponding height values of the low slope parts of the object.

for i=(201:255);%the range of the intensity included is from the flatten part 201 to all the above intensity (up to 255).

[Rrcom ,Cccom]= find(SEM_se_mu2>=i&SEM_se_mu2<i+1);% find the positions of the SEM points which values are equal to i.

sizeRrcom=size(Rrcom);

Fmeanfull=zeros(1,sizeRrcom(1));

Fmeanfull=Fsecantvecco(Rrcom+(Cccom-1)*(RZ-4));%find the corresponding secant points which are calculated from the input height image.

Fmean=trimmean(Fmeanfull,25);%exclude outliers and average the other values to reduce the noise.

if ~isnan(Fmean)%plot the value of the SEM (i) against the corresponding mean secant value later for curve fitting.

SEM_mean_1(mun)=i+0.5;

Fmean_1(mun)=Fmean;

mun=mun+1;

end

end

figure(1);

SEM_X_se= polyfit(Fmean_1,SEM_mean_1,1);%curve fitting is used to obtain the coefficients.It is the same as that of the last part.

plot(Fmean_1,SEM_mean_1,'*');

```
save('SEM_X_se.txt','SEM_X_se','-ascii');
```

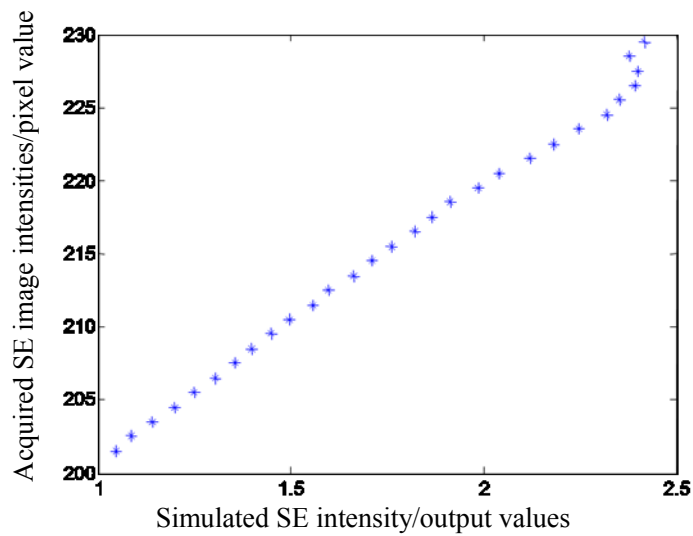


Figure E-1: *The relationship between the SEM intensity and the corresponding secant values*

%The code for quantitatively reflected the improvement of the result. It is a kind of the correlation coefficient method which has been discussed above.

```
clear
```

```
H_ideal=textread('Ideal.txt');
```

```
H_improve=textread('result_I.txt');
```

```
H_Orignal=textread('result_O.txt');
```

```
recorr_1=corr2(H_ideal,H_improve);
```

```
recorr_2=corr2(H_ideal,H_Orignal);
```

```
disp(recorr_1);
```

```
disp(recorr_2);
```

Appendix F: the Facet model used to obtain the simulated images

%the function that can obtain the Fsecant image form the height image

%the function is obtained by the Facet model

function Fyin=Fsecant(zzz)

