Charged particle imaging methods for CD metrology of sub 22nm 3D device structures

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CHARGED PARTICLE IMAGING METHODS FOR CD METROLOGY OF SUB 22NM 3D DEVICE STRUCTURES

By

Aron Cepler

A Dissertation

Submitted to the University at Albany, State University of New York

in Partial Fulfillment of

the Requirements for the Degree of

Doctor of Philosophy

College of Nanoscale Science and Engineering

2013
CHARGED PARTICLE IMAGING METHODS FOR CD METROLOGY OF
SUB 22NM 3D DEVICE STRUCTURES

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ABSTRACT

Critical dimension scanning electron microscopes (CD-SEMs) are used to perform highly accurate dimensional metrology on patterned features. In order to ensure optimal feedback for process control, it is necessary that these tools produce highly reproducible measurements. As the smallest device features continue to shrink, and new challenging high aspect ratio (HAR) structures are being introduced, gaps are appearing between process control measurements that are necessary for high volume manufacturing and the capabilities of the CD-SEM. Two possible routes for solving this problem include improvement of the existing CD-SEM technology or the replacement of the CD-SEM.

With improved tool monitoring techniques, the uncertainty in the tool measurements may be reduced, leading to an improvement in the tool performance. By using a carefully designed test structure (such as a pseudorandom dot array), the Contrast Transfer Function (CTF) of a given tool can be decoupled from the specimen information, allowing for characterization of the imaging system itself. Test samples are fabricated using nanoimprint lithography and are imaged in a variety of CD-SEMs in order to measure the performance of the microscopes. This technique is used successfully to identify when the tool is not performing optimally, as well as to monitor the performance of a tool over time and match the performance of different tools.

Research is being made into CD-SEM replacement technologies, among them, ion microscopy. The Helium Ion Microscope’s (HeIM) higher depth of focus than the CD-SEM could be advantageous for the imaging of HAR structures. Studies were conducted in order to determine what imaging signals will be the most useful for CD-metrology and to evaluate the damage that the beam will do to the sample. A technique was developed to determine the depth which that signals were able to escape from the HAR structures, using a series of images acquired with varied tilts. This allows the abilities of the SEM and HeIM to image the bottoms of deep contact holes is compared, and Monte Carlo modeling is used to gain further insights into the process. In our tests, the HeIM outperformed the SEM, but it was unable to detect signals from the bottoms of all of the deep contact hole structures fabricated for this study. Modeling results show for SEM imaging of contact holes, signals should be able to escape from the hole, but they will almost completely be obscured by noise.
ACKNOWLEDGEMENTS

I would like to extend my thanks to many people who have helped me along this journey, with the disclaimer that this is by no means a comprehensive list.

First, thanks to my advisor for shepherding me through my studies over the past several years, and thanks to Professors Diebold, Huang and Lifshin and Dr. Bryan Rice for being a part of my committee and for their suggestions and critiques which have helped to strengthen this work.

I’d like to thank my entire family for its support over these past several years. I would not be here today without the support of my wife. My PhD has a journey which can trace its origins to the day my father gave me an article from the New York Times’ Science Section on carbon nanotubes, which first piqued my interest in this burgeoning field of nanotechnology. Special thanks is due to my parents and my wife for proofreading the many drafts of this work.

I would like to extend thanks to my colleagues from my first internship at the US Naval Research Laboratory’s Advanced Laser Processing group, including Moshe Kasser, Alberto Piqué, Ray Auyeung, Heungsoo Kim, Nick Charipar, and Vic Cestone. It was at NRL where I first learned to do research and where I began to develop the skills that have served me in the course of my graduate studies.

During my studies at the University at Albany’s College of Nanoscale Science and Engineering, I have been indebted to some of my fellow students, including Zachary Robinson, Everett Comfort, Ben Backes, Dan Steinke and Steve Olson. I must also extend thanks to Miguel Rodriguez, Tom Murray, Brian Taylor, Stephen Stewart, Steven Warfield and John Winchell of CNSE and Art Haberl and Wayne Skala of the Ion Beam Laboratory.

The bulk of my time as a grad student at CNSE has been spent as an intern in SEMATECH, and I express my thanks to the members of the Mask Cleaning Group and the Metrology Division, taking note of the assistance I received from Abbas Rastegar, Arun John, Jae Choi and Byunghoon Lee (Mask Cleaning Group) and Ben Bunday, Aaron Cordes, Hugh Porter and Abraham Arceo (Metrology). Feedback was also appreciated from SEMATECH Metrology’s Program Advisory Group (PAG).

I learned a great deal in my invaluable conversations and collaborations with András Vladár and John Villarrubia of NIST. Finally, thanks to Eric Solecky and Allan Minns of IBM for help with tool access.
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LIST OF ACRONYMS

CD               Critical Dimension
SEM              Scanning Electron Microscope
CD-SEM           Critical Dimension Scanning Electron Microscope
eV               Electron volt
keV              kilo-electron volt
LWR              Linewidth roughness
ITRS             International Technology Roadmap for Semiconductors
CTF              Contrast Transfer Function
E-T              Everhart-Thornley (Detector)
PMT              Photomultiplier Tube
NFG              Term used to describe unsatisfactory result
MCP              Microchannel Plate
TLD (TTL)        Through Lens Detector (Through The Lens detector)
SNR (S/N)        Signal to noise ratio
OTF              Optical Transfer Function
TLA              Three Letter Acronym
PSD              Power spectral density
MTF              Modulation Transfer Function
FFT              Fast Fourier Transform
PTF              Phase Transfer Function
FZP              Fresnel Zone Plate
NIL              Nano imprint lithography
SPC              Statistical Process Control
HeIM (HIM)       Helium Ion Microscope
BSI              Backscattered Ion

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LIST OF MICROSCOPES USED

Make and Model (Tool Owner)

General Imaging

- LEO 1550 (CNSE)
- Hitachi CG-4000 (CNSE)
- Carl Zeiss ORION+ Helium Ion Microscope (Carl Zeiss Microscopy)
- FEI Nova NanoSEM 600 (CNSE)
- Hitachi S9380-II (SEMATECH)

Tool Performance Measurements

- Hitachi S9830-II (SEMATECH)
- LEO 1550 (CNSE)
- Applied Materials Verity 4i (Not CNSE)
- FEI Helios (NIST)

Contact Hole Depth Measurements

- LEO 1550 (CNSE)
- Carl Zeiss ORION+ Helium Ion Microscope (Carl Zeiss Microscopy)
Chapter 1    Introduction

1.1  CD-Metrology

   Critical dimension (CD) metrology is widely used in the semiconductor industry. It is used to monitor lithographic processes as well as to evaluate new lithographic processes, by measuring features such as line widths or contact hole diameters (and comparing them to the intended values) [1]. When these measurements are taken, it is important that the measurements be highly accurate and precise (where accuracy is defined as the agreement of the measurement result with the true value and precision is the repeatability of the measuring process [2]), in order to determine that the lithographic processes are working correctly in order to create features on the computer chip that act as intended.

   The Scanning Electron Microscope (SEM) is used widely as an imaging device when the sizes of the features to be examined fall below the capabilities of the optical microscope. The SEM sweeps an electron beam back and forth across the surface of a sample. As the electron beam enters the surface, it can generate secondary and backscattered electrons. Those electrons that escape the surface can then be captured by electron detectors. The point-to-point variations in the yield of the secondary electron emissions (which are dependent on materials as well as topography) as the beam dwells on each location are used to form the image [3].

   One common CD metrology tool in use in the semiconductor industry today is the CD-SEM. The CD-SEM is a type of SEM that is customized and optimized for one purpose: Measuring features on wafers. Whereas many conventional SEMs are very versatile, capable of operating at many different conditions and are equipped with chambers that can fit many different types of samples, the CD-SEM is designed from the
ground up to make specific types of measurements on wafers. Wafers are loaded using a robot arm that removes it from the sample carrier and places it in the chamber (as opposed to samples in analytical SEMs which are manually inserted in the tool each time). Whereas many analytical SEMs can be operated across a wide range of energies (for example, 1-30 keV), the CD-SEM is optimized to run only at low voltages (500 eV – 3 keV), in order to minimize sample damage and charging effects. Specialized software allows a layout file (a map containing the locations of all of the features on the wafer) to be loaded and recipes set up so that the tool can go from point to point on the wafer and make automated measurements (such as pitch, linewidth roughness (LWR, the variation in the width of the line), etc.). In order to minimize operator variation and error, as much of the imaging and measuring process as possible is automated [4].

1.1.1 CD-Measurements with the CD-SEM

The CD-SEM is used to make many different types of measurements, including linewidth ("CD"), pitch (distance from the start of one line to the start of another), and LWR. Examples of these measurements are shown in Figure 1, Figure 2 and Figure 3. These parameters are important to monitor, as variations in the physical dimensions of certain features may result in changes to the electrical performance of the device. For example, a single line can be fabricated for use as a gate for multiple transistors on a chip [5]. The shrinking of device dimensions has led to the need for overlay and multiple exposures (double patterning), and problems with processing have been known to lead to the phenomena of “pitch walk” [6] [7]. Variations in the LWR have been shown to result in changes to the gate length for transistors, which can have effects on the threshold voltages and leakage currents of the device [5].
Figure 1: Example linewidth measurements

Top: Width measured at bottom (61.48 nm)
Bottom: Width measures at top (48.67 nm)

FOV of each image is 675 nm
**Figure 2:** Example pitch measurements

Top: Left pitch  
(107.97nm)  
Bottom: Right pitch  
(108.12nm)  

FOV of each image is 675 nm
1.2 Image Formation in the SEM

For the purposes of this work, it is helpful to discuss a few of the many processes that are a part of the process of forming an image with the SEM. Specifically, the topics of electron scattering, electron detectors, charging, and digital signal processing are addressed.

1.2.1 The Interaction Volume

As the primary electrons in the beam enter the sample, they lose energy and scatter. The amount of energy lost per unit length is the stopping power [3]. The electrons undergo both electronic stopping and nuclear stopping. During the electronic stopping phase, the electrons undergo inelastic collisions with the electrons that surround the atoms in the material, resulting in the loss of energy without major changes in its direction. During the nuclear stopping phase, the electrons will be deflected
electrostatically by the nuclei of the atoms in the material, and significant changes in
direction may occur [8]. The combination of scattering events which both change and do
not change the direction of the primary electrons results in an interaction volume which
starts out narrow and then gets wider below the surface. When the primary electron loses
energy, secondary electrons can be generated. If the SEs are generated close enough to
the surface, they may escape and be captured by the detector. This escape depth is
generally within 10 nm of the surface, although it differs based on material type. It is
important to note that this does not only refer to the top surface, but any surface,
including edges. However, even if the primary electron has scattered far from the initial
beam impact point, it can still generate SEs which will appear to be from the initial
impact point. As the size of the features being examined in CD-metrology has shrunk,
this becomes more of a problem, as illustrated in Figure 4. The interaction volume for a
SEM exposure with a beam energy of 800 eV and a beam size of 1 nm is calculated with
CASINO [9]. This result is graphically outputted, which allows it to be scaled and
overlaid over an image. The left image represents a structure which has a width of 250
nm and a depth of 250 nm. The right image represents a fin-type structure, with a top
width of 10 nm, bottom width of 15 nm and a height of 30 nm. It can be seen that while
the interaction volume only occupies a small fraction of the larger feature (left image), it
easily spreads across most of the width of the fin (right image), such that even when the
SEM beam is impinging the center of the feature, signals may be detected that were
generated near the edges.
1.2.2 Charging in the SEM

When an electron beam impacts a material, it can create SEs and BSEs, assuming that the initial energy of the primary electrons is above a minimum value. As the beam energy increases from the minimum value, more SEs and BSEs are created, up to a point where the yield curve reaches a maximum. After this point, the total yield begins to decrease, as the range of the primary electrons is increasing and therefore the signal electrons are generated at depths which are farther into the material.

When secondary and backscattered electrons are generated, this will have an effect on the charge of the specimen. If the total yield (SE yield ($\delta$) + BSE yield($\eta$)) is less than one, there will be fewer electrons that escape the sample than primary electrons which entered it. Consequently, the charge of the sample will become more negative. If

![Figure 4: Comparison of interaction volume to size of feature](image)

Both images show an interaction volume (plotted with CASINO) for an 800 eV electron beam (1nm beam size) into silicon.
Left: 250nm x 250nm feature
Right: Fin-type structure with 10nm top width, 15nm bottom width and 30nm height.
the total yield is greater than one, more electrons escape the sample as compared to the number of primary electrons which enter it, and the charge of the sample will become more positive. The ideal imaging conditions are when the total yield is approximately equal to one. In this case, this avoids some of the pitfalls associated with sample charging. For example, if the sample charges negatively, the primary electron beam can be deflected. If the sample charges positively, some SEs which initially are able to escape from the surface may be attracted back to it and therefore not be detected. As the total yield increases and decreases (as the beam energy is increased from the minimum value), it passes through unity twice. These “crossover” points are commonly denoted E₁ and E₂, and they are illustrated in Figure 5. E₁ is normally at an energy that is too low for SEM operation, and therefore the E₂ energy level (normally between 0.4 keV – 4 keV, depending on the type of material) is typically desired for imaging [3].

1.2.3 Electron Detectors

One typical electron detector is the Everhart-Thornley (ET) detector, and it is used to attract electrons and amplify the signal. This detector is shown in Figure 6. It consists of a collection grid, scintillator, light guide and a photomultiplier tube. A
positive bias is placed on the collection grid (typically around 200-300 V) in order to attract the secondary electrons. Behind the collection grid is the scintillator, which has a very large voltage (around 10 keV), in order to attract the electrons from the collector. The scintillator is able to take electrons and output corresponding photons. The photons travel down the light guide to the photomultiplier tube (PMT). The PMT multiplies the amount of photons and sends them to an amplifier, converting them back to an electronic signal [3].

Figure 6: Everhart-Thornley Electron Detector

F: Collection grid (also referred to as a Faraday cage)
S: Scintillator
LG: Light guide
PM: Photo multiplier tube
B: Backscattered electrons
SE: Secondary electrons

Figure taken directly from reference [2].

Another common detector is the microchannel plate (MCP). This has the advantage of being small in size, but has the marked disadvantage of having a finite lifetime compared to the E-T. The MCP contains a series of small holes (~6-20µm in diameter) embedded in a small glass plate. The signal gain is dependent of the ratio of the length to the diameter of the channel [4] [10].

The location of the detector plays an important role in image formation. The detector may be positioned off to the side, in order to allow large samples to be placed in the chamber (without risking them hitting the detector). Often, the detector is placed
within the final objective lens, where it is referred to as an inlens detector, or a through the lens detector (TLD or TTL), shown in Figure 7. When the sample is placed very close to the detector, the magnetic field from the final objective lens can surround the sample as well. This magnetic field helps to direct the electrons up towards the lens and can greatly increase the capture efficiency of the detector.

