Electroquasistatic Sensors for Surface and Subsurface Nano-
Imaging of Integrated Circuit Features

by

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Abstract

The following thesis relates to the design, simulation, and testing of electroquasistatic (EQS) sensors to be used for feature/defect location and imaging. The aim of this thesis is to launch an investigation into the use of EQS sensor arrays for non-destructive evaluation and quality control purposes for integrated circuit industry applications. Research into three specific areas serves as the primary focus of the thesis:

1.) The use of EQS sensors to penetrate the surface of doped silicon and locate p-n junctions and doped wells. Arrays of coplanar EQS sensors are scanned laterally over the surface of a doped silicon bulk at a fixed scan height. Electric fields from the driven EQS sensor array are capable of penetrating the surface of the semiconductor when sensors are operated at a frequency comparable to its charge relaxation break frequency. It is demonstrated through finite element method (FEM) simulations that voltage-driven EQS electrodes can couple into the p-n junction without making any direct electrical contact with the semiconducting bulk. A new methodology for locating p-n junctions is presented where the currents on these voltage-driven sensors are monitored for harmonic distortion due to the junction's nonlinear drift/diffusion carrier dynamics. With sensors located over a p-n junction at a scan height of 200 nm and driven at 1GHz, the ratio of the second harmonic current to the fundamental current on a sensor is shown to exceed 9%. Such an IC imaging technique could prove to be useful for verification and detection of fabrication errors, externally monitoring current flows, as well as detecting hidden Trojan circuits that might be present.

2.) The use of EQS sensors to locate and image surface features and contaminant objects on photomasks. Motivation for research into this area comes from the desire to be able to locate and remove contaminant particles that might be present on extreme ultraviolet lithography (EUVL) photomasks used in the mass production of next-generation integrated circuits. FEM simulation results demonstrate the sensitivity of EQS sensor arrays in detecting various contaminant particles located
in a 100nm wide by 70nm deep gap in the absorber layer of an EUVL photomask. A millimeter-scale, in-lab experiment using capacitive sensors is performed with sensors and materials having similar aspect ratios and electrical properties to those simulated. Experiments demonstrate both the capabilities and limitations of sensors in detecting various objects located in a trenches milled out of aluminum. Additionally, a discussion of the need for low-noise pickup circuitry to interface with sensors is presented.

3.) An investigation into the inversion of sensor transimpedance response signals into predicted feature/defect profiles. In this case study, an inverse electromagnetic sensor problem is solved by training a radial basis function artificial neural network (RBF-ANN) to accurately approximate the forward mapping of the physical dimensions (width and depth) of a high aspect ratio trench in doped silicon into a sensor’s transimpedance response as the sensor array scans past the trench at a fixed scan height. This is an example of the type of inverse problem that might be encountered in an EQS array microscope and one possible approach to its solution. The function-approximation network is then inserted into an iterative signal inversion routine which converges to a prediction for the trench’s dimensions, given a measured transimpedance response. The routine is capable of predicting trench dimensions to within 1% of their actual value.

In all three cases, research involves extensive finite element method (FEM) simulations of sensor performance using COMSOL Multiphysics.

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I have many people to thank for making the last two years at MIT both a rich and enjoyable experience.

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1 Introduction

This thesis is an investigation into the potential use of electroquasistatic (EQS) impedance sensors as an inspection and imaging tool for the integrated circuit industry. Large arrays of individually addressable EQS sensors could provide the integrated circuit industry with a new class of fast-scanning imaging tools to aid in the quality control of integrated circuits and photolithography equipment. This thesis launches an investigation into several different case studies that evaluate the sensitivity of EQS sensors in detecting both surface and subsurface features and contaminant objects that are typical to an integrated circuit. Both forward and inverse EQS problems are considered. Although this thesis focuses solely on EQS sensors, there exists an entire dual class of magnetoquasistatic (MQS) sensors. MQS sensors are particularly advantaged over EQS sensors when detecting features in highly conducting substrates due to the capabilities of magnetic fields to see beneath the surface of conductors at very low frequencies [1-5].