global RZ CZ

```
Fyin=6.776e-21.*(1.235e35.*(31.0.*zzz(1:(RZ-4),1:(CZ-4)) - 44.0.*zzz(1:(RZ-4),2:(CZ-3)) +  
44.0.*zzz(1:(RZ-4),4:(CZ-1)) - 31.0.*zzz(1:(RZ-4),5:(CZ-0)) - 5.0.*zzz(2:(RZ-3),1:(CZ-4)) -  
62.0.*zzz(2:(RZ-3),2:(CZ-3)) + 62.0.*zzz(2:(RZ-3),4:(CZ-1)) + 5.0.*zzz(2:(RZ-3),5:(CZ-0)) -  
17.0.*zzz(3:(RZ-2),1:(CZ-4)) - 68.0.*zzz(3:(RZ-2),2:(CZ-3)) + 68.0.*zzz(3:(RZ-2),4:(CZ-1)) +  
17.0.*zzz(3:(RZ-2),5:(CZ-0)) - 5.0.*zzz(4:(RZ-1),1:(CZ-4)) - 62.0.*zzz(4:(RZ-1),2:(CZ-3)) +  
62.0.*zzz(4:(RZ-1),4:(CZ-1)) + 5.0.*zzz(4:(RZ-1),5:(CZ-0)) + 31.0.*zzz(5:(RZ-0),1:(CZ-4)) -  
44.0.*zzz(5:(RZ-0),2:(CZ-3)) + 44.0.*zzz(5:(RZ-0),4:(CZ-1)) -  
31.0.*zzz(5:(RZ-0),5:(CZ-0))).^2 + 1.235e35.*(31.0.*zzz(1:(RZ-4),1:(CZ-4)) -  
5.0.*zzz(1:(RZ-4),2:(CZ-3)) - 17.0.*zzz(1:(RZ-4),3:(CZ-2)) - 5.0.*zzz(1:(RZ-4),4:(CZ-1)) +  
31.0.*zzz(1:(RZ-4),5:(CZ-0)) - 44.0.*zzz(2:(RZ-3),1:(CZ-4)) - 62.0.*zzz(2:(RZ-3),2:(CZ-3)) -  
68.0.*zzz(2:(RZ-3),3:(CZ-2)) - 62.0.*zzz(2:(RZ-3),4:(CZ-1)) - 44.0.*zzz(2:(RZ-3),5:(CZ-0)) +  
44.0.*zzz(4:(RZ-1),1:(CZ-4)) + 62.0.*zzz(4:(RZ-1),2:(CZ-3)) + 68.0.*zzz(4:(RZ-1),3:(CZ-2)) +  
62.0.*zzz(4:(RZ-1),4:(CZ-1)) + 44.0.*zzz(4:(RZ-1),5:(CZ-0)) - 31.0.*zzz(5:(RZ-0),1:(CZ-4)) +  
5.0.*zzz(5:(RZ-0),2:(CZ-3)) + 17.0.*zzz(5:(RZ-0),3:(CZ-2)) + 5.0.*zzz(5:(RZ-0),4:(CZ-1)) -  
31.0.*zzz(5:(RZ-0),5:(CZ-0))).^2 + 2.178e40).^(1./2);
```

End

%the $0.5 \cdot \cos(\theta) + 0.5 \cdot \sin(\theta) \cdot \cos(\chi_N)$ function that can obtain the image
form the height image

%the function is obtained by the Facet model

function Fyin=FFcosquan_adNEW_halfpi(zzz)