![Figure 7: Through the Lens Detector](image)

By placing the sample close enough to the final objective lens such that the sample is within the lens’s magnetic field, the magnetic field can greatly increase the efficiency of the collection of the electrons. Figure taken directly from reference [3].

Whereas the analytical SEM may only use a single detector to form an image, the CD-SEM uses a different detector scheme in order to capture as many of the escaping secondary electrons as possible. By positioning the detectors as close to the sample (and as close to the optic axis) as possible, the best detector efficiency can be achieved. The proximity allows the magnetic field from the lens to extend around the sample, increasing the collection efficiency [1].
1.2.4 Digital Signal Processing

No image forming device can perfectly represent an object. The impulse response of a digital signal processing system is a term that is used to describe how a signal that enters the system exits a system. Assuming that the incoming signal is a delta function, a perfect system would yield a delta function as an output. This of course is not the case in reality. What is more likely to happen is that the incoming signal (in our example, a delta function) would be smoothed and spread out by the system. In imaging, the impulse response of the system is referred to as the point spread function (PSF) [11].

The image in the SEM is formed with the convolution of the intensity distribution in the object with the spread function of the microscope, as shown in (1), where $i(x,y)$ is the intensity distribution in the object, $f(x,y)$ is the spread function of the microscope, and $i'(x,y)$ is the intensity distribution in the image [12].

$$i'(x,y) = i(x,y) \otimes f(x,y) \quad (1)$$

1.3 Modeling and Simulation Tools used for SEM Studies

When studying the processes which are involved in scanning electron microscopy, there are a number of simulation and modeling tools which can be used. Two programs that were made by a group at the National Institute for Standards and Technology (NIST) are of particular use for this work and will be explained here. These are Artimagen [13] and JMONSEL [14].

1.3.1 Artimagen

Built by Petr Cizmar at NIST, the Artimagen (Artificial Scanning-Charged-Particle-Microscope Image Generator) program takes an image (or designs one using the program’s tools) and adds a series of SEM-like effects in order to create an image that
has the appearance of a realistic SEM micrograph. The program may apply a specified PSF (including an amount of defocus and/or astigmatism), as well as noise and vibration. For structures created by the program itself, it can model the “edge-effects” that is present in SEM imaging (although it cannot do this for imported image files). An example of how an input image looks after Artimagen is used to apply a PSF with small amounts of blur and astigmatism, in addition to noise and vibration, is shown in Figure 8.

![Example of Artimagen-processed image](image)

**Figure 8:** Example of Artimagen-processed image

Left: Original input image. Right: Outputted image after defocus, astigmatism, noise and vibrations were added with Artimagen.

### 1.3.2 JMONSEL

Whereas Artimagen is primarily an image processing program which modifies images to appear as if they had been imaged in a SEM, JMONSEL (Java MONte Carlo Simulator of Secondary ELectrons) works very differently. After a user specifies the geometry and material composition of the sample, JMONSEL performs a series of finite element analysis steps and follows the primary electrons as they enter the material, lose energy, generate backscattered and secondary electrons, and scatter, until their energy
falls below a threshold level (typically ~50 eV). These processes take into account the mean free path of electrons in the material (the average distance between scattering events), the stopping power of the material, as well as how the electron trajectories are effected upon intersection with a material boundary (between two solid materials, for example, or between a solid and vacuum). JMONSEL generates SEs when an electron which is moving at a fast enough speed transfers enough energy from itself to a sample electron such that it now has the ability to move. If an electron is able to escape from the sample into the vacuum, it is assumed that it will travel in a straight line, unless an external extraction voltage is applied (which is commonly the case in many CD-SEMs and is an option in JMONSEL).

JMONSEL can also monitor charging phenomena in insulating parts of the sample. Finite element analysis periodically solves for the electrostatic potentials associated with these charges and specified boundary conditions (such as grounded wafer and externally imposed fields). Electron trajectories take the effects of the fields into account. By monitoring the electrons that exit the material and are captured, the electron yields can be found at each point and are plotted as line scans. Figure 9 shows trajectory plots for electrons incident on copper and silicon surfaces. Below the blue line is the material (above is vacuum). The black lines show electron trajectories in the surface while the red lines show trajectories of electrons which have escaped the surface boundaries.
1.4 Methods for improving performance

According to the International Technology Roadmap for Semiconductors (ITRS) 2012 Update (Metrology) [15], there are no known manufacturable solutions for achieving inline non-destructive process control for the 20nm node. Additionally, an IBM-led study [16] established that the necessary resolution of the CD-SEM should be approximately 1.5% of the minimum feature size, and that the CD-SEM resolution has not been meeting this requirement. This is illustrated graphically in Figure 10, which shows that as the industry moves to smaller nodes, the increases in CD-SEM resolution have not kept up with the necessary resolution for CD-SEM inspection.

**Figure 9:** Trajectory plots for electron beam (2 keV beam energy) impinging on edges of target materials.

Left is copper, right is silicon. Above the blue line is vacuum, below is the material. The fields of view are 150 nm x150 nm. The incoming beam is not shown. Figure taken directly from reference [88].
In order to improve the performance of the CD-SEM, it is proposed that methodologies for improved tool monitoring and diagnosis of imaging conditions be implemented. In addition to that, an alternative technology, ion microscopy, is discussed and compared to the CD-SEM. This will be discussed later, in Chapter 6.

**Figure 10:** Comparison of CD-SEM resolution with 1% of minimum design rule over time.

Figure taken directly from reference [16].

In order to improve the performance of the CD-SEM, it is proposed that methodologies for improved tool monitoring and diagnosis of imaging conditions be implemented. In addition to that, an alternative technology, ion microscopy, is discussed and compared to the CD-SEM. This will be discussed later, in Chapter 6.

**Chapter 2  Improved tool monitoring and diagnosis of tool conditions**

The need is seen to monitor the performance of the tools in order to identify aberrations in the image. Additionally, a need is seen for improved ability to match the performance of different CD-SEMs (whether they are from different manufacturers or simply different units). Current matching techniques involve a significant amount of
measurements and tool time [17]. These needs may be met with the Contrast Transfer Function (CTF), a mathematical function which can be used to quantitatively determine the performance of a CD-SEM.

Digital signal acquisition devices always have an effect on the signal that they are measuring [18] [11]. In the case of the CD-SEM, the CTF can be used in order to measure the effect that the microscope is having on the final image. Once the effect is measured, there are a number of actions that can be taken with that data. One possibility is to identify a specific part of the microscope which may be causing an image defect (for example, using the CTF in order to determine if a certain type of aberration corrector needs to be adjusted). Additionally, the CTF can be monitored over time in order to evaluate the performance of the CD-SEM over time, and the CTF could be measured on multiple tools in order to compare the performance of different CD-SEMs with each other.

2.1 Evaluating the Performance of Electron Microscopes

2.1.1 Resolution

When comparing the performance of imaging devices, such as the electron microscope, the one term that is normally used the most to describe a device is its resolution. Resolution is classically defined with the Rayleigh Criterion, stating that “Two monochromatic spectra should be regarded as resolved when the maximum of one spectrum coincides with the minimum of the other one [19].” Other definitions of the term resolution include the “minimum spacing at which two features of the specimen can be recognized as distinct and separate” [3], and the distance between adjacent detection points [20].
There are a variety of techniques used to measure the resolution of the SEM. They include the point-to-point resolution method, edge resolution method, and gap resolution method. These methods are illustrated in Figure 11 [19].

![Figure 11: Different Types of Resolution Measurements](image)
Left to Right: Gap resolution, Point-to-point resolution, and Edge resolution measurements
Figure based on reference [13].

There are problems with all of these techniques. The techniques rely on having samples that have specific features that allow the resolution measurements to be made. Additionally, they also only make use of a small amount of the pixels in the overall image. The techniques are highly dependent on the sample chosen (both on its topography as well as its material properties). Another issue is that even if two images are found to have the same resolution, it does not necessarily mean that the images are of the same quality.

In addition to resolution, other metrics used when discussing image quality include sensitivity, the signal-to-noise ratio and the information limit.
2.1.2 Sensitivity
Sensitivity is defined as the smallest change in a variable for which the instrument shows a measurable response [20]. For example, if two materials are in close physical proximity, and they have similar secondary electron yields, the sensitivity of the tool would determine if the two materials could both be identified.

2.1.3 Signal-to-noise ratio
In digital image processing, signal is defined as how one parameter is related to another parameter [11]. In the case of the CD-SEM, the signal being measured is how the electron yield varies with position. If the same area was measured multiple times and a histogram was plotted showing the signal levels measured at one specific pixel, it would be Gaussian in nature. The standard deviation of this Gaussian function is referred to as the noise. The noise is defined as “the random fluctuations which occur in the signal from a particular pixel in the image, even under conditions where the incident beam, the sample, and the recording conditions are kept constant. [21]”

Another way to find the noise of a system is to acquire an image of a highly uniform surface that has no unique features (for example, a polished silicon wafer) and find the standard deviation of the pixel intensities, as shown in Figure 12, [22].

As the noise is related to the signal, the ratio between the two is used as a metric, the signal-to-noise ratio (SNR). The Rose Criterion states that for an average user to be able to distinguish between objects in an image and the background of the image, the change in the signal should be at minimum five times greater than the noise level [3]. This is not a physical law (it is based on a study of observers), but it helps to illustrate the concept that a minimum SNR is necessary to make out detail in an image, and the higher
the SNR, the better. The sources of noise can be from many varying components, ranging from the detectors to stray electric fields interfering with the column.

Typically, images that are acquired using a faster frame time appear to have more noise than images acquired over a longer frame time. The frame time is a function of the pixels in the image and the dwell time per pixel, as shown in Table I.

![Figure 12: Signal to Noise Ratio](image)

<table>
<thead>
<tr>
<th>Signal</th>
<th>Noise</th>
</tr>
</thead>
</table>

Left: SEM image of a piece of polished Si wafer
Right: Histogram of the signal from the SEM image. Figures adapted from reference [16]

As the beam spends more time on each pixel, it collects more signal, helping to increase the SNR. The downside to this is that one has to assume the presence of mechanical vibrations, and as the beam is kept in one place, the sample is motion. This means that the signal from one pixel can actually be the average signal from multiple locations [23]. Additionally, higher dwell times may result in increased amounts of photoresist shrinkage [24] or carbon contamination and should therefore be avoided when possible.
The information limit (or cut-off frequency) corresponds to the spatial frequency where the magnitude of the signal becomes indistinguishable from the noise floor. Any features that are smaller than the corresponding feature size cannot be detected by the microscope [25].

<table>
<thead>
<tr>
<th>Field of View (pixels)</th>
<th>128 x 128</th>
<th>256 x 256</th>
<th>512 x 512</th>
<th>1024 x 1024</th>
<th>2056 x 2056</th>
</tr>
</thead>
<tbody>
<tr>
<td>Dwell time per pixel (µs)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.1</td>
<td>0.00</td>
<td>0.01</td>
<td>0.03</td>
<td>0.10</td>
<td>0.42</td>
</tr>
<tr>
<td>0.8</td>
<td>0.01</td>
<td>0.05</td>
<td>0.21</td>
<td>0.84</td>
<td>3.38</td>
</tr>
<tr>
<td>3</td>
<td>0.05</td>
<td>0.20</td>
<td>0.79</td>
<td>3.15</td>
<td>12.68</td>
</tr>
<tr>
<td>6</td>
<td>0.10</td>
<td>0.39</td>
<td>1.57</td>
<td>6.29</td>
<td>25.36</td>
</tr>
<tr>
<td>12</td>
<td>0.20</td>
<td>0.79</td>
<td>3.15</td>
<td>12.58</td>
<td>50.73</td>
</tr>
<tr>
<td>24</td>
<td>0.39</td>
<td>1.57</td>
<td>6.29</td>
<td>25.17</td>
<td>101.45</td>
</tr>
<tr>
<td>30</td>
<td>0.49</td>
<td>1.97</td>
<td>7.86</td>
<td>31.46</td>
<td>126.81</td>
</tr>
<tr>
<td>60</td>
<td>0.98</td>
<td>3.93</td>
<td>15.73</td>
<td>62.91</td>
<td>253.63</td>
</tr>
<tr>
<td>90</td>
<td>1.47</td>
<td>5.90</td>
<td>23.59</td>
<td>94.37</td>
<td>380.44</td>
</tr>
</tbody>
</table>

A minimum threshold current is necessary to produce a signal with a SNR that is statistically valid. This is shown in (2),

$$I_{th} = \frac{k}{C^2 \tau DQE} \quad (2)$$

where $I_{th}$ is the minimum threshold current (amps), $k$ is a constant determined in part by the pixel density in the image, $\tau$ is the time to record one frame and DQE is the quantum efficiency (collection efficiency) of the detector [26].
2.1.4 Contrast

Contrast is defined with (3)

\[ C = \frac{S_2 - S_1}{S_2 + S_1}, \quad S_2 > S_1 \]  \hspace{1cm} (3)

where \( C \) is contrast, and \( S_1 \) and \( S_2 \) are signals that respectively represent the lightest and darkest shades in the image [3]. An image is comprised of measurements of signal at every pixel. The variations in contrast between pixels are what consist of the information in the image.

2.1.5 Relations between Noise, Contrast and Resolution

The terms noise, contrast, and resolution all have different definitions, but they are interrelated. This is illustrated in Figure 13, which shows three sets of waveforms (in this example, the waveforms are offset sine curves). The top set is the original data, whereas the middle and bottom sets show the effects of different amounts of additive noise. A routine is used in Microsoft Excel which outputs a set of numbers with a specified mean and standard deviation. The results from this routine are multiplied by the original waveform values to create the noisy datasets. After adding noise, each curve is rescaled so its maximum value is unity. The calculated contrast between the maximum value of the curves and the location of where they intersect, using (3), will change based on the amount of noise added. The contrast for the top set of curves is calculated as \((1-.7071)/(1+.7071) = 0.171\). The contrast for the middle set of curves is calculated as \((1-.633)/(1+.633) = 0.224\), and the contrast for the bottom set of curves is calculated as \((1-.493)/(1+.493) = 0.339\). The results of these calculations show that the noise and contrast values of a system are interrelated. Additionally, even though the contrast of the
system is increasing along with noise, one cannot necessarily state that the increased contrast is helpful in observing the system.

Figure 14 shows how adding even more noise to the original waveforms shown in Figure 13 make it difficult to find the resolution of the system, based on the definition from [3], as it cannot be easily determined where the “two features of the specimen can be recognized as distinct and separate.” This shows the relationship between the noise and resolution terms, as when the noise is increased, it may be difficult to obtain an accurate measurement of the resolution of the system.
Figure 13: Examining the effects of noise on the contrast and resolution
2.1.6 Contrast Transfer Function

There is another method of evaluating the performance of the SEM that conveys more information than just a simple resolution or SNR term. This method incorporates the information limit and also makes use of every pixel in the image. This is the Contrast Transfer Function.