Current applications of both EQS and MQS sensors include, but are not limited to: detection of buried objects such as metallic and non-metallic landmines [1]; humidity and moisture sensing [3]; determining absolute electrical and magnetic properties and characterization of layered, heterogeneous materials [3, 4, 6]; measuring corrosion, aging, and cracking in structures [5, 7]; and proximity detection [8]. The electromagnetic operation of the sensors presented in this thesis is governed by the same fundamental set of equations as those described in the various applications above but provide new applications and methodologies for feature/defect detection and imaging.
1.1 Theory and Background of Electromagnetic Sensors

Given the breadth of applications in which electromagnetic sensors are used, it is appropriate to first describe their theory of operation at a fundamental level. The well-known and well-tested Maxwell’s Equations that describe the coupling between electric and magnetic fields and their sources are listed in differential form:

\[ \nabla \times \vec{E} = -\frac{\partial \vec{B}}{\partial t} \quad (1.1) \]
\[ \nabla \times \vec{H} = \vec{j} + \frac{\partial \vec{D}}{\partial t} \quad (1.2) \]
\[ \nabla \cdot \vec{D} = \rho_f \quad (1.3) \]
\[ \nabla \cdot \vec{B} = 0 \quad (1.4) \]
\[ \nabla \cdot \vec{j} + \frac{\partial \rho_f}{\partial t} = 0 \quad (1.5) \]

where \( \vec{E} \) is defined as the electric field vector in \([V/m]\), \( \vec{H} \) the magnetic field intensity vector in \([A/m]\), \( \vec{D} \) the electric displacement vector in \([C/m^2]\), and \( \vec{B} \) the magnetic flux density in \([T]\). The source terms \( \vec{j} \) and \( \rho_f \) represent the free current density in \([A/m^2]\) and the free volume charge density in \([C/m^3]\), respectively. Equation (1.5) is simply the source continuity equation. For linear, homogeneous media, these vector fields are related through the following set of constitutive relations:

\[ \vec{D} = \varepsilon \vec{E} \quad (1.6) \]
\[ \vec{B} = \mu \vec{H} \quad (1.7) \]
\[ \vec{j} = \sigma \vec{E} \quad (1.8) \]

where \( \varepsilon \) is the electrical permittivity of the medium, \( \mu \) the magnetic permeability, and \( \sigma \) the electrical conductivity.
For problems in which sensor sizes are much smaller than the free space wavelength of electromagnetic waves that propagate at the sensors' operating frequency, Equations (1.1)—(1.5) can be decoupled and broken into two sets of approximate equations: electroquasistatics (EQS) and magnetoquasistatics (MQS). These equations are:

EQS

\[ \nabla \times \vec{E} \approx 0 \] (1.9)

\[ \nabla \cdot \vec{D} = \rho_f \] (1.10)

\[ \nabla \cdot \vec{j} + \frac{\partial \rho_f}{\partial t} = 0 \] (1.11)

MQS

\[ \nabla \times \vec{E} = -\frac{\partial \vec{B}}{\partial t} \] (1.12)

\[ \nabla \times \vec{H} \approx \vec{j} \] (1.13)

\[ \nabla \cdot \vec{B} = 0 \] (1.14)

\[ \nabla \cdot \vec{j} \approx 0 \] (1.15)

The EQS set of equations are used when the dominant sources are charges creating electric fields, while the MQS equations govern situations where the dominant sources are currents creating magnetic fields. In this quasistatic approximation, time-varying electric and magnetic fields no longer serve as source terms, and consequently, the equations do not describe the propagation of electromagnetic waves. This is appropriate as all electrically driven elements under consideration in a quasistatic regime are extremely poor at radiating electromagnetic waves.