global RZ CZ

```
Fyin=(0.5.*(1.546e19.*zzz(1:(RZ-4),2:(CZ-3)) - 1.089e19.*zzz(1:(RZ-4),1:(CZ-4)) -
1.546e19.*zzz(1:(RZ-4),4:(CZ-1)) + 1.089e19.*zzz(1:(RZ-4),5:(CZ-0)) +
1.757e18.*zzz(2:(RZ-3),1:(CZ-4)) + 2.178e19.*zzz(2:(RZ-3),2:(CZ-3)) -
2.178e19.*zzz(2:(RZ-3),4:(CZ-1)) - 1.757e18.*zzz(2:(RZ-3),5:(CZ-0)) +
5.973e18.*zzz(3:(RZ-2),1:(CZ-4)) + 2.389e19.*zzz(3:(RZ-2),2:(CZ-3)) -
2.389e19.*zzz(3:(RZ-2),4:(CZ-1)) - 5.973e18.*zzz(3:(RZ-2),5:(CZ-0)) +
1.757e18.*zzz(4:(RZ-1),1:(CZ-4)) + 2.178e19.*zzz(4:(RZ-1),2:(CZ-3)) -
2.178e19.*zzz(4:(RZ-1),4:(CZ-1)) - 1.757e18.*zzz(4:(RZ-1),5:(CZ-0)) -
1.089e19.*zzz(5:(RZ-0),1:(CZ-4)) + 1.546e19.*zzz(5:(RZ-0),2:(CZ-3)) -
1.546e19.*zzz(5:(RZ-0),4:(CZ-1)) + 1.089e19.*zzz(5:(RZ-0),5:(CZ-0)) +
1.476e20))./(1.235e35.*(31.0.*zzz(1:(RZ-4),1:(CZ-4)) - 44.0.*zzz(1:(RZ-4),2:(CZ-3)) +
44.0.*zzz(1:(RZ-4),4:(CZ-1)) - 31.0.*zzz(1:(RZ-4),5:(CZ-0)) - 5.0.*zzz(2:(RZ-3),1:(CZ-4)) -
62.0.*zzz(2:(RZ-3),2:(CZ-3)) + 62.0.*zzz(2:(RZ-3),4:(CZ-1)) + 5.0.*zzz(2:(RZ-3),5:(CZ-0)) -
17.0.*zzz(3:(RZ-2),1:(CZ-4)) - 68.0.*zzz(3:(RZ-2),2:(CZ-3)) + 68.0.*zzz(3:(RZ-2),4:(CZ-1)) +
17.0.*zzz(3:(RZ-2),5:(CZ-0)) - 5.0.*zzz(4:(RZ-1),1:(CZ-4)) - 62.0.*zzz(4:(RZ-1),2:(CZ-3)) +
62.0.*zzz(4:(RZ-1),4:(CZ-1)) + 5.0.*zzz(4:(RZ-1),5:(CZ-0)) + 31.0.*zzz(5:(RZ-0),1:(CZ-4)) -
44.0.*zzz(5:(RZ-0),2:(CZ-3)) + 44.0.*zzz(5:(RZ-0),4:(CZ-1)) -
31.0.*zzz(5:(RZ-0),5:(CZ-0))).^2 + 1.235e35.*(31.0.*zzz(1:(RZ-4),1:(CZ-4)) -
5.0.*zzz(1:(RZ-4),2:(CZ-3)) - 17.0.*zzz(1:(RZ-4),3:(CZ-2)) - 5.0.*zzz(1:(RZ-4),4:(CZ-1)) +
31.0.*zzz(1:(RZ-4),5:(CZ-0)) - 44.0.*zzz(2:(RZ-3),1:(CZ-4)) - 62.0.*zzz(2:(RZ-3),2:(CZ-3)) -
68.0.*zzz(2:(RZ-3),3:(CZ-2)) - 62.0.*zzz(2:(RZ-3),4:(CZ-1)) - 44.0.*zzz(2:(RZ-3),5:(CZ-0)) +
44.0.*zzz(4:(RZ-1),1:(CZ-4)) + 62.0.*zzz(4:(RZ-1),2:(CZ-3)) + 68.0.*zzz(4:(RZ-1),3:(CZ-2)) +
62.0.*zzz(4:(RZ-1),4:(CZ-1)) + 44.0.*zzz(4:(RZ-1),5:(CZ-0)) - 31.0.*zzz(5:(RZ-0),1:(CZ-4)) +
5.0.*zzz(5:(RZ-0),2:(CZ-3)) + 17.0.*zzz(5:(RZ-0),3:(CZ-2)) + 5.0.*zzz(5:(RZ-0),4:(CZ-1)) -
31.0.*zzz(5:(RZ-0),5:(CZ-0))).^2 + 2.178e40).^(1./2);
```

end

%the $0.5 \cdot \cos(\theta) - 0.5 \cdot \sin(\theta) \cdot \cos(\chi_N)$ function that can obtain the image
form the height image

%the function is obtained by the Facet model

function Fyin=FFcosquan_muNEW_halfpi(zzz)