Figure 14: The original reference waveforms shown in the top plot from Figure 13 is reproduced. In the bottom plot, a large amount of noise has been added. With this much noise, it is difficult to assess the resolution of the system, using the definition from reference [3], as it cannot be easily determined where the “two features of the specimen can be recognized as distinct and separate.”
Chapter 3  The Contrast Transfer Function

The Contrast Transfer Function (CTF) is a mathematical function that shows how spatial frequencies present in the object are transferred by the microscope to the image. Rather than just examining one number that hopefully corresponds to the information limit of the tool, the analyst can see how faithfully every spatial frequency is represented in the final image. Two definitions of resolution are used when evaluating the CTF. One definition of resolution is where the scaled transfer function falls to 10% of its maximum value. Another definition is the feature size where the transfer function falls into the noise floor (Information Limit may be a more appropriate term in this case). The reasoning behind this definition is that the transfer function shows how all spatial frequencies are transferred from the object to the image, not just one frequency that corresponds to a resolution (10% of max) term. In Figure 15, two example curves are shown. The dashed line shows the transfer function for an optical system where the lowest spatial frequencies are transferred quite well, and then the performance drops off quickly towards zero at higher spatial frequencies. The solid line shows the transfer function for an optical system that does not transfer the lower spatial frequencies as well as the dashed line, but it transfers the higher spatial frequencies much better. Both of the imaging systems represented might be advantageous for different applications, even though they have the same resolution value.
In order to derive the CTF, it is necessary to introduce the Fourier transform, which transforms a function of time or distance to that of frequency. The Fourier transform $F(s)$ of the function $f(x)$ and its inverse transform are shown in (4) and (5). Commonly, the function of time or distance is represented with a lowercase designation $f(x)$ and the function of frequency is represented with an uppercase designation $F(s)$.

$$F(s) = \int_{-\infty}^{\infty} f(x)e^{-i2\pi xs}dx$$  \hspace{1cm} (4)$$

$$f(x) = \int_{-\infty}^{\infty} F(s)e^{i2\pi xs}ds$$  \hspace{1cm} (5)$$

Figure 15: Example Transfer Functions
Two arbitrary example transfer functions. They represent imaging systems with the same resolution value, but different performances. Figure adapted from reference [13]. The imaging device corresponding with the dashed line has superior information transfer at the lower spatial frequencies, but the imaging device corresponding with the solid line has superior information transfer at the higher spatial frequencies, after the dashed curve has already gone to zero.

3.1 Derivation of CTF
In order to derive the CTF, it is necessary to introduce the Fourier transform, which transforms a function of time or distance to that of frequency [27]. The Fourier transform $F(s)$ of the function $f(x)$ and its inverse transform are shown in (4) and (5). Commonly, the function of time or distance is represented with a lowercase designation $f(x)$ and the function of frequency is represented with an uppercase designation $F(s)$. 

$$F(s) = \int_{-\infty}^{\infty} f(x)e^{-i2\pi xs}dx$$  \hspace{1cm} (4)$$

$$f(x) = \int_{-\infty}^{\infty} F(s)e^{i2\pi xs}ds$$  \hspace{1cm} (5)$$
Section 1.2.4 discussed that the image was formed by taking the convolution of the intensity distribution of the object with the spread function of the microscope, and that equation is reproduced here.

\[ i'(x,y) = i(x,y) \otimes f(x,y) \quad (1) \]

According to the convolution theorem [27], the transform of a convolution is the product of the transforms, as shown in (6).

\[ I'(s) = I(s)F(s) \quad (6) \]

The Fourier transforms of the spread function \( f(x,y) \), object \( i(x,y) \) and image \( i'(x,y) \) are noted here as \( F(s) \), \( I(s) \) and \( I'(s) \), where \((x,y)\) represent position and \((s)\) represents spatial frequency. The Fourier transform of the spread function is defined as the Optical Transfer Function (OTF), as shown in (7).

\[ I'(s) = I(s)OTF(s) \quad (7) \]

The OTF can be seen as the ratio between the Fourier transfers of the image and the object. The OTF consists of two components, the magnitude and the phase. The amplitude is represented by the Contrast Transfer Function (CTF), and the phase is represented by the Phase Transfer Function (PTF), as shown in (8).

\[ OTF(s) = CTF(s)e^{i\cdot PTF(s)} \quad (8) \]

The specific form of the OTF used in this type of work is not necessarily found by the Fourier transform of the PSF. It may be found by taking the Power Spectral Density (PSD), or the square of the magnitude of the FFT term. The CTF is the response of an imaging system to a square wave pattern [28]. Additionally, as the detectors on a SEM do not capture the phase of the electrons, the PTF term is not relevant (this is a stark contrast to the transmission electron microscope, where the phase of the electrons is incredibly
important). As the PSD involves taking the complex conjugate of the term, the exponential PTF term drops out, as shown in (8). This derivation includes common mathematical steps such as $e^{a+bi} = e^a(cos(b) + isin(b))$, $(\sin^2(x) + \cos^2(x) = 1)$ and $\exp(0) = 1$.

$$PSD = CTF(s)e^{i\cdot PTF(s)}CTF(s)e^{-i\cdot PTF(s)}$$ \hfill (9)a

$$PSD = |CTF(s)|^2e^0(\cos PTF + i \sin PTF)e^0(\cos PTF - i \sin PTF)$$ \hfill b

$$PSD = |CTF(s)|^2e^0e^0(\cos^2 PTF + \sin^2 PTF)$$ \hfill c

$$PSD = |CTF(s)|^2$$ \hfill d

Ideally, the microscope would fully transfer all of the spatial frequencies in the object to the image, and the corresponding CTF would be equal to unity at all spatial frequencies. However, that is not possible for a variety of factors. Even if every possible aberration was corrected, there is still diffraction in the electron beam. This diffraction causes the probe size to increase, and it makes it more difficult to transfer information from the higher spatial frequencies.

The diffraction limited case is derived in references [19] and [29], and is shown in (10).

$$CTF(s) = \frac{2}{\pi} \left\{ \cos^{-1}\left(\frac{s}{2}\right) - \frac{s}{2} \left[1 - \left(\frac{s}{2}\right)^2\right]^{1/2} \right\}$$ \hfill (10)

In addition to diffraction, there are many other contributions that contribute to poor information transfer, including defocusing, astigmatism, tool vibration, electromagnetic interference in the column, chromatic and spherical aberration. Figure 16 illustrates the case of unity, the diffraction limited case, as well a real CTF measured on a SEM.
3.2 Noise and Image Formation

Equation (1) showed how the image is formed by the convolution of the object information with the PSF.

\[ i'(x, y) = i(x, y) \otimes f(x, y) \quad (1) \]

This is an approximation, which neglects the contributions of noise. The contribution of noise can be seen with Equation (11) [30].

\[ i'(x, y) = i(x, y) \otimes f(x, y) + n \quad (11) \]

This equation shows that in addition to the convolution of the object information with the PSF, the presence of noise still adds to the image. There can be many sources of noise, including the electron gun and the tool electronics.


3.3 Terminology

A transfer function is typically defined as the ratio between an output and an input. The ideal OTF is the ratio between the respective Fourier transforms of the image and the object, and the CTF separates the amplitude of the OTF from the phase information. Because the analysis done in this work does not take the effect of the noise into account, the function used cannot be stated to be the true CTF. It may be more properly referred to as an approximation of the CTF, or as an “experimental CTF”. Additionally, many sources in the literature make use of different terms to describe this function. Yashuck et. al. uses the term Modulation Transfer Function when they use the PSD of an image of a pseudorandom dot array to measure the performance of an SEM [31]. Moody et. al. simply referred to the “1D Power Spectral Density Estimation” [32]. Some work by Joy refers to the same analytic function as the experimental transfer function, Optical Transfer Function, and the Contrast Transfer Function [26] [33]. Due to the confusion as to the correct term to use in the community, as well as the fact that the work done here does not factor in noise (using (1) instead of (11), it is necessary to explicitly state the use of the term “Contrast Transfer Function” in this work is actually referring to an approximation of the CTF, not the true CTF.

3.4 CTF Examples

Although the process of acquiring a SEM image is a real-space process, with the microscope constructing an image based on the detected electron yields as the beam dwells across various pixels in the image, the SEM can also be modeled as a Fourier filter [34], with information present at different spatial frequencies passed by the SEM from the object to the image in accordance with the capabilities of the filter. As shown in Figure 17 (in which 1-D line profiles are used for ease of illustration), the process can be
modeled as imaging system first taking a Fourier transform of the object and multiplying that result by its CTF. The product is then back transformed from Fourier space to form the image [12].

Another example that can serve to illustrate the concept of the CTF is the square wave. The square wave can be calculated by taking a summation of the odd terms of the infinite series shown in (12).

\[
 f(x) = 0.5 + \sum_{n=1}^{\infty} \frac{\sin\left(\frac{\pi n}{2}\right)}{\pi n} \cos(2\pi xn) 
\]  

(12)

When the function is approximated by summing from n=0 to n=19, the square wave can be seen, as shown in Figure 18. This can only be achieved by summing the
terms with equal weighting, i.e. all the spatial frequencies are passed equally from the object to the image. When the frequencies are not passed equally, the summation changes, as shown in Figure 19.

**Figure 18:** Approximation of a square wave by summing of \( f(x) \), \( n=0 \) to \( n=13 \), with all components weighted equally.

**Figure 19:** Effect of weighting the different series of the Fourier expansion differently

Solid series: Approximation of a square wave by summing of \( f(x) \), \( n=0 \) to \( n=13 \), with all components weighted equally.
Dashed series: Approximation of a square wave by summing of \( f(x) \), \( n=0 \) to \( n=13 \), with higher spatial frequency components receiving less of a weighting than lower spatial frequency components.
For the series with different weightings, many measurements would not yield an accurate result. Taking the series where all the terms are added equally to be our “object,” and the series where many of the terms are weighted differently to be our “image,” the CTF for this system is calculated and shown in Figure 20. As the system moves to higher spatial frequencies, the magnitude of the CTF decreases.

In order to illustrate for the reader how different CTFs can produce different images, an example is produced below. For the object, a 1024 x 1024 pixel slice of Van Gogh’s *Starry Night* is used, and it is subjected to two different arbitrary CTFs, as shown in Figure 21. In Figure 22, the images that are produced with the two example CTFs are shown, and it can be seen that they are not perfect representations of the object. By subtracting the image from the object, the information that has been lost in our example imaging process can be seen.

**Figure 20:** Transfer function, with the unequal weighting summation as the image and the equal weighting summation as the object.
Figure 22: Comparing how the image is effected by two different CTFs
Top: Images that are produced by multiplying the Fourier transform of the object with the CTFs
Bottom: Image formed by subtracting the image from the object. This shows what information is not present in the image which was present in the object.
It has been shown how imaging tools with different CTFs can produce different images. It can also be shown that imaging tools with different CTFs can produce different measurements of the same features. An image of silicon lines is modified to produce two new images with the CTFs shown in Figure 23. The original image and the modified images are shown in Figure 25, and the corresponding linewidth measurements from the images are shown in Table II, where it can be clearly seen that differences in the CTF can have an effect on the CD-measurements. The images are modified by taking their Fourier transforms, multiplying them by the example CTFs, followed by taking an inverse Fourier transform of the product. The CD-measurements are done using an offline measurement routine provided by the manufacturer of the tool. While the specifics of the algorithm may be proprietary, it can be assumed that the process is similar to the following method. For a specific number of locations defined by the user across the line, a profile is analyzed. The minimum and maximum intensities of the edges are found, and the algorithm places the edge of the line at a magnitude of the step determined by the user. For example, if the user sets a threshold of 75%, the edge location is determined to be at the coordinate which corresponds with the intensity value of 75% of the maximum. This is shown in Figure 24.
Figure 23: Example CTFs used to modify images of silicon lines.

Figure 24: Illustration of linewidth measuring procedure. The line profile is measured, and the maximum and minimum points are found (the minimum is labeled as 0% in this figure). A threshold is chosen by the operator (here, 75% of the maximum). The software identifies the location where the value of the line profile is equal to the threshold and declares that location to be the edge location.
Table II: Comparison of Linewidth Measurements with Different CTFs

<table>
<thead>
<tr>
<th>Image</th>
<th>Linewidth</th>
<th>Percent Change from Original</th>
</tr>
</thead>
<tbody>
<tr>
<td>Original</td>
<td>228.7 nm</td>
<td></td>
</tr>
<tr>
<td>CTF 1</td>
<td>229.5 nm</td>
<td>0.35%</td>
</tr>
<tr>
<td>CTF 2</td>
<td>230.7 nm</td>
<td>0.87%</td>
</tr>
</tbody>
</table>

Figure 25: CD-SEM images of silicon lines modified by example CTFs

- Top left: Original image
- Top right: Result after original is modified by CTF 1
- Bottom: Result after original is modified by CTF 2
3.5 Software Solution for Finding the Contrast Transfer Function

Before commencing with Fourier analysis of an image, it can be helpful to perform a “windowing” procedure. This is done to eliminate artifacts that will manifest in the frequency domain which are due in part to the fact that the image is not periodic [35] [36] [11]. Because the image is not periodic, an abrupt step is introduced which requires many high frequencies to model [37]. These high frequencies manifest as the horizontal and vertical lines seen in the FFT of a non-windowed image, as shown in Figure 27.

The specific window used in this work is pictured in Figure 26, and is represented in (13).

![Figure 26: Example of window function that is used to modify images prior to Fourier analysis.](image)

The intensity of the window \( w \) is calculated at points \((u,v)\). The variable \( M \) represents the number of pixels in each dimension of the image (assumed to be a square for these purposes).

\[
w(u, v) = \cos \left( \frac{\pi}{2} \left[ \frac{2u}{M} - 1 \right] \right) \cdot \cos \left( \frac{\pi}{2} \left[ \frac{2v}{M} - 1 \right] \right)
\]

(13)
In order to generate the CTF, a software package called SMART-J is used [38]. SMART-J is a plugin that works with the image analysis program ImageJ [39]. SMART-J creates a region of interest (for example, 512x512 pixels) and takes uses a FFT algorithm to calculate the Fourier transform of the image. A radial intensity profile is
then taken, which measures half of the region of interest (in this case, 256 pixels), and rescaled so that the spatial frequency range goes from the minimum frequency of $\frac{1}{2}$ up to twice the maximum number of pixels (in this case, 512). The radial integration is done in order to increase the SNR, and for these purposes it is assumed that the PSF and the corresponding CTF are radially symmetric. For display purposes, the magnitude of the data may be rescaled to vary between 0 and 1, and the spatial frequency is inverted in order to give the corresponding feature size, so a “resolution” term can be easily seen from the graph. However, for some applications, rescaling the dataset is not necessary and can even be harmful to the data analysis, in which case the raw (unscaled) magnitudes are used. For higher spatial frequencies (smaller feature size numbers), the plot may level off. At this point, the information limit has been reached, as the noise is greater than the data.