The sensors described in this thesis are governed by the EQS set of equations; however, as stated previously, there also exists an entire class of analogous MQS-governed sensors useful for the detection of surface and subsurface features and objects. This thesis did not investigate the use of MQS sensors, because the original goal of this thesis was to detect features and objects that are
described electrically by their relative permittivity and electrical conductivity; moreover all materials considered in this thesis have relative permeability, $\mu_r = 1$. For a detailed description of the operation of MQS sensors and the duality between EQS and MQS sensors, sources [1-5, 7, 9] are suggested readings.

Because we treat the curl of the electric field as zero under the EQS approximation, we can write the electric field as the gradient of a scalar potential:

$$\vec{E} = -\nabla \phi$$  \hspace{1cm} (1.16)

By taking the divergence of the above equation and applying the constitutive relationship from Equation (1.6), one can see that the scalar potential obeys Poisson’s Equation (1.17), and in source-free regions where $\rho_f = 0$, Equation (1.17) reduces to Laplace’s Equation (1.18):

$$-\nabla \cdot \nabla \phi = \nabla \cdot \vec{E}$$  

$$-\varepsilon \nabla^2 \phi = \nabla \cdot \vec{D}$$

$$\nabla^2 \phi = -\frac{\rho_f}{\varepsilon}$$  \hspace{1cm} (1.17)

$$\nabla^2 \phi = 0 ; \; \rho_f = 0$$  \hspace{1cm} (1.18)

A consequence of Laplace’s Equation for planar sensor arrays excited with a spatial periodicity is that solutions for the scalar potential $\Phi$ have evanescent fields that decay exponentially in the direction orthogonal to the sensor plane, even in the absence of a lossy medium. The range of these evanescent fields is proportional to the electrode size and spacing [3, 4]. Figure 1-1 illustrates an EQS sensor with sensitivity at multiple penetration depths [4].

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Present generation quasistatic sensors utilize various coplanar electrode layouts to investigate materials at multiple depths of penetration. Electrodes are often interdigitated (EQS) or meandered (MQS) to achieve excitation patterns with desired periodic spatial wavelength(s) [1, 3-5, 10, 11]. Figure 1-2 shows a generic interdigital EQS sensor where one of the two interdigitated combs is driven by a source voltage, $V_D$, and the current on the other comb, $I_S$, is measured [4]. Such sensors are useful for the nondestructive testing and evaluation (NDT/NDE) of materials, as well as measuring absolute electrical properties [3, 11].
EQS sensor electrodes are typically excited by a known, time-varying voltage with sensor currents measured to determine terminal impedances/admittances (alternatively, electrodes can be driven by a known current with terminal voltages measured). For a given position in space, the current-voltage relation on a sensor is a function of the local electrical properties (permittivity $\epsilon$ and conductivity $\sigma$) of the material(s) near the sensor.

Consider, for instance, the canonical parallel plate capacitor shown in Figure 1-3(a) with plate area, $A$, and spacing, $d$.

![Figure 1-3: Parallel plate capacitor (a) opened to form fringing field capacitor (b).](image)

Ignoring fringing field effects in this parallel-plate configuration, the complex terminal admittance, $Y_{cap}$, is determined by $\epsilon$ and $\sigma$ between the two plates, where the capacitive susceptance goes as:

$$
Imag\{Y_{cap}\} = \frac{\omega \epsilon A}{d}
$$

and the conductance goes as:

$$
Real\{Y_{cap}\} = \frac{\sigma A}{d}
$$
By opening up the capacitor plates into a co-planar geometry, an intentional fringing field sensor is formed, where \( Y_{cap} \) is now a function of the material(s) surrounding the electrodes. The co-planar geometry is convenient when scanning sensors over a material under test at a fixed height. As driven electrodes are scanned over the surface of the material under test, terminal currents vary as local material properties change. Objects, features, and material interfaces can be detected by monitoring these variations in the sensors' currents.