global RZ CZ

```
Fyin=(0.5.*(1.089e19.*zzz(1:(RZ-4),1:(CZ-4)) - 1.546e19.*zzz(1:(RZ-4),2:(CZ-3)) +  
1.546e19.*zzz(1:(RZ-4),4:(CZ-1)) - 1.089e19.*zzz(1:(RZ-4),5:(CZ-0)) -  
1.757e18.*zzz(2:(RZ-3),1:(CZ-4)) - 2.178e19.*zzz(2:(RZ-3),2:(CZ-3)) +  
2.178e19.*zzz(2:(RZ-3),4:(CZ-1)) + 1.757e18.*zzz(2:(RZ-3),5:(CZ-0)) -  
5.973e18.*zzz(3:(RZ-2),1:(CZ-4)) - 2.389e19.*zzz(3:(RZ-2),2:(CZ-3)) +  
2.389e19.*zzz(3:(RZ-2),4:(CZ-1)) + 5.973e18.*zzz(3:(RZ-2),5:(CZ-0)) -  
1.757e18.*zzz(4:(RZ-1),1:(CZ-4)) - 2.178e19.*zzz(4:(RZ-1),2:(CZ-3)) +  
2.178e19.*zzz(4:(RZ-1),4:(CZ-1)) + 1.757e18.*zzz(4:(RZ-1),5:(CZ-0)) +  
1.089e19.*zzz(5:(RZ-0),1:(CZ-4)) - 1.546e19.*zzz(5:(RZ-0),2:(CZ-3)) +  
1.546e19.*zzz(5:(RZ-0),4:(CZ-1)) - 1.089e19.*zzz(5:(RZ-0),5:(CZ-0)) +  
1.476e20))./(1.235e35.*(31.0.*zzz(1:(RZ-4),1:(CZ-4)) - 44.0.*zzz(1:(RZ-4),2:(CZ-3)) +  
44.0.*zzz(1:(RZ-4),4:(CZ-1)) - 31.0.*zzz(1:(RZ-4),5:(CZ-0)) - 5.0.*zzz(2:(RZ-3),1:(CZ-4)) -  
62.0.*zzz(2:(RZ-3),2:(CZ-3)) + 62.0.*zzz(2:(RZ-3),4:(CZ-1)) + 5.0.*zzz(2:(RZ-3),5:(CZ-0)) -  
17.0.*zzz(3:(RZ-2),1:(CZ-4)) - 68.0.*zzz(3:(RZ-2),2:(CZ-3)) + 68.0.*zzz(3:(RZ-2),4:(CZ-1)) +  
17.0.*zzz(3:(RZ-2),5:(CZ-0)) - 5.0.*zzz(4:(RZ-1),1:(CZ-4)) - 62.0.*zzz(4:(RZ-1),2:(CZ-3)) +  
62.0.*zzz(4:(RZ-1),4:(CZ-1)) + 5.0.*zzz(4:(RZ-1),5:(CZ-0)) + 31.0.*zzz(5:(RZ-0),1:(CZ-4)) -  
44.0.*zzz(5:(RZ-0),2:(CZ-3)) + 44.0.*zzz(5:(RZ-0),4:(CZ-1)) -  
31.0.*zzz(5:(RZ-0),5:(CZ-0))).^2 + 1.235e35.*(31.0.*zzz(1:(RZ-4),1:(CZ-4)) -  
5.0.*zzz(1:(RZ-4),2:(CZ-3)) - 17.0.*zzz(1:(RZ-4),3:(CZ-2)) - 5.0.*zzz(1:(RZ-4),4:(CZ-1)) +  
31.0.*zzz(1:(RZ-4),5:(CZ-0)) - 44.0.*zzz(2:(RZ-3),1:(CZ-4)) - 62.0.*zzz(2:(RZ-3),2:(CZ-3)) -  
68.0.*zzz(2:(RZ-3),3:(CZ-2)) - 62.0.*zzz(2:(RZ-3),4:(CZ-1)) - 44.0.*zzz(2:(RZ-3),5:(CZ-0)) +  
44.0.*zzz(4:(RZ-1),1:(CZ-4)) + 62.0.*zzz(4:(RZ-1),2:(CZ-3)) + 68.0.*zzz(4:(RZ-1),3:(CZ-2)) +  
62.0.*zzz(4:(RZ-1),4:(CZ-1)) + 44.0.*zzz(4:(RZ-1),5:(CZ-0)) - 31.0.*zzz(5:(RZ-0),1:(CZ-4)) +  
5.0.*zzz(5:(RZ-0),2:(CZ-3)) + 17.0.*zzz(5:(RZ-0),3:(CZ-2)) + 5.0.*zzz(5:(RZ-0),4:(CZ-1)) -  
31.0.*zzz(5:(RZ-0),5:(CZ-0))).^2 + 2.178e40).^(1./2);
```

end