A MATLAB routine was written which mimics the output of the SMART plugin from ImageJ. This was done for speed (the MATLAB routine loads and completes faster than SMART) as well as for ease of modifying the program. Some changes were made to the routine that differ from SMART’s operation, but the overall principles remain the same. A five pixel moving average is used to smooth the plots. The code used is shown in the Appendix (Chapter 9).

When the FFT of an image is found, the information present spans many orders of magnitude. Any attempt to display this graphically will result in an image that is mostly black with some bright pixels in the center. For purposes of visualization, whenever FFTs are shown in this work, the log of the image is shown.
3.6 Interpreting the Contrast Transfer Function

Figure 28 shows an example set of CTFs. The vertical axis shows the magnitudes of the CTF. The horizontal axis shows the feature size. This is the inverse of the spatial frequency, which allows the use of length units instead of frequency units, for the purpose of making it easier to quickly analyze the performance of the microscope.

Initially, the transfer functions start at high values, and then they begin to decline. This corresponds with the fact that at higher spatial frequencies, less of the information is fully transferred from the object to the image. At one point, the magnitudes of the functions may stop decreasing and level off. At this point, the noise is overcoming the actual signal, and the information limit has been reached.

In Figure 28, datasets two and three level off. These represent the noise levels. Two things to take into consideration are the point where they hit the noise floor, and the magnitude of the noise. Dataset 3 reaches the noise floor at a larger feature size than dataset 2. In addition, dataset 2 represents an image with more noise than dataset 3, as its noise floor is at a higher magnitude than the other.

If one wishes to use resolution (with the definition of the feature size where the magnitude has fallen to 10% of the maximum value) to compare these features, it would yield erroneous results. In the case of the datasets in Figure 28, the 10% resolution value for dataset 2 is in the noise floor, while dataset 3 does not even fall to 10%. This illustrates why it is important to specify what metric is being used to compare images (information limit vs. 10% resolution value), and more importantly, why the CTF can show more detail than a simple resolution number.
In addition to simply plotting multiple CTFs on the same graph, there are other ways of comparing them which can make it easier to see the differences between two conditions. If one CTF is plotted on the x-axis and another on the y-axis, one can compare the slope (which would be a slope of one if the functions were exactly equal). The difference in the CTFs can be plotted as a function of spatial frequency in order to identify where the functions are similar and where they diverge. These are shown in Figure 29.

**Figure 28**: Example datasets to illustrate how to interpret plots of the Contrast Transfer Function. The portions of the curves which are flat at the higher spatial frequencies (smaller feature sizes) represent the noise floor.

In addition to simply plotting multiple CTFs on the same graph, there are other ways of comparing them which can make it easier to see the differences between two conditions. If one CTF is plotted on the x-axis and another on the y-axis, one can compare the slope (which would be a slope of one if the functions were exactly equal). The difference in the CTFs can be plotted as a function of spatial frequency in order to identify where the functions are similar and where they diverge. These are shown in Figure 29.
3.7 Test Structures for Finding the Contrast Transfer Function

Ideally, all spatial frequencies represented in the object would be fully transferred to the image by the SEM. The use of this technique requires specific test samples which contain uniform information across the frequency range, in order to measure the performance of the tool at all spatial frequencies. Therefore, when a Fourier transform is taken of images of the test samples, the frequencies present should only reflect information from the microscope itself, not from the samples. Some samples which meet

---

**Figure 29: Other ways to compare CTF Datasets**

Top: Plot of CTF A on x-axis and CTF B on y-axis. Solid line is 1:1 trend line for reference. Bottom: Plot of the difference between the CTFs for comparison purposes
this criterion include Fresnel Zone Plates (FZPs), as well as samples that have random feature sizes and placement, such as pseudorandom dot arrays, or sputtered materials.

3.7.1 Ideal Test Structures

The ideal random dot array would result in every pixel in the image having a different value. Such a sample would result in a mostly flat transfer function, as illustrated in Figure 36. This holds true if the arrangement of the dots is random, or if the arrangement is fixed and the intensity of the dots is random, as shown in Figure 30.

![Figure 30: Comparison of two ideal random dot arrays.](image)

In the top left array, every pixel has a random value. In the top right array, the layout of the pixels is random (with each occupied location having the same intensity). The corresponding CTFs of the profiles show that both are flat across the spatial frequency range. The random dot arrays used for the CTF calculation were 1024x1024 pixels, although the figures shown here are 64x64 pixels, with the smaller sizes picked for display purposes.
The basis behind this behavior is that if every pixel is different, there is no periodicity found with any structures in the random dot array, and therefore, in the Fourier spectrum, no individual spatial frequency should be present more than any other. The ideal random dot array (with every pixel being having a different value) shown in Figure 36 was constructed with a MATLAB routine based on an algorithm found in [40] and [41].

In order to verify this, a random dot array was constructed (with the location of the dots, not the intensity as the random variable), and the spacings between all of the dots were found. The number of times a particular spacing occurred was plotted as a function of the distance between the points. This plot was normalized by the distance between the points as well to account for the fact that as the spacings get larger, the dots will be spread out along a greater radius. This function shows the probability of finding a given spacing per unit area. The random dot array and the plot are shown in Figure 31. The plot is mostly flat, showing all spacings are equally present. The plot falls in magnitude towards the higher numbers of spacings. The largest distance spacings are not present in the same amounts as the lowest distance spacings, due to the fact that the sample size is finite, and dots in the center of the array do not have specific neighbors at the largest spacings as compared to dots at the edge, which can have specific neighbors at much farther distances.
A Fresnel Zone Plate is shown in Figure 32. Fresnel Zone Plates have been used previously by research groups for CTF studies due to their “wide and flat Fourier spectrum” [34] [42]. The design rule for the FZP is that every ring (and the space between every ring) must have the same area. This should result in a flat Fourier spectrum, where every spatial frequency contributes equally.

**Figure 31:** Examining the number of times that different spacings occur between all dots in the random dot array.

Left: Random dot array. Right: Plot of the number of times that the spacings occur. This plot is a probability distribution of finding a neighboring dot at any position, and may be interpreted as a histogram with a bin size of 1 pixel.

**Figure 32:** Example of a Fresnel Zone Plate
To illustrate this, a 1D example is used. This is shown in Figure 33, where the magnitude is plotted as a function of distance from the origin \( r \). If the FZP is plotted as a function of radial distance from the origin \( r^2 \), \( f(r^2) \) becomes a function consisting of periodic rectangles, as shown in Figure 34, also referred to as a rectangle function.

![Figure 33: One dimensional profile of the FZP, plotted as distance from the origin.](image1)

![Figure 34: One dimensional profile of the FZP, plotted as radial distance from the origin.](image2)

The Fourier transform of a rectangle function is a sinc function, where \( \text{sinc}(x) = \frac{\sin(x)}{x} \), except where \( x = 0 \), in which case \( \text{sinc}(0) = 1 \). The Fourier transform of the rectangle function (shown in Figure 34) is shown in Figure 35. This plot shows a mostly flat Fourier transform in the low spatial frequency range, and the magnitude tails off into the higher spatial frequencies, where it might be expected that the Fourier transform would have a zero value. This is due to the fact that high spatial frequency components are necessary to represent the rectangles in the frequency domain.

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The CTFs for an ideal random dot array and FZP are shown in Figure 36. As expected from the plots shown in Figure 30 and Figure 36, the CTF for the ideal random dot array is mostly flat across the entire spatial frequency range, but the CTF for the ideal FZP tails off at high frequencies. As the tail off is likely due to the need for high frequencies to represent the sharp rectangles, this may not be present in the FZPs of fabricated structures which will likely have rounded edges.
Figure 36: Ideal samples for CTF Measurement and their corresponding plots
Top Left: Random dot array, generated using MATLAB code. A random number algorithm is used to decide if a location is “occupied” by a dot (has a value of 0 or 1).
Top Right: Fresnel Zone Plate (FZP). The area of each ring (and the space between each ring) is identical.
Bottom: Transfer functions for the random dot array and the FZP
3.7.2 Fabrication of Test Structures

For this work, the test structures were constructed with nanoimprint lithography (NIL) on 300mm silicon wafers, using the Imprio 300 tool (Molecular Imprints, Incorporated). NIL uses a rigid “stamp” to create a pattern in a soft photoresist material that has been deposited on to a silicon wafer. This technique has been shown to create features as small as 5 nm [43], although the capabilities of the unit used for this work were closer to 20nm. Two sets of FZPs were printed. One set had an outer ring width of 25nm, and the other had a width of 22nm. Several sets of random dots were printed, including isolated dots with diameters of 30nm and 22nm. Another set of dots was printed which also used 22nm diameters, but the dots were placed very close together, resulting in overlap of many of the dots.

In order to fabricate these structures, an initial resist layer is spun onto the silicon wafer. The exact resist used is proprietary, but it is known that it contains some combination of an acrylic ester, acrylate, as well as a crosslinking agent and a photoinitiator. Next, the imprint template is pressed directly into the resist layer, transferring the pattern. The template does not press all the way through the resist, leaving a resist layer below the pattern. This layer serves to promote adhesion between the patterned resist and the substrate below. As it is in contact with the resist, there is a brief UV curing step. This is followed by the etching step which transfers the pattern to the wafer. The process flow is diagrammed in Figure 37.
Figure 37: Process flow of the sample fabrication.

Top: Resist layer is spun onto wafer.
Middle: After imprint template is applied, the pattern is transferred, leaving an untouched layer of photoresist to promote adhesion.
Bottom: After etching, pattern is transferred to the silicon.
The dashed line represents the original location of the photoresist/silicon interface.
Initial results of the photoresist patterns for the FZPs are shown in Figure 38, and of the pseudorandom dots in Figure 39. These images were acquired with a Hitachi S9380-II CD-SEM.

![Figure 38: Fresnel Zone Plates fabricated with Nanoimprint lithography (photoresist)
Left: Fresnel Zone Plate with smallest ring intended to be 22nm wide. This did not print successfully. Field of view is 1.125 µm
Right: Fresnel Zone Plate with smallest ring intended to be 25nm wide. The outermost ring, which should be the narrowest, appears to be larger than the ring it surrounds. Field of view is 900nm](image)

There are problems with how the Fresnel Zone Plate structures printed, which can lead to a serious issue when using them for CTF measurements. The basis behind the use of the FZP structure assumes that every ring prints correctly. If one ring does not print correctly, the design rule which mandates that every ring have the same area is violated. Additionally, the large number of edges in the feature (due to the number of separate rings as opposed to a single planar surface) result in the prevalence of edge-effects that were discussed in Section 1.2.1, which also act to disrupt the periodicity of the FZP.
With regards to the dot arrays, the photoresist patterns printed as designed. However, the isolated 30nm and 22nm dots did not survive the etching process. The 22nm dots with overlap were printed successfully, as shown in Figure 40. This is likely due to the fact that the larger features which were created in the locations where the dots overlapped acted to shield the smaller dots from the etch gases during the reactive ion etching step. This image was acquired with a Hitachi CG-4000 CD-SEM.

**Figure 39: Pseudorandom dot arrays fabricated with Nanoimprint lithography (photoresist)**
Left: Random dot array, 30 nm diameters  Middle: Random dot array, 22nm diameters. Right: Random dot array, 22nm diameters, with overlap. All images captured with a field of view of 675nm.

**Figure 40: Etched Random Dot Array**
Etched random dot array. The field of view is 1.350 µm
When examining the transfer function of this pattern, it can be seen that it is not nearly as flat as the transfer function from the ideal random dot array, as shown in Figure 41.

In order to obtain a relevant measure of the performance of the SEM, it is necessary to measure the test pattern at the same imaging conditions that the tool would be using to take its measurements (for example, fields of view between 500nm up to 2 microns, with a nm/pixel ratio approaching 1). Taking these magnifications into account, and combining this with the fact that the smallest feature that could be created in the photoresist was 22nm (although after etching, the smallest dots appeared to be closer to 14nm), it is not possible to take an image of an ideal random dot array using the samples fabricated for this work. If an image of the etched silicon random dot array was acquired at a low magnification, it would approach the level of randomness needed, but it would only measure how the microscope is performing at that low level of magnification, which is information of limited usefulness.
3.7.3 Comparing CTFs for dots with different pixel sizes

As it has been seen that the pseudorandom dot arrays that can be produced for this work do not have anywhere near the ideal CTF profile, it is helpful to explore how structures that contain dots which are inevitably larger than a single pixel can be used for these applications, including the examination of how they would respond to similar image defects (e.g. similar amounts of defocus). Using Cizmar’s Artimagen program [13], it is possible to create artificial images of circular features with specified pixel sizes and pixel densities. Images were generated with tightly packed small dots (varying in size between 2-3 pixels) and large dots (varying in size between 10 and 30 pixels), and the images were compared to the ideal random dot image, as shown in Figure 42.
Figure 42: Artificially generated random dot arrays and their CTFs

Top row: Random dot arrays with dot sizes of 2-3 pixels (left) and 10-30 pixels (right)
Bottom row: CTF curves comparing the ideal random dot array with the random dot arrays in the top row.
It can be seen that neither of the simulated dot images have nearly as flat a CTF as the ideal random image, although the CTF profile from the image with 2-3 pixel-sized dots does have a flat region for a large spatial frequency range. Given that a lack of periodicity in the arrangement of the features results in a flat CTF profile (as no singular spatial frequency is present more than any other), the fact that the CTF profiles are not uniform over the entire spatial frequency range suggests that there is periodicity present in their arrangements.

It is helpful to consider how the profiles will be changed when the images are subjected to a two pixel blur. This is illustrated in Figure 43. In all of the images, the change in the CTF can be plainly seen, and the CTF profile from the blurred image falls below that of the original around the spatial frequency corresponding with 35 inverse pixels.
Figure 43: Comparing the effect of a two-pixel blur on the CTFs of various test images.

Top row (L-R): Original images (Ideal random distribution, 2-3 pixel sized dots, 10-30 pixel sized dots)

Middle row: Images subjected to a two pixel blur

Bottom row: CTF curves comparing the original and blurred images. The original dataset is the thin black line, and the blurred dataset is the thicker red line.
3.7.4 Evaluating the Fabricated Random Dot Samples

The goal of the random dot array was to create a structure with as little periodicity in the arrangement of the dots as possible, leading to a nearly flat CTF profile. As has been shown, this type of structure was not able to be fabricated for this work. It is necessary to confirm that the structures still have some degree of randomness, so that acquiring images of the dots from different locations within the array would not result in measurements of different CTF values. To this end, several images were acquired of the random dots from five different locations, each with the same imaging conditions, as shown in Figure 44. As shown in the plot, the measured CTFs from each location are very similar. Therefore, it is determined that the different structures in each image are not resulting in different measurements and the samples are appropriate for use.
Comparing CTFs for images of dots in different locations within the random dot array

![Graph showing Contrast Transfer Function Magnitude vs Feature Size (nm)](image)

**Figure 44:** Examining the “randomness” of the random dot array

Top row: Images of random dot array, acquired with a FOV of 675nm. Each image was acquired with the same imaging conditions.
Bottom: Comparing the CTFs from images of random dots measured at five different locations.