This process is often described as solving the forward problem. Forward sensor problems are in general well-posed in that for a given geometry a unique sensor current response exists. The inverse problem is then to determine absolute material properties or absolute locations of features and objects from the sensor current response. These problems are in general ill-posed, as there does not necessarily exist a single unique solution for a given sensor current response [12]. An illustration of this forward/inverse problem cycle is provided in Figure 1-4.

1.2 Scanning Force Microscopy Methods

Scanning force microscopy (SFM) or atomic force microscopy (AFM) is one of the leading tools for imaging materials at the nanoscale. In general, SFM methods work by scanning (typically raster-scanning) a sharp probe tip over the surface of a
sample, and creating an image of that sample, where the contrast agent for the image comes from variations in a measurable force/interaction between the probe tip and the surface of the material [13-15]. In 1984, Matey and Blanc of RCA Laboratories invented scanning capacitive microscopy (SCM) where they utilized pre-developed instrumentation and pickup circuitry from the RCA CED VideoDisc player [14]. SCM is similar to AFM but specifically targets changes in the electrostatic capacitance between the probe tip and the surface. An image is created by monitoring local changes in capacitance between the probe tip and the sample or a conducting surface under the sample. The capacitance is a function of electrode and sample geometry, as well as the local permittivity of the sample.

While there have been many different approaches toward improving scanning probe microscopy methods—primarily with respect to probe shape, probe guarding, pickup circuitry, and image reconstruction—what has remained common amongst all of the groups attempting to develop high-resolution nanometer scale images via AFM/SCM methods is the use of a single sense electrode. A well known and well documented drawback of the single sense electrode (both guarded and unguarded implementations) is its inherent lack of ability to image/characterize the sample in all three dimensions. While it is possible to scan a single probe over a surface with high lateral resolution and precise vertical control, such a configuration does not provide information for characterizing into the depth of the material under evaluation. Consequently, AFM/SCM images are only capable of providing accurate maps of surface topology and near-surface material properties [13-15].

Another drawback of SCM is that it requires access to an electrical contact beneath the sample being imaged. EQS/MQS arrays are capable of imaging samples without making any direct electrical contact as they work by monitoring the fringing field effects between two or more sensors in the array and how they respond to changes in the sample’s bulk electrical properties.
Large arrays of EQS/MQS electrodes could potentially provide a new class of inspection tools that can quickly scan nanoscale samples (photolithography equipment, ICs, biological samples, etc.) for features, defects, and contaminants at speeds far above the capabilities of current, single-probe technologies due to massive array parallelism. This thesis considers the ability of small arrays (less than ten electrodes) of EQS sensors to detect both surface and subsurface features and objects.

1.3 Thesis Overview

The aim of this thesis is to launch an investigation—solving both forward and inverse problems—into the potential use of EQS sensor arrays for nondestructive evaluation, imaging, and quality control purposes for integrated circuit industry applications. Research into three specific core areas will serve as the primary focus of the thesis:

1.) The use of EQS sensors to penetrate the surface of doped silicon and locate junctions
2.) The use of EQS sensors to locate and image sub-micron-scale surface features and contaminants
3.) An investigation into the inversion of sensor current response signals for determining exact feature dimensions and imaging purposes

In all cases sensors are coplanar and operate at a fixed height over the surface of the material under evaluation.

The first case study is presented in “Chapter 2: Subsurface Sensor Application: Locating a p-n Junction.” This case study serves as a primary investigation into a potentially new technology for mapping and imaging semiconductor devices. The results of this case study are intended to serve as a building block for future research into this new technology. The work comprising this chapter makes use of the commercially available finite element method (FEM)
software package COMSOL Multiphysics [16]. Simulations demonstrate how fringing fields from driven EQS sensors can couple into doped semiconducting substrates by operating sensors at a frequency comparable to the charge relaxation time of the silicon. It is demonstrated how p-n junctions in the substrate can be located by monitoring steady-state sensor currents for harmonic distortion.

The second area of focus is presented in “Chapter 3: Locating Surface Features and Contaminants.” This case study is an investigation into the use of EQS electrode arrays for quickly scanning surfaces for unwanted contaminant particles. One specific application that motivates research into this area is locating and removing contaminant particles on photomasks used in the mass production of integrated circuitry. Section 3.1 provides simulation results of the sensitivity of a EQS sensor array to various contaminant particles located in a gap in the absorber layer of an extreme ultraviolet lithography (EUVL) photomask. Section 3.2 presents the results of a macroscopic-scale laboratory experiment to confirm the results of Section 3.1. Laboratory experiments are performed where samples have similar aspect ratios and material properties to the simulated EUVL masks. Section 3.3 discusses the need for low-noise pickup circuitry for detecting sub-nano-amp variations in sensor currents as they scan past photomask contaminants and surface features.

These first two case studies deal solely with solving well-posed forward problems. The third core area presented in “Chapter 4: Sensor Signal Inversion through a Radial Basis Function Artificial Neural Network” provides one specific algorithm for solving an inverse problem for feature detection and imaging. In Chapter 4 a radial basis function artificial neural network (RBF-ANN) is trained to accurately predict the forward mapping of a feature's physical dimensions into a sensor's impedance response as it scans past the feature. The RBF-ANN is first trained with a small database of COMSOL simulation results to act as a forward function-approximation network. Once the RBF-ANN is trained, it is integrated
into an iterative signal inversion routine that can accurately predict a feature's dimensions when provided a sensor's impedance response and an initial guess.

Thesis results are summarized in "Chapter 5: Conclusions and Suggestions for Future Work."
2 Subsurface Sensor Application: Locating a p-n Junction

This chapter describes how a p-n junction can be detected in a doped semiconductor substrate with an array of non-contact EQS sensors. This case study is a primary investigation into a new methodology for mapping and testing semiconductor devices. The results in this chapter are intended to serve as a building block for future investigation into this technology. Locating device junctions by coupling into them through an air gap could allow for new, fast scanning microscopy methods for IC imaging. IC imaging is useful for verification and detection of fabrication errors as well as detecting hidden Trojan circuits that might be present [17].

This chapter makes use of the commercially available COMSOL Multiphysics finite element method (FEM) simulation package [16]. Two different geometries are simulated in COMSOL to evaluate sensor performance. In both cases, sensors are driven with an AC voltage and held at a fixed height over the surface of a doped silicon substrate. Sensor currents are then measured and monitored for harmonic distortion caused by the junction’s nonlinear drift-diffusion dynamics.

Results demonstrate how EQS sensors’ fringing fields can couple into doped semiconducting substrates by operating sensors at a frequency comparable to the charge relaxation time of the silicon bulk. The frequency bandwidth over which these junctions are detectable is presented, illustrating both the capabilities and limitations of EQS sensors for such an application.
2.1 The p-n Junction Diode

The p-n junction is a fundamental component of many semiconductor devices including diodes, solar cells, and transistors. A p-n junction is the interface between a positively doped p-type region (where there exists a greater concentration of free holes than free electrons), and a negatively doped n-type region (where there exists a greater concentration of free electrons than free holes). The abrupt discontinuity in carrier concentrations that exists when the two regions meet forms a device with a nonlinear current-voltage relationship.