### 3.7.5 Comparing CTFs for FZPs with Different Amounts of Rings

When using the FZPs, a characteristic which should be specified is the minimum number of rings needed in the FZP in order for it to be suitable for use as a test sample.

For this purpose, FZPs were created using Adobe Illustrator with different amounts of rings. Two test FZP samples are shown along with their respective CTFs in Figure 45. The respective plots from both FZPs do have distinctive flat regions in their CTFs,
however, while the FZP with 50 rings has a singular flat region, the FZP was 12 rings has two. This seems to imply that 12 rings is below the minimum design rule needed for use of the FZP pattern for this study. When fewer rings are present, the rings which are present are thicker, and therefore there may not be enough higher spatial frequency components to result in a flat CTF profile. This is problematic due to the difficulty of producing the necessary amount of rings at the dimensions needed in order to acquire an image of the FZP at conditions that are similar to those commonly used by the CD-SEM. For a 50 ring FZP, the outermost rings are between 2-5 pixels (depending if the image is 512x512 or 2048x2048 pixels in size).
In Figure 46, the CTF if a CD-SEM image of an FZP is compared with that of an ideal FZP. This images was acquired with a Hitachi S9380-II CD-SEM. While it is clear that the fabricated sample does not have as many rings as the ideal sample, there is still a flat portion of the visible, indicating that the sample may be able to be used for the experiments. Even if there was no flat portion, as long as the sample is thoroughly characterized, it may be used, as the goal of the experiments is to look at changes in the profile.
Chapter 4  Using the Contrast Transfer Function to Evaluate CD-SEM Performance - Image Defect Detection

In order to test the feasibility for using this technique to identify when the CD-SEM was not operating at optimal performance, images were acquired of the test samples while modulating different parameters, including defocus, astigmatism and aperture alignment. As CD-SEMs are designed for automated operation with only a specific type of sample, the tools are not designed for the operator to make adjustments (as is the case with most analytical SEMs). Consequently, instead of specifying a working distance in units of length, the focus is controlled by adjusting the volts applied to a lens. Similarly, the astigmatism and aperture alignment are modulated in units of mA. The CD-SEMs (Applied Materials Verity 4i) were used at a facility belonging to an individual member company of SEMATECH.

Figure 46: Comparison of ideal FZP from Figure 36 to image of FZP from a CD-SEM.
The actual size of the SEM image is not of interest here, only the trend of its CTF
4.1 Focus Modulation

Figure 47 shows CTF profiles for a defocus series. An image of the FZPs was acquired with the autofocus condition, and then images were taken with defocuses of one, two and three volts. It can be seen that as the defocus is increased, the trend of the CTF curve is to drop in magnitude and move towards the lower spatial frequency range.

Figure 47: Effects of focus modulation on the tool performance.
4.2 Effect of Astigmatism on the CTF

The primary beam has a Gaussian profile, and it can be approximated with a two-dimensional Gaussian function, as shown in (14), (15), (16) below.

\[
f(x, y) = \frac{1}{2\pi \sigma_x \sigma_y} \exp \left( -\frac{1}{2} \left( \frac{x'^2}{\sigma_x^2} + \frac{y'^2}{\sigma_y^2} \right) \right) \tag{14}
\]

\[
x' = s(x \cos(\varphi_s) + y \sin(\varphi_s)) \tag{15}
\]

\[
y' = \frac{1}{s}(-x \sin(\varphi_s) + y \cos(\varphi_s)) \tag{16}
\]

where \( f \) is the profile, \( s \) is the coefficient of astigmatism, and \( \varphi_s \) is the direction of the astigmatism [13]. The effect of astigmatism is to skew the image, stretching it in one direction at the expense of the other (instead of the beam converging to a circle, it converges to an oval, as seen in Figure 48).

**Figure 48:** Effect of astigmatism on electron beam

<table>
<thead>
<tr>
<th>Left</th>
<th>Middle</th>
<th>Right</th>
</tr>
</thead>
<tbody>
<tr>
<td>Highly stigmated beam in one direction.</td>
<td>Highly stigmated beam in other direction.</td>
<td>Beam corrected for astigmatism. [2]</td>
</tr>
</tbody>
</table>

Astigmatism in the SEM can occur as the result of asymmetries in the lens. The asymmetries can be caused by things like machining errors (whether in the factory, or machining caused by careless operators ramming their samples into the pole piece) or dirty apertures.
In contrast to defocus, the effect of astigmatism on the PSF (and therefore, the CTF) is a non-symmetric one. Therefore, integration over 360° is not appropriate in this case. The procedure must therefore include both a step which finds the direction of the astigmatism and its magnitude. Shown in Figure 49 are examples of images with different astigmatism ratios (x'/y') as well as different directions of astigmatism $\varphi_s$. The images were created with Artimagen.

![FFT examples with different astigmatism ratios and directions](image)

**Figure 49:** FFTs from images with different astigmatism ratios and directions.  
Top, Left to Right: Ratio 1.5, 45°, Ratio 1.5, 90°, Ratio 2.0, 45°.  
Bottom, Left to Right: Ratio 2.0, 90°, Ratio 5.0, 60°, Ratio 5.0, 130°.

As the 360° integration was done to improve the SNR of the CTF, it must be determined what sized integration is necessary in this case. If the integration is too large, different regimes could be averaged together, producing incorrect data. There should be some integration, however, in order to increase the SNR. Images in Figure 50 graphically show a few different sized angular integrations. It is seen that integrations of
$5^\circ$ and $10^\circ$ fall within the major axis of the stigmated region, but for a $50^\circ$ integration, more is incorporated when the shape has changed. It can be seen in Figure 49 that for smaller astigmatism ratios, wider integrations can be used. When comparing the integrated radial profiles in the CTF plot in Figure 50, one can see that the plots for the $5^\circ$ and $10^\circ$ integrations follow the same overall path, but there is divergence for the $50^\circ$ integration, as it has incorporated regions that are not part of the desired region of interest.

**Figure 50:** Different Integration Angles for CTF Calculations  
Top Row - Left: $5^\circ$ Integration.  Middle: $10^\circ$ Integration.  Right: $50^\circ$ Integration  
Bottom: CTFs calculated from the respective radial slices
For the purposes of this thesis work, the identification of the orientation of the FFT and its magnitude are done manually. Others have done work to automate this process, and if interested the reader is directed to review reference [36].

Once the major axis has been identified, the astigmatism analysis is completed by comparing the CTFs from the major and minor axes. The greater the divergence between the profiles from the two axes, the greater the astigmatism. This is shown in Figure 51. The left plot is from the image with the stigmation ratio of 5.0. On the major axis, the noise floor starts at a much higher spatial frequency than that of the minor axis. The spike in the plot associated with the minor axis at the high spatial frequencies is due to the intersection of the radial profile with the fringes seen in Figure 50. The right plot is from an image with a stigmation ratio of 1.5, and it can be seen that while there is a noticeable difference between the major and minor axes, it is much less for this smaller astigmatic ratio.

![Comparison of CTF plots from images with different amounts of astigmatism](image)

**Figure 51:** Comparison of CTF plots from images with different amounts of astigmatism
Left: Plots from image with stigmation ratio of 5.0
Right: Plots from image with stigmation ratio of 1.5
In order to determine the minimum amount of astigmatism that could be detected with this technique, artificial images were generated which had astigmatism ratios of 1.025/1, 1.05/1 and 1.1/1. Their corresponding CTFs are shown in Figure 52. The astigmatism present in the image with an astigmatism ratio of 1.025/1 cannot be easily determined from the corresponding plot. However, for larger amounts of astigmatism, the differences between the radial integrations along the major and minor axes of the ellipse can be seen, and the astigmatism can be detected.
Using a LEO 1550 SEM, an image was acquired of an FZP with an arbitrarily large amount of astigmatism. Upon examining the image and its FFT in Figure 53, an

**Figure 52:** Evaluations of artificial images with different astigmatism ratios to identify minimum amount of astigmatism that can be detected with this technique.

- **Top left:** CTFs from artificial image with astigmatism ratio of 1/1 (No astigmatism added).
- **Top right:** CTFs from artificial image with astigmatism ratio of 1.025/1. At this point, it is difficult to see a difference in the CTF curves, so the astigmatism is not detected.
- **Bottom left:** CTFs from artificial image with astigmatism ratio of 1.05/1. At this point, a small amount of divergence may be seen between the two curves in the region where the magnitudes drop sharply.
- **Bottom right:** CTFs from artificial image with astigmatism ratio of 1.1/1. At this point, the divergence between the two curves can be easily seen, and the astigmatism in the corresponding image can be identified.
elliptical region can be seen in the FFT, which is consistent with the behavior of the artificial images shown in the previous section.

Using a CD-SEM, small amounts of astigmatism were introduced, and images were captured at iterations between 0.1 mA and 10 mA away from the auto-stigmatization-correction point (at the original setpoint, the current going through the stigmation coil was approximately 36 mA). Given how the CD-SEM already contains an auto-calibrate function for astigmatism, the goal of this portion of the work was to see if CTF techniques could be used to detect small amounts of astigmatism, even before the effect was easily visible by eye to an operator. In this set of experiments, a clearly elliptical region was not visible in the FFT for any of the images acquired. This implies that the technique is not sensitive enough to identify astigmatism at the levels tested on the CD-SEM, even for stigmation of 10 mA. This is shown in Figure 54.
4.3 Aperture Misalign

Experiments were performed to see if it was possible to use the CTF to identify small amounts of aperture misalignment on the CD-SEM. The initial aperture control setting for one direction was 14.06 mA, and this was altered in small steps between 0.1 and 1.0 mA (with autocalibration, the initial aperture control setting was 14.06 mA). CTF
analysis of the images is able to show a direct correlation between the imaging performance and the aperture misalignment, as shown in Figure 55.

![Graph showing Contrast Transfer Function (CTF) magnitude vs. Feature Size (nm) for different aperture misalignment scenarios.](image)

**Figure 55:** Use of CTF measurements to identify aperture misalignment

### 4.4 Analysis of CTF Trends

One of the goals of this work is to see if different types of image defects have different CTF behaviors. While the results do not show characteristic behaviors for different image defects in a single plot (as shown in Figure 56, where CTFs for arbitrary amounts of aperture misalign and defocus show the same overall behavior), different behaviors can be seen if the parameters are modulated and the trends are examined.
Section 0 reviewed different ways to analyze the CTF curve, including subtracting two different CTF curves and plotting the difference as a function of spatial frequency. If this difference was normalized to the magnitude of one of the datasets, it is similar to a contrast measurement and we can examine the “contrast” of the CTF curves to further examine their trends. This is done to compare the CTF curves for the defocus series and the aperture misalignment series, as shown in Figure 57. Each imaging condition is compared with the autocalibration condition (the autofocus and the automatic aperture alignment). The top plot shows the defocus series and the bottom shows the aperture misalignment. It can be seen that as the defocus increases, each subsequent series is

Figure 56: Comparing CTFs for arbitrary amounts of aperture misalign and defocus. This plot shows how the type of image defect cannot necessarily be identified from single CTF profiles of each condition, as the profiles for these two different types of image defects do not have any distinguishing characteristics from each other.
smaller in magnitude and moves towards lower spatial frequencies (higher feature sizes). The behavior for the aperture misalignment series is different. Although each subsequent misalignment lowers the magnitude, we do not see the curve shift towards different spatial frequencies. Here, we see a difference in the trends of the behaviors for the two types of image defects.

4.5 Use of the CTF to identify vibrations

Using a frequency generator and a set of amplifiers, a SEM was deliberately subjected to vibrations in order to determine if the CTF could be used to detect vibrations. This work was done at that National Institute of Standards and Technology in Gaithersburg, MD, using an FEI Helios. The position of the speakers was varied
(distance from the tool, height of the speakers, side of the tool), as was the amplitude and the frequency of the wave, and the waveform.

Similar to the case of astigmatism, the vibrations are a non-symmetric feature, so the procedure for finding the CTF in this case must first involve analysis of the FFT to determine the proper orientation and amount of radial integration. This is shown in Figure 58.

**Figure 58: Image of Sample Subjected to Vibrations, and Different Angular Slices of FFT**
- Top left: Image of test sample without vibrations. Image is windowed. FOV is 317nm.
- Top right: FFT of top left image.
- Bottom left: Image of test sample subjected to vibrations. Image is windowed. FOV is 317nm.
- Bottom middle: FFT of top left image, highlighting an angular slice of 30°, centered at 90°
- Bottom right: FFT of top left image, highlighting an angular slice of 30°, centered at 180°
In Figure 59, the effect of 23.5 Hz vibrations using a square waveform are evaluated. Comparing the data from the images without vibrations to the data from the image with vibrations, the CTF slice around the 180° angle showed no difference. However, a sharp difference was seen for vibrations around the 90° angle.

![Figure 59: CTF Vibration Study](image)

CTF plot comparing the angular slices from the images that were and were not subjected to external vibrations. In these tests, the speakers were placed on the floor in front of the microscope, approximately 1.5 feet away from the tool. In the analysis program used, 90° corresponds to the major (vertical) axis and 180° corresponds to the minor (horizontal) axis.

In this study, it was found that the type of waveform used had a significant impact on the vibrations seen in the SEM. Waveforms tested include the sine wave, square wave, triangle wave and ramp, as shown Figure 60. When vibrations with the sine
waveform were applied, there was very little effect seen in the SEM. This is likely due to vibration controls built into the tool.

![Waveforms](image)

**Figure 60: Different Waveforms Used**
Left to right: Sine, square, triangle and ramp waveforms.

The specific frequency of the vibrations was also found to have an effect on the tool. When the frequencies were similar to the frame rate, the vibrations were found to be much more severe, whereas when the frequencies were not near the frame rate, no evidence of the vibration was seen in the image or the CTF.

### 4.6 Effect of Acquisition Time on the CTF

When deciding on the time that the electron beam dwells on each individual pixel in the image, there are a number of issues that must be considered. On the one hand, by selecting a condition where the electron beam spends more time dwelling on each pixel, the SNR will be improved. However, with the additional time spent on each pixel, the more one must assume that the sample is moving (due to vibrations), resulting in a blurring of the image. Additionally, with more dwell time, one may expect the sample to be exposed to more carbon contamination or, in the case of photoresist, beam-induced shrinkage.