The two ways in which electrical current can flow in a semiconductor are due to carrier drift and carrier diffusion. Carrier drift exists due to the Coulombic force experienced by free charge carriers (electrons and holes) under the influence of an electric field, while carrier diffusion is the natural tendency for free carriers to flow along a concentration gradient in an attempt to equilibrate. The total current density for holes inside a semiconductor \( J_p \) is simply the sum of these two currents:

\[
J_p = J_{p,\text{drift}} + J_{p,\text{diffusion}}
\]

\[
J_p = q\mu_p E - qD_p \nabla p
\]  

(2.1)

(2.2)

and the total current density for electrons \( J_n \) is:

\[
J_n = J_{n,\text{drift}} + J_{n,\text{diffusion}}
\]

\[
J_n = q\mu_n E + qD_n \nabla n
\]

(2.3)

(2.4)

where \( p \) and \( n \) are the concentrations of holes and electrons in \([1/cm^3]\), \( \mu_p \) and \( \mu_n \) are the hole and electron mobilities in \([cm^2/V\cdot s]\) (taken to be positive numbers), \( D_p \) and \( D_n \) are the hole and electron diffusivities in \([cm^2/s]\), and \( q \) is the magnitude of charge of an electron \( (1.602(10^{-19})[C]) \), all satisfying the Einstein Relation:
\[ \frac{D_p}{\mu_p} = \frac{D_n}{\mu_n} = \frac{kT}{q} \] 

(2.5)

With \( \vec{J}_p \) and \( \vec{J}_n \) defined as such, the total free current density \( \vec{J} \) is then:

\[ \vec{J} = \vec{J}_p + \vec{J}_n \]

\[ \vec{J} = q(\mu_p p + \mu_n n)\vec{E} + q(-D_p \nabla p + D_n \nabla n) \]

(2.6)

When a p-n junction is formed, the steep gradients in carrier concentrations cause free hole and electrons to diffuse across the junction. Figure 2-1 (a)-(c) illustrates this. As a result, each region is no longer charge neutral and a space charge layer begins to form on each side of the junction (Figure 2-1(d)). This charge imbalance produces an electric field across the junction that acts to "push" holes and electrons—via carrier drift—back up the concentration gradient as seen in Figure 2-1 (e). This region of charge imbalance is known as the depletion region. Static equilibrium is achieved when carrier drift balances out carrier diffusion. Under static equilibrium, there then exists a built-in potential across the p-n junction even when the diode is unexcited by an external source shown in Figure 2-1 (f) [18].

When the diode is excited by an external voltage source, it is no longer under static equilibrium. Under forward bias—where the p-region potential is excited at a higher potential than the n-region—free holes in the p-region and free electrons in the n-region are pushed toward the depletion region. As the bias is increased, the depletion region narrows and the built-in electric field is unable to balance carrier diffusion across the junction; at a large enough forward biasing potential, diffusion then overcomes drift and the diode can conduct significant current. Under reverse biasing conditions, where the p-region potential is excited at a lower potential than the n-region, free holes in the p-region and free electrons in the n-region are now...
pulled away from the depletion region. Consequently, the diode fails to conduct a significant current across the junction (unless the potential is increased to such a high level that the diode breaks down [18]). Since the diode conducts differently under forward and reverse bias, it forms a device with a nonlinear current—voltage relationship. For a more detailed explanation on p-n junction physics, the sources [18, 19] are suggested readings.

Figure 2-1: p-n Junction under static equilibrium.
2.2 Coupling into a p-n Junction Diode through an Air Gap

A p-n diode can be repeatedly turned on and off by applying a sinusoidal voltage to a terminal pair that is electrically connected to the diode's two differently doped regions. This creates a terminal current that is inherently nonlinear. If we look at the frequency spectrum of this diode current, we would see that there exist contributions to the total current at integer multiples of the fundamental drive frequency. We say that the diode current then experiences a harmonic distortion where this harmonic distortion is solely due to the nonlinear drift-diffusion barrier between the p-type and n-type regions described in the previous section.