A series of images was acquired with different cycle times, using the LEO 1550 SEM. The images and their corresponding transfer functions are shown in Figure 61. When analyzing the transfer functions, several conclusions can be made. The image
captured with the fastest cycle time appears to be the noisiest of the images based on a quick visual inspection of the image. The transfer function for that image is flat in the highest spatial frequency range, and its magnitude is greater than that than both of the other series, suggesting that the noise has overpowered all other information at the highest spatial frequency range. The image that was captured with a 20 second cycle time is the least grainy of the images. Its corresponding transfer function decreases in magnitude almost all the way to the highest spatial frequency, suggesting that there is information content there (which is not overcome by noise). The peaks shown in the transfer function between the feature sizes of 5-8nm correspond to the vibrations which can be seen in the image. Whereas the vibrations experiments shown in section 4.5 showed the results of a significant amount of vibrations applied, this experiment shows that the CTF can detect much smaller vibrations.
Chapter 5  Using the Contrast Transfer Function to Monitor CD-SEM Performance

5.1 Using the CTF to Monitor the Performance of the CD-SEM over time

Figure 62 shows the performance of one specific CD-SEM (Hitachi S9380-II), monitored at multiple different times over the course of a year. This monitoring was done using images of the random dot array, from a photoresist wafer (before etching), using the isolated 22 nm dots. The trend is very similar for all of the tests, but there are small differences in certain spatial frequency ranges.
This work shows that the tool performance can be monitored over time with this technique. However, as this tool was heavily utilized, it was not possible to perform a substantial series of measurements in order to correlate this with other tool performance data.

### 5.2 Matching
Currently, efforts to match the results of multiple CD-SEMs are time consuming and can be difficult to interpret. In order to perform matching experiments, the same sample is measured multiple times. This is problematic, because the operator must be
able to determine if subsequent differences in the measurements are due to drifts in the tool’s performance, or to contamination (carbon deposition) buildup on the location being measured. While most CD-SEMs do have auto-calibration routines to adjust the focus, stigmation, and aperture alignment, the routines only are functional if the parameters have drifted a small amount.

Images of the random dot array were acquired on four CD-SEMs (all CD-SEMs used for this section were Applied Materials Verity 4i’s), using identical imaging parameters on each tool (autofocus condition, beam current, acquisition time, etc.). Based on analysis of the CTF curves from four CD-SEMs, the tools can be separated into two groups. CD-SEM 4 and CD-SEM 2 appear to outperform CD-SEM 1 and CD-SEM 3. This assessment is based on which CTF profiles have the highest magnitude, as shown in Figure 63. It should be stated that there is an overlap between the data from CD-SEM 4 and CD-SEM 2 in some areas, however, the data from CD-SEM 4 is greatest in the areas where they do not overlap. Results from the facility’s matching measurements are shown in Table III. The matching techniques at this facility involve taking a tool out of production for tens of hours each month in order to take a large amount of measurements. The results from these measurements are compared to the expected values. If the measurements differ, the question must be asked, what is causing this discrepancy? This could be due to various problems with the tool, or even carbon contamination on the sample which are changing its physical dimensions. The table shows the difference from specification for horizontal and vertical measurements, plus the sum in quadrature (\( R = (\text{horizontal}^2 + \text{vertical}^2)^{1/2} \)). The results from the CTF measurements and the matching measurements are shown in Table IV. The best CD-SEM from the CTF measurements is
CD-SEM 4 and CD-SEM 2 (as the two CTF profiles are very close and difficult to distinguish with certainty), and the best from the sum of the matching measurements is CD-SEM 2.

![Graph showing contrast transfer function magnitude vs feature size for four CD-SEMs.](image)

**Figure 63:** Matching data from four CD-SEMs of the same make and model, from images of the random dot arrays. All images were acquired with the same imaging conditions.
### Table III: Matching Measurements over Multiple Tools

<table>
<thead>
<tr>
<th></th>
<th>Horizontal Drift (nm)</th>
<th>Vertical Drift (nm)</th>
<th>Total Drift (added in quadrature)</th>
<th>Amount of drift worse than best (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>CD-SEM 1</td>
<td></td>
<td></td>
<td></td>
<td>Measurements not available</td>
</tr>
<tr>
<td>CD-SEM 2</td>
<td>0.16</td>
<td>0.21</td>
<td>0.26</td>
<td>Best</td>
</tr>
<tr>
<td>CD-SEM 3</td>
<td>0.32</td>
<td>-0.06</td>
<td>0.32</td>
<td>23.1%</td>
</tr>
<tr>
<td>CD-SEM 4</td>
<td>0.26</td>
<td>0.1</td>
<td>0.28</td>
<td>7.7%</td>
</tr>
</tbody>
</table>

### Table IV: Comparing CTF Results with Matching Measurements

<table>
<thead>
<tr>
<th>Metric</th>
<th>Best Tool Performance</th>
</tr>
</thead>
<tbody>
<tr>
<td>Horizontal Drift</td>
<td>CD-SEM 2</td>
</tr>
<tr>
<td>Vertical Drift</td>
<td>CD-SEM 3</td>
</tr>
<tr>
<td>Total Drift</td>
<td>CD-SEM 2</td>
</tr>
<tr>
<td>CTF</td>
<td>CD-SEM 4 &amp; CD-SEM 2</td>
</tr>
</tbody>
</table>

The matching measurements are on the order of magnitude of $10^{-10}$ nm, which is in the noise floor for the CTF measurements. If this work was to be redone, the images of the random dot array should be taken at higher magnifications, so the units of interest do not fall within the noise floor of the image.

### Chapter 6  Ion Microscopy

For both electron and ion microscopes, the size of the imaging probe can be described by (17) [3],

$$d_p = \sqrt{d_o^2 + d_d^2 + d_s^2 + d_s^2} \quad (17)$$
where $d_p$ is the probe size, $d_G$ is the contribution from the brightness of the source, $d_d$ is the contribution from diffraction, $d_c$ is the contribution from chromatic aberration and $d_s$ is the contribution from spherical aberration.

The different contributions to the probe size can be found using (18), (19), (20), and (21) [3].

$$d_G = \sqrt{\frac{4I_p}{\beta \pi^2 \alpha^2}}$$  \hspace{1cm} (18)$$

$$d_d = \frac{0.61 \ h}{\alpha \ mv}$$  \hspace{1cm} (19)$$

$$d_c = C_c \frac{\Delta E}{E_0}$$  \hspace{1cm} (20)$$

$$d_s = \frac{1}{2} C_s \alpha^3$$  \hspace{1cm} (21)$$

where $\beta$ is the brightness, $i_p$ is the probe current, $\alpha$ is the convergence angle, $h$ is Planck’s Constant, $m$ is the mass of the particle, $v$ is the velocity of the particle, $C_c$ and $C_s$ are the coefficients of chromatic and spherical aberration, respectively, $E_0$ is the beam energy and $\Delta E$ is the energy spread.

By using particles which have significantly more mass than electrons, the smaller wavelength of the particle will contribute to a significantly smaller probe size. Additionally, different scattering behaviors will result in an interaction volume that is much smaller than that of the SEM, both parallel and perpendicular to the surface. The result of these factors is that ion microscopes will have a much smaller spot size than that of the SEM (and signals generated from this spot will be coming from a smaller area), contributing to a much better “resolution” metric. However, there are significant
concerns regarding damage. In order to keep sputter damage to a minimum, light ions (such as hydrogen, helium and neon) are of interest, as opposed to the much heavier gallium ions [44]. Even with the use of light ions to avoid sputter damage, there is still a risk that at high doses (in this context, the term dose refers to the amount of beam exposure in a given area, in units of electrons/cm² or ions/cm², and high doses refer to the orders of magnitude of $10^{17}$ ions/cm² and greater), there is a risk that the helium atoms may accumulate and “bubbles” may form under the surface [45]. At the time of the writing of this report, Carl Zeiss Microscopy is the only manufacturer with a light ion microscope in the market. The ORION Helium Ion Microscope (HeIM or HIM) uses positive helium ions for imaging (neon may be used with this microscope for applications where more sputtering is required). Interest has been expressed in the use of hydrogen ions (protons), but to date this microscope is not commercially available (although a prototype was built in the 1970s [46]). Samples imaged with a proton microscope would have similar SE yields compared to that of HeIM imaging [47], and less of a danger of sample damage due to sputtering and “bubble formation” [48]. There are differences between the structures of the HeIM as compared to the CD-SEM, which are shown in Figure 64. These differences include the sources used (HeIM uses an atomically sharp trimer structure for a tip, and the combination of a high extraction voltage and the presence of the helium gas create the beam, whereas the CD-SEM uses a conventional Schottky emitter) and the detector scheme (the detector for the HeIM is located off-axis and the detector for the CD-SEM is on-axis).
It is helpful to evaluate the signals that are produced by ion bombardment with materials that are typical in the semiconductor industry in order to determine which would be the most useful in metrology. As a prelude to experiments done for this work, a compilation of data from the literature indicated that secondary electrons were the most promising signal for metrology due to their high yield (the ion-induced SE yield is larger than electron-induced SE yields for their respective energy ranges of interest) [47] [49].

The HeIM and CD-SEM are similar in principle but have many differences. It can be seen that the HeIM’s source is exposed to a partial pressure of gas, whereas the CD-SEM’s source is not. Additional differences of note include the fact that the detector for the HeIM is off-axis and the detector for the CD-SEM is on-axis.

**Figure 64:** Cross sectional schematic comparing HeIM and CD-SEM. HeIM, left [48] and CD-SEM, right [1]. The HeIM and CD-SEM are similar in principle but have many differences. It can be seen that the HeIM’s source is exposed to a partial pressure of gas, whereas the CD-SEM’s source is not. Additional differences of note include the fact that the detector for the HeIM is off-axis and the detector for the CD-SEM is on-axis.

### 6.1 Analysis of Signals

It is helpful to evaluate the signals that are produced by ion bombardment with materials that are typical in the semiconductor industry in order to determine which would be the most useful in metrology. As a prelude to experiments done for this work, a compilation of data from the literature indicated that secondary electrons were the most promising signal for metrology due to their high yield (the ion-induced SE yield is larger than electron-induced SE yields for their respective energy ranges of interest) [47] [49].
Backscattered ions (BSIs) were found to have quite low yields [51] and consequently are not expectedly to contribute strongly to a measured signal. A recent study of ionoluminescence found that some materials which experience luminescence in the SEM do not necessarily do so in the HeIM, due to the smaller interaction volume, which results in a smaller region where the excitation processes may occur and therefore less total excitations (the interaction volume of HeIM is much smaller than that of the CD-SEM, as explored in reference [44]) and possible implantation of defects from the beam [52]. Additionally, as the ions in the beam are moving at a speed that is orders of magnitude below that of the electrons in the SEM beam, characteristic x-rays are unlikely to be generated in any measureable quantities [49] [53]. It is helpful to review that when comparing electrons and ions, the velocity of the particles is a more appropriate metric of comparison than the energy of the particles [49]. Due to the heavier mass, a helium ion with an energy of 40 keV has the same velocity as an electron with an energy of 5.48 eV and therefore is unable to excite characteristic x-rays.

An apparatus was designed to measure SE yields on certain materials of interest, including silicon, SiO$_2$, photoresist and HfO$_2$ (20Å thin film on a silicon substrate). Due to equipment constraints, quantitative measurements were only able to be made using a neon ion source, in the energy range between 6-10 keV. This work was done at the University at Albany’s Ion Beam Laboratory, using a duoplasmatron source which created beams with a current around 1 nA. The apparatus was designed based on designs in reference [47], and a schematic of the design is shown in Figure 65. The measured SE yields are shown in Figure 66. The SE yield can be found by taking the number of emitted SEs and dividing them by the amount of incoming ions. Neglecting the
contribution of backscattered ions to the measured current (due to the very low backscattered ion yields), the total current can be found by summing the currents measured at the target and at the collector box. Dividing the current measured at the collector by the sum of the collector and target current allows one to calculate the SE yields.

Figure 65: Schematic of apparatus used to measure secondary electron yields

The sample plate is placed inside a collector box. The currents from the sample plate and the collector box are measured (the plate and the box are electrically isolated from each other) in order to calculate the SE yield. To aid in the collection of electrons, a positive voltage is put on the collector box. In order to make sure that emitted electrons do not return to the sample, the sample is negatively biased.
It can be seen that the measured SE yields for SiO$_2$ are much less than those of HfO$_2$. This is partially attributed to the fact that the HfO$_2$ is a thin film on top of a silicon layer, whereas the SiO$_2$ is much thicker. When SEs are generated in the SiO$_2$, the high resistivity of the material prevents electrons from deeper in the material from filling the holes. Consequently, as additional SEs are generated, many of them will fill these holes instead of escaping from the material and being detected [54]. As the HfO$_2$ sample is a thin film on top of a silicon layer (which has much less resistivity than SiO$_2$), holes which are formed by the generation of SEs are more easily filled by electrons migrating from the bulk silicon, and consequently additional SEs are able to escape the material instead of filling the holes.

In addition to the quantitative measurements, relative SE and BSI yields were measured by bringing the samples to a HeIM demonstration unit in at the manufacturer’s (Carl Zeiss Microscopy) facilities in Peabody, MA. Images of all of the samples were acquired with the same imaging conditions (including the same beam current, acquisition
time, brightness and contrast settings), and the average brightness in each of the images was compared. SE yields were measured with the Everhart-Thornley detector, while BSI yields were measured with a multi-channel plate at beam energies of 20, 30 and 40 keV. The results are shown in Figure 67. It can be seen that in the energy range of interest, the SE yields are increasing with energy while the backscattered yields are decreasing.

![Figure 67: Relative secondary electron and backscattered ion yields for helium ion impingement on materials of interest](image)

### 6.2 Damage Studies

In order to further examine the suitability for HeIM as a possible replacement for CD-SEM, tests were done in order which involved exposing a variety of samples to large doses of helium ions in order to see at what point damage occurred. Samples used for this work included lines etched in amorphous silicon, lines etched in photoresist and contact holes etched through an oxide layer. The samples were imaged several times in a row without moving in order to monitor the effect of dosing the sample. The linewidth measurements were made manually using ImageJ. Static measurements for lines of silicon are shown in Figure 68 and Figure 69. This shows substantial amounts of damage.
at the high doses used, although these doses are at least an order of magnitude higher than typical imaging conditions would need to be. The process does not appear to be energy dependent. The series of static measurements of photoresist lines is shown in Figure 70 and measurements are shown in Figure 71. The lines undergo a great deal of shrinkage, which appears to be greater than the shrinkage which takes place in the CD-SEM [24]. Charging is also a factor here, as it can be seen how much the field of view moved over the course of the static imaging.

![Images of etched silicon lines in the HeIM](image)

**Figure 68:** Static imaging of etched silicon lines in the HeIM

Top left: First image of series, dose of $3.82 \times 10^{16}$ ions/cm$^2$
Top right: $15^{th}$ image of series, dose of $5.73 \times 10^{17}$ ions/cm$^2$
Bottom: $25^{th}$ image of series, dose of $9.56 \times 10^{17}$ ions/cm$^2$
Figure 69: Change in linewidth as a function of dose for HeIM-imaged silicon lines

Figure 70: Static imaging of photoresist lines in HeIM.

Note the amount that the beam shifted over the course of the images due to charging.
Chapter 7    CD-Metrology of Contact Holes: Comparing SEM and Ion Microscopy for a Specific Application

Many different applications in high volume manufacturing (HVM) of semiconductors require the inspection of high aspect ratio (HAR) features [55] [56]. In addition to 3D memory features, logic contacts and shallow trench isolations (STIs) must be inspected during the lithographic process. This inspection should be able to monitor the sidewall roughness, hole profiles, the top and bottom critical dimensions (CD), as well as be able to detect the presence of residues on the bottom or sides of the hole.

New vertical architectures that are being developed for memory devices by integrate circuit manufacturing are posing new challenges in metrology [15]. Many of these features are HAR holes or trenches in silicon, oxide, or multiple alternating layers of the two. A non-destructive technique for process control is necessary for these
features, in order to allow monitoring of measurements such as top and bottom diameters, as well as the sidewall roughness and the amount of any tapering.

A barrier to SEM based metrology on HAR features is complex charging phenomena, which have been the topic of study by many research groups [57] [58] [59] [60]. As stated earlier, CD-SEMs typically operate with a beam energy in the range of 500 eV - 800 eV. At these conditions, the electrons from the primary beam terminate tens of nanometers below the surface. As the primary beam electrons enter the material, secondary electrons (SEs) are generated. Those SEs generated within the escape depth of the material (typically around 5nm for metals and around 50nm for insulators [3]) may escape, leaving the surface layer charged positively. This positive layer on the top surface of the layer that the hole is etched through helps to create an extraction field to help SEs escape from the hole bottom. However, this is partially counteracted by a negative charge layer (from the primary electrons which have reached the end of their range, typically around 10-20 nm below the surface of the oxide). SEs are also generated at the bottom of the hole when it is struck by the primary electron beam. However, many of those SEs will accumulate on the sidewall of the hole, and it is only after enough SEs accumulate at the sidewalls and create enough negative charge to repel more SEs from reaching the sidewalls that SEs are able to escape the hole.

The HeIM uses a primary beam of positively charged helium ions instead of electrons to probe the sample [61]. During the process of imaging the contact hole sample, SEs are generated as the primary beam ions enter the oxide. SEs that are generated close enough to the surface may be able to escape, which results in the accumulation of a layer of positive charge near the surface. However, as the primary
beam is made of positive ions, there is no negative charge layer that accumulates below the oxide surface to counteract the positively charged surface, as in the case of the SEM. Additionally, as compared to the SEM, the HeIM has a smaller probe size, higher magnitude brightness and a smaller convergence angle [44] [50].

During imaging, the primary beam is focused to the smallest point possible, but the beam is still considered to be “in focus” when its size is less than a factor of two larger than the size of the beam at the smallest point (this is referred to as the zone of least confusion) [3]. The classical equations used to define the DOF assume that the limitations are based on a CRT screen with a fixed pixel size of 0.1mm [62]. This is no longer applicable in the cases of modern microscopes, which allow the user to choose from multiple options for the amounts of pixels in the image. Additionally, the equations used a term for the magnification of the image, which is problematic due to the fact that many microscopes have different calibrations for the magnification factor. A more appropriate term than magnification is the field of view (FOV) of the image.

A common size of the image is 512 x 512 pixels. If an image is taken with a FOV of 1µm (an appropriate FOV for the imaging of the contact holes), this corresponds to a pixel size of 1.95nm. By focusing the beam to the size of one pixel, it can be stated that any information acquired from locations where the beam size was less than 3.9nm would be in focus. Estimations of the convergence angles for the HeIM and the SEM are 1mR and 5mR, respectively [50]. The depth of focus (DOF) can be calculated with

\[
DOF = 2 \times \frac{\text{beam size}}{\tan \alpha}
\]

where \( \alpha \) is the convergence angle (in radians). The results of the calculations for FOVs of 1µm and 500 nm are shown in Table V. These calculations show that the DOF of the
HeIM is far superior to that of the SEM, which is very useful for the imaging of deep structures, and that the DOF must be taken into account when choosing a technique for imaging HAR structures.

| Table V: Calculated depth of focus for SEM and HeIM |
|-----------------|-----------------|
| Field of view   | Depth of Focus  |
| SEM             | 1 µm            | 780 nm          |
| HeIM            | 1 µm            | 3900 nm         |
| SEM             | 500 nm          | 390 nm          |
| HeIM            | 500 nm          | 1950 nm         |

While the smaller probe size and the higher DOF make the HeIM seem promising for contact hole imaging, there are potential drawbacks. The HeIM has been shown to cause significant damage to samples at high doses [45]. Additionally, charging phenomena may also pose a detriment in this case. In electron microscopy, there are energy levels where the negative charge from the beam can be balanced with positive charge on the surface, as was shown earlier in Figure 5 (the $E_1$ and $E_2$ crossover points). However, in ion microscopy, as the beam itself is positive, there are no energy levels where the charge would cancel. There are methods for compensating for charging in the HeIM (for example, the use of an electron flood gun), but these methods are nontrivial. Additionally, as the SE yields are higher for HeIM than for SEM in the energy range in which the tools operate [49], positive charging on the surfaces and the sidewalls may be much greater than the case of the CD-SEM, and this could result in SEs being attracted back to the surface instead of escaping to the detector.

7.1 Experiments
In order to study this problem, a set of samples was fabricated. This included large arrays of contact holes which were 150 µm wide. The contact holes were etched through
a 500nm layer of SiO₂, terminating at a silicon substrate. Holes with different dimensions were fabricated, with top diameters ranging from 140 nm down to 60 nm. The holes taper and have a smaller bottom diameter than top diameter. A schematic of the sample is shown in Figure 72 along with a cross-sectional SEM image of an array of contact holes. Experiments were designed to see if it was possible to conclusively discern if the signal from the bottom of the hole was able to be successfully extracted.

![Figure 72: Contact hole samples](image)

Left: Schematic of contact hole sample. Right: Cross sectional SEM image of array of contact holes. The bumpy areas at the top of the holes are material left over from the cross sectional SEM sample preparation procedure and are not present in top-down imaging.

Unless there is a clear topographic feature at the bottom of a contact hole, it is not possible to conclusively determine if the bottom is successfully imaged from a single top-down micrograph. Although some images may look like they clearly show the bottom of the hole, that is not necessarily the case. Figure 73 shows two example CD-SEM images of contact holes, where it may appear that the bottoms are being imaged, but this
conclusion cannot be reached by simply looking at the images. These images were acquired with a Hitachi S9380-II CD-SEM.

![CD-SEM images of contact holes.](image)

From these top down images, it cannot be determined if the bottoms of the holes are being imaged successfully.

Figure 73: CD-SEM images of contact holes.

What appears to be relevant information about the bottom of the hole may in fact be SE$_{2s}$ generated far from the beam impact point (An SE$_2$ is a secondary electron which is not generated by the primary beam (this is termed an SE$_1$), but instead is generated by a backscattered electron/ion [3]), or even noise from the tool electronics [63]. In order to determine if any signal is escaping from the hole at all, it is necessary to establish what pixel intensity corresponds to the level of zero signal intensity. This can be found by blanking the beam during a portion of the scan, and then comparing the brightness level in the blanked part of the image to that of the hole. By blanking the beam during the scan, one can find the zero level of the signal from the secondary/backscattered electrons (or, in the case of the HeIM, backscattered ions). If the signal level from the blanked part of the scan is very similar to that of the bottom of the hole, it may be inferred that no
signal is escaping. Even if it appears that the bottom is visible, the maximum depth that the signal is detected from may not correspond with the bottom of the hole.

In order to determine the maximum depth that the signal is coming from, the sample may be imaged at two different tilt angles. By examining line profiles from the image and comparing the locations where the sidewall apparently intersects with the bottom, as shown in Figure 74, the lateral shift can be measured and used to estimate the depth that the signal is coming from.
An assumption is made that when the sample is tilted by a small angle (between 1° and 5°), the signals are able to escape from the same depth. This assumption allows one to construct an isosceles triangle, as shown in Figure 75, and using elements of basic
trigonometry, one is able to calculate the depth that the signals are emanating from. The calculation is derived from the Law of Sines, as shown in (23)

\[
\frac{\sin A}{a} = \frac{\sin D}{d}
\]

(23)

where angle A is the tilt angle, distance a is the distance that the perceived bottom moves and distance d is the calculated depth.

![Figure 75: Schematic of the tilt measuring calculation.](image)

For the HeIM imaging studies, the work was done using an Orion Plus Helium Ion Microscope, manufactured by Carl Zeiss Microscopy. Tests were done at beam energies around 35 keV, using both the Everhart-Thornley (ET) detector for secondary electrons and a microchannel plate (MCP) for backscattered ions. The detectors were located off-axis. The highest doses applied were calculated to be in the order of magnitude of 16 µC/cm², which is significantly less than the damage threshold of 1.6x10⁴ µC/cm² found in prior studies [64] for this material set and energy level.

As a CD-SEM with a calibrated tilt capability was not available for these experiments, a traditional SEM (LEO 1550, also manufactured by Carl Zeiss Microscopy) was used for these experiments. The SEM was operated at a low energy of 800 eV, in order to mimic the low-voltage operating condition of the CD-SEM. An on-
axis inlens-type SE detector was used, and the sample was exposed to continuous scanning of the electron beam at a low magnification for two minutes in order to charge the surface positive and create an extraction field to aid in the escape of the signals from the inside of the holes [57]. Combined with the large field of view, the long time period of two minutes was used in order to reach a state where the surface charge would reach a steady state.

7.2 Results – Analysis of Signal Levels

In order to ascertain if the signal coming from the hole bottoms was due to signal electrons or due to instrument noise, the signal was blanked during some parts of the scan in order to determine the zero signal level, and the intensity levels were measured in the blanked areas and compared to the intensity levels in the holes. The images are shown in Figure 76 and the intensity levels are shown in Table I. This shows that for the backscattered ion case, the signal from the holes is barely any greater than the portion of the image where the beam was blanked, whereas for the other detectors, there is signal which is greater than the zero level being detected.

<table>
<thead>
<tr>
<th>Table VI: Comparison of signal levels from center of holes and blanked region</th>
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<tbody>
<tr>
<td></td>
</tr>
<tr>
<td>Blanked Area</td>
</tr>
<tr>
<td>Center of Hole</td>
</tr>
</tbody>
</table>
For the cases of the images of the holes acquired with the SEM using the inlens detector and the HeIM using the E-T detector, the intensity level in the center of the holes was many times greater than that of the intensity in the blanked area. However, for the image that was acquired with the HeIM using the MCP detector (to detect backscattered ions), the signal level from within the holes was very similar to that of the blanked area,
which implies that the signal being detected from the holes in this case is negligible. This is likely due to the fact that the backscatter yield for ion bombardment is extremely low [51].

### 7.3 Results – Depth Calculations

![Graph showing calculated depths of contact holes](image)

**Figure 77:** Calculated depths of contact holes known to be 500nm deep with tilt method

Figure 77 shows the calculated depths that signals were detected from the 500 nm deep contact holes. The results show that the signals detected with the HeIM (using the Everhart-Thornley detector) came from much deeper in the hole as compared to the SEM for all of the geometries tested. The depth calculated from the imaging of the widest holes approaches the expected depth of the holes and suggest that the HeIM was able to image the bottom (within the probable margins of error for the technique and the lithography). It has been suggested that the HeIM results could be improved by use of an on-axis detector (which would have a higher collection efficiency than the off-axis Everhart-Thornley detector) [65].
7.4 Modeling – JMONSEL

Simulations were done using the JMONSEL tool which was introduced in Section 1.3.2. By using simulations, the ability is gained to quickly vary the sample geometry in order to examine trends in the experimental data in a manner that is much faster and more cost effective than fabricating additional sets of samples.

Several conditions were simulated with a variety of sample geometries. Holes of different depths were simulated (500 nm, 700 nm and 900 nm), as well as holes of different widths (top/bottom radii of 70 nm/50 nm, 50 nm/35 nm and 35 nm/20 nm). The hole width dimensions were designed to be similar to that of the samples used. Additionally, simulations were designed that added a small cylindrical “particle” to the bottom of the hole, with a radius of 10 nm and a height of 10 nm. If the shape of the particle could be seen in the line profile, the signal from the hole bottom can be extracted. Particles were defined as either silicon or copper.

One set of simulations compared line profiles from scans of holes of varying widths. Two sets of geometries were used, one with a bottom particle made of copper and another with a bottom particle of silicon. Line profiles showing total yield (BSE + SE) are displayed in Figure 78. The total yield is used (instead of just the SE or BSE yield) due to the somewhat arbitrary distinction JMONSEL uses to divide the electrons that reach its detector between SEs and BSEs. Additionally, some CD-SEM detectors likely use a combination of SEs and BSEs to make up the image.

For the holes with the widest top radius, the bottom particle is reflected in the line scan. As the holes get narrower, the signal from the particle decreases. In the narrowest holes, it can barely be seen. Additionally, there is a much stronger detection of signal from the copper particle than from the silicon particle. This is likely due to the fact that
the BSE yield of Cu is much higher than that of Si. Therefore, based on examination of the line scans, it can be determined that the higher energy BSEs are able to escape, although it is more difficult for the lower energy SEs to escape from the bottom of the hole.

Another set of simulations compared line profiles from scans of holes with a constant radius and varying depths. The holes had a top radius of 70 nm and a bottom radius of 50 nm, and the depths included 500 nm, 700 nm, and 900 nm. Copper particles were placed at the hole bottoms, and the beam energy was held at 500 eV. Line profiles for this simulation are shown in Figure 79. The profiles indicate that the copper particle can be detected at the bottom of a 500 nm deep hole, but as the hole becomes deeper it becomes more difficult for the signal at the bottom to be detected.
Figure 78: Simulated line profiles as a function of width, without added noise.
Top left: Top radius of 70 nm with a Cu marker particle
Middle left: Top radius of 50 nm with a Cu marker particle
Bottom left: Top radius of 35 nm with a Cu marker particle
Top right: Top radius of 70 nm with a Si marker particle
Middle right: Top radius of 50 nm with a Si marker particle
Bottom right: Top radius of 35 nm with a Si marker particle
The simulated results shown thus far do not reflect any noise, which will be a part of any realistic SEM image. A quantitative way of displaying the effect of noise on the measurements is by plotting expected measurement noise and signal as a function of a parameter of interest (e.g., hole size) on the same graph. The parameter range under which a feature is detectable can be chosen based on the choice of a criteria (for example, the Rose Criterion (S/N = 5), or even S/N = 1). For our purposes, to detect a marker particle on the bottom of a contact hole, the difference in the signal yields between the marker and the hole bottom must be greater than the noise level. The expected noise depends on the number of incident electrons per pixel \( n \), which is calculated according to \( (24) \)

\[
n = \frac{A \tau}{e}
\]  

(24)

with \( A \) the beam current, \( \tau \) the total time the beam spends on a, and \( e \) is the magnitude of the electron charge. The number of electrons per pixel will vary with imaging conditions. For our calculations, the parameters used are a beam current of \( A = 10 \text{ pA} \) and a time \( \tau = 0.126 \mu\text{s} \) (using a frame acquisition time of 0.033 seconds, and 512 × 512 pixels in each frame), conditions that are very similar to that of the CD-SEM. With these assumptions, \( n \)


**Figure 79:** Simulated line profiles as function of depth, without added noise. Holes vary in depth from 500 nm (left) to 700 nm (center) to 900 nm (right)
is approximately 8 electrons per pixel multiplied by the number of pixels and frames in the image (with 16 or 32 being a common amount of frames).

If the electron yield on the marker particle is $y_{mp}$, the yield from the remainder of the bottom of the hole is $y_b$, and the number of incident electrons per pixel is $n$, the noise is calculated according to (25)

$$\text{Noise} = 1.45 \sqrt{\frac{y_{mp} + y_b}{n}}$$

(25)

A coefficient would not be needed if the noise was only based on a Poisson distribution. This is not the case here, as some of the electron emission events are correlated. For example, a BSE that leaves the bottom surface may impact the sidewalls and create multiple SE$_2$s. The value of 1.45 for the coefficient was derived from the simulation data by John Villarrubia at NIST.

This calculation can be applied to the line profiles to display the effect of noise on the scan. For each data point in the line profile, a MATLAB routine takes the original (noiseless) value and multiplies it by a random number, using the original value as the mean and the noise value as the standard deviation. Figure 80 displays line profiles of scans from simulations of contact holes with a top radius of 70 nm and a silicon particle at the bottom of the hole. If only one frame makes up the image, the particle at the hole bottom cannot be discerned (and therefore, SEs from the hole bottom are not detected). However, if an image is acquired by integrating a substantial number of frames, evidence of the particle is seen in the linescan and hence state that SEs from the bottom are being detected.
The results of the detectability calculations are shown in Figure 81. Each plot shows a signal level and corresponding noise levels for images with different numbers of frames. The detectability calculations are plotted as functions of hole depth or hole radius. When the signal plot is greater than the noise plot, it is assumed that the signal can be detected. For a silicon particle, the signal is so weak that one would need to integrate more than 128 frames to see a signal from the widest hole. The copper particle is much easier to detect because it emits more BSEs. Figure 81 (bottom left) shows the detectability as a function of hole depth. It is shown that a 500 nm deep hole is barely detectable with 8 frame integrations.
7.5 Summary of Contact Hole Imaging

The use of HeIM for imaging contact holes etched through a deep layer of an insulating material was evaluated and compared to the case of low voltage SEM. The DOF for HeIM is superior to that of the SEM, which is helpful for imaging of high aspect ratio structures. For the holes etched through a 500 nm layer of oxide, it outperformed the low voltage SEM, detecting a signal from deeper in the hole. However, with the possible exception of the widest holes tested, the HeIM was not able to detect the bottoms...
of all of the holes tested. Based on modeling results, the SEM signal is very weak and for many cases will be obscured by noise.

Chapter 8 Conclusions and Future Work
As the semiconductor industry continues to require the manufacture of smaller and smaller features, monitoring the outcome of the fabrication process becomes even more important. Additionally, as the progress in the capabilities of the CD-SEM has not been increasing as much as many in the industry feel is necessary to keep pace with the smaller device structures, it is necessary to increase the amount of monitoring done to the CD-SEM in order to wring the best performance out of it possible. The ability of the Contrast Transfer Function to monitor tool performance and identify when the tool is not performing optimally is demonstrated. While the samples used are not ideal, the random dot arrays still allow the measurements to be taken, and it was shown that moving around on the random dot array does not affect the measurements. Potential is shown for the use of this technique for matching the results of different tools. For this work to continue, more work should be put into developing a better random dot array with different fabrication techniques (for example, e-beam lithography), which could yield tool performance results that are more decoupled from the sample behavior than the currently available samples. If an ideal sample was used, the CTF could be extracted and applied to other images, with the goal of taking artificially generated images and outputting images that appear as they would have had they been imaged with the tool. Many CD-SEMs contain built in samples for calibration purposes, and a well-built random dot array could be a valuable choice for a built in auto-calibration target.
The development of light ion microscopy brings with it new possibilities for CD-metrology, which may include the supplementation or the replacement of the CD-SEM. Helium Ion Microscopy has been shown by others to have a smaller beam size and interaction volume as compared to the SEM, but this work shows the amount of physical damage that the HeIM imparts to samples must be taken into consideration when choosing a metrology technique. The depth of focus and high SE yields of HeIM make it promising for contact hole imaging, but the tool is still limited by the use of an off-axis Everhart-Thornley detector. Additionally, JMONSEL simulations showed that BSEs are much more likely to escape from contact holes than SEs. The further development of microscopes with other light ions (mainly protons) is awaited as a new enabling technology which could solve many of the problems associated with the CD-SEM but avoid the damage associated with the HeIM.
Works Cited


[58] H. Abe, S. Babin, S. Borisov, A. Hamaguchi, A. Iyanchikov, M. Kadowski and Y. Yamazaki, "Time dependence of SEM signal due to charging: measurements and


Chapter 9  Appendix – MATLAB Code for Finding the CTF

In MATLAB, the % character is used to signify a comment.  %% is used to easily separate the sections.

clearvars

%% Load Files
%load input file for CTF, read it into variable ARRAY
image_0=double(imread('windowed-dots_lumFOV_4i_AF.tif'));
image_1=double(imread('windowed-dots_lumFOV_4i_app-1.tif'));
image_2=double(imread('windowed-dots_lumFOV_4i_n2voltFocus.tif'));

image_0=imcrop(image_0, [0 0 1024 1024]);
image_1=imcrop(image_0, [0 0 1024 1024]);
image_2=imcrop(image_0, [0 0 1024 1024]);

%Find the size of the array
array = image_0;
[M N] = size(array);

%% Windowing
max0 = max(max(image_0));
image_0 = image_0/max0;
max1 = max(max(image_1));
image_1 = image_1/max1;
max2 = max(max(image_2));
image_2 = image_2/max2;

array = image_0;
[M N] = size(array);

midpoint=M/2;

w1 = cos(linspace(-pi/2, pi/2, M)); %linspace: draws a line from -pi/2 to pi/2 with M pixels.
w2 = cos(linspace(-pi/2, pi/2, N)); %Taking a cosine of this sets a value of zero at the extremeties
w = w1' * w2;
image_0 = array.*w;

array=image_1;
image_1 = array.*w;
array=image_2;
image_2 = array.*w;

%% Specify information about size of image.  CODE ASSUMES SQUARE IMAGE!!!
imageSizeNM = 1000;  %FOV, nm.  675nm = 200kX on Hitachi CD-SEM
imageSizePIXELS = 1440; % FOV, pixels. Uses number found on prior line
pixelsPerNM = imageSizePIXELS / imageSizeNM; % pixels per nm
mR = (M + N) / 4;
pixConvert = (0.5 - 1/(2*mR))/mR;

% Find the center
midpoint=M/2;
% Windowing
maxArray = max(max(array));
array = array/maxArray;

% initialize results array
results=zeros(midpoint,4);

% meanZero: The central pixel of the FFT is the average brightness. By % subtracting the average value, we remove that from the data.
array = array - mean2(array);

% Take Fourier transform of CTF-file
F_array = abs(fft2(array)).^2; % PSD
% shift origin to center
F_array=fftshift(F_array);

%% Radial Distribution - Extract CTF from input file
for m = 1:M
    for n = 1:N
        R=floor(sqrt((m-midpoint)^2+(n-midpoint)^2))+1;
        if R==0
            R=1;
        end
        if R>midpoint
            R=midpoint-1;
        end
        results(R,1)=results(R,1)+1;
        results(R,2)=results(R,2)+F_array(m,n);
    end
end
for i=1:midpoint
    results(i,2)=abs(real(results(i,2)/results(i,1)));
% divide real part of the magnitudes by the number of times that value was found
    results(i,1)=i;
% rewrite column with values 1-256
end
for i=1:midpoint
    results(i,3) = (i*pixConvert*pixelsPerNM); % spatial frequency
    results(i,4) = 1/(i*pixConvert*pixelsPerNM); % inverse spatial frequency
for j=1:midpoint
    x_axis(j)=results(j,1);
    x_axis_calibrate(j)=results(j,4);
    CTF_real(j)=results(j,2);
end

maxReal = max(max(CTF_real));
minReal = min(min(CTF_real));

maxOrderofMagnitude = floor(log(abs(maxReal))./log(10)) + 1;
minOrderofMagnitude = floor(log(abs(minReal))./log(10)) - 1;

%% Next data set
%initialize results array
results=zeros(midpoint,4);
array=image_1;
%Find the size of the array
[M N] = size(array);
%Find the center
midpoint1=M/2;
results=zeros(midpoint1,4);

% meanZero: The central pixel of the FFT is the average brightness.
By
% subtracting the average value, we remove that from the data.
array = array - mean2(array);

%Take Fourier transform of CTF-file
F_array = abs(fft2(array)).^2;  %PSD
%shift origin to center
F_array=fftshift(F_array);

%% Specify information about size of image. CODE ASSUMES SQUARE
% IMAGE!!!
imageSizeNM = 1000;          %FOV, nm. 675nm = 200kX on Hitac
imageSizePIXELS = 1440;      %FOV, pixels. Uses number found on prior
                             % line
pixelsPerNM = imageSizePIXELS / imageSizeNM;  %pixels per nm
mR = (M + N) / 4;
pixConvert = (0.5-1/(2*mR))/mR;

%% Radial Distribution - Extract CTF from input file
for m = 1:M
    for n = 1:N
        R=floor(sqrt((m-midpoint1)^2+(n-midpoint1)^2))+1;
        if R==0
            R=1;
        end
        if R>midpoint
            R=midpoint-1;
        end
        results(R,1)=results(R,1)+1;
for i=1:midpoint1
    results(i,2)=abs(real(results(i,2)/results(i,1))); %divide real part of the magnitudes by the number of times that value was found
    results(i,1)=i; %rewrite column with values 1-256
end

for i=1:midpoint1
    results(i,3) = (i*pixConvert*pixelsPerNM); %spatial frequency
    results(i,4) = 1/(i*pixConvert*pixelsPerNM); %inverse spatial frequency
end

for j=1:midpoint1
    x_axis_calibrate1(j)=results(j,4);
    CTF_real1(j)=results(j,2);
end

%% Next data set
%Find the size of the array
array=image_2;
[M N] = size(array);
%Find the center
midpoint2=M/2;
%initialize results array
results=zeros(midpoint2,4);

% meanZero: The central pixel of the FFT is the average brightness. By
% subtracting the average value, we remove that from the data.
array = array - mean2(array);

%Take Fourier transform of CTF
F_array = abs(fft2(array)).^2; %PSD
%shift origin to center
F_array=fftshift(F_array);

%% Specify information about size of image. CODE ASSUMES SQUARE IMAGE!!!
imageSizeNM = 1000; %FOV, nm. 675nm = 200kX on Hitachi CD-SEM
imageSizePIXELS = 1440; %FOV, pixels. Uses number found on prior line
pixelsPerNM = imageSizePIXELS / imageSizeNM; %pixels per nm
mR = (M + N) / 4;
pixConvert = (0.5-1/(2*mR))/mR;

%% Radial Distribution - Extract CTF from input file
for m = 1:M
    for n = 1:N
        R=floor(sqrt((m-midpoint2)^2+(n-midpoint2)^2))+1;
        if R==0
            R=1;
        end
        if R>midpoint
            R=midpoint-1;
        end
        results(R,1)=results(R,1)+1;
        results(R,2)=results(R,2)+F_array(m,n);
    end
end

for i=1:midpoint2
    results(i,2)=abs(real(results(i,2)/results(i,1))); %divide real part of the magnitudes by the number of times that value was found
    results(i,1)=i; %rewrite column with values 1-256
end

for i=1:midpoint2
    results(i,3) = (i*pixConvert*pixelsPerNM); %spatial frequency
    results(i,4) = 1/(i*pixConvert*pixelsPerNM); %inverse spatial frequency
end

for j=1:midpoint2
    x_axis_calibrate2(j)=results(j,4);
    CTF_real2(j)=results(j,2);
end

%% Smoothing

CTF_real_smooth = CTF_real;
CTF_real_smooth1 = CTF_real1;
CTF_real_smooth2 = CTF_real2;

for j=2:midpoint-1
    CTF_real_smooth(j) = (CTF_real(j-1)+CTF_real(j)+CTF_real(j+1))/3;
    CTF_real_smooth1(j) = (CTF_real1(j-1)+CTF_real1(j)+CTF_real1(j+1))/3;
    CTF_real_smooth2(j) = (CTF_real2(j-1)+CTF_real2(j)+CTF_real2(j+1))/3;
end

CTF_real = CTF_real_smooth;
CTF_real1 = CTF_real_smooth1;
CTF_real2 = CTF_real_smooth2;
%% Compile results into one variable
for j=1:midpoint
    CTF_total(1,j)=x_axis_calibrate(1,j);
    CTF_total(2,j)=CTF_real(j);
    CTF_total(3,j)=CTF_real1(j);
    CTF_total(4,j)=CTF_real2(j);
end
% csvwrite('CTF-apertureMi
salign.csv', CTF_total);

%% Display results
figure
CTF_real_plot = loglog(x_axis_calibrate, CTF_real);
hold all
CTF_real_plot1 = loglog(x_axis_calibrate1, CTF_real1);
hold all
CTF_real_plot2 = loglog(x_axis_calibrate2, CTF_real2);

ylim([10^minOrderofMagnitude  10^maxOrderofMagnitude]);
set(gca, 'XDir', 'reverse', 'Color', [0.8,0.8,0.8]);
set(gcf, 'Color', 'white');
set(CTF_real_plot, 'Color', 'black', 'LineWidth', 2.5);%, 'Marker', '+');
set(CTF_real_plot1, 'Color', 'red', 'LineWidth', 2.5, 'LineStyle', ':');%, 'Marker', 'diamond');
set(CTF_real_plot2, 'Color', 'yellow', 'LineWidth', 2);
xlabel('Feature Size (nm)', 'FontSize', 15);
ylabel('Contrast Transfer Function Magnitude', 'FontSize', 15);
legend('Best Conditions', 'Aperture Misalign', 'Defocus');