The challenge of this chapter is to determine if p-n junctions can be coupled into and turned on and off by driven EQS electrodes without making any direct electrical contact to either of the p-type or n-type regions. One can imagine scanning an array of two (or more) voltage driven EQS electrodes at a fixed height over the surface of a semiconductor that has doped into it several p-type and n-type regions that form nonlinear drift-diffusion barriers at each of their interfaces. If these electrodes are positioned so that they are not over the top of any junctions—for instance they might be over top of a large p-type bulk region with no n-type wells doped into it—then the current on these sensors will be linear and experience no harmonic distortion whatsoever. However, if two of these sensors are located over the top of a p-n junction, then they might manage to couple into that junction, repeatedly turning it on and off over time causing harmonic distortion in the sensor currents. One can then imagine scanning a massive array of these electrodes over the surface of a semiconductor and monitoring the individual sensor currents for harmonic distortion. This concept could then provide a new, fast-scanning method for mapping and imaging the semiconducting layers of an integrated circuit, where doped wells and junctions are located by looking for these higher harmonics in the sensors' current responses.
Two different geometries were simulated in COMSOL to investigate the ability and sensitivity of EQS sensors in locating a p-n junction. The setup and the results of each of these two case studies are summarized in Sections 2.3—2.6.

2.3 FEM Model #1 Setup

2.3.1 Geometric Properties

A geometry was drawn in COMSOL to represent a silicon p-n junction diode with an air-filled region interfacing one of the diode's sides. The simulation was performed using two-dimensional solvers for simplicity, so all results presented in this chapter are in per-unit-depth format. This first geometry under evaluation is shown in Figure 2-2 with important geometric dimensions listed in Table 2-1.
Figure 2-2: COMSOL geometry #1 to be analyzed.

Table 2-1: Key geometric dimensions for geometry #1

<table>
<thead>
<tr>
<th>Dimension</th>
<th>Length [μm]</th>
</tr>
</thead>
<tbody>
<tr>
<td>silicon region horizontal dimension</td>
<td>5</td>
</tr>
<tr>
<td>air-filled region horizontal dimension</td>
<td>6</td>
</tr>
<tr>
<td>p-type region vertical dimension</td>
<td>6</td>
</tr>
<tr>
<td>n-type region vertical dimension</td>
<td>6</td>
</tr>
<tr>
<td>sensor horizontal dimension</td>
<td>0.2</td>
</tr>
<tr>
<td>sensor vertical dimension</td>
<td>2.75</td>
</tr>
<tr>
<td>sensor-silicon air gap</td>
<td>0.1</td>
</tr>
<tr>
<td>sensor-sensor inner edge-to-edge spacing</td>
<td>1.8</td>
</tr>
</tbody>
</table>
2.3.2 Physical Properties

The silicon region was doped to represent a p-n junction at the interface shown in Figure 2-2. In the interest of achieving numerical convergence in COMSOL, an abrupt, discontinuous "step-junction" was not specified; rather, the dopant concentration function, $N$, was described using a Gaussian function with a very steep drop-off constant, $c_d$:

$$
N = \begin{cases} 
2N_{D_{n_{\text{max}}}}e^{-\left(\frac{y-y_1}{c_d}\right)^2} - N_{A_{p_{\text{max}}}}, & y > y_1 \\
N_{D_{n_{\text{max}}}}, & y \leq y_1 
\end{cases} 
$$

(2.7)

where $N_{D_{n_{\text{max}}}}$ is the maximum donor (n-type) doping concentration and $N_{A_{p_{\text{max}}}}$ is the maximum acceptor (p-type) doping concentration. A negative value for $N$ indicates a doping of acceptor atoms, while a positive value indicates a doping of donor atoms. By specifying the dopant concentrations in this manner, a p-n step junction is created with a smooth but still steep concentration function rather than a sharp, discontinuous function over several orders of magnitude ($N$ changes on the order of $10^{22}$ [1/m$^3$] across the junction).

The relevant physical parameter values assigned to the silicon region are listed in Table 2-2.

**Table 2-2: Electrical parameters used in FEM simulation**

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>$N_{D_{n_{\text{max}}}}$: maximum n-type doping</td>
<td>$10^{16}$</td>
<td>[1/cm$^3$]</td>
</tr>
<tr>
<td>$N_{A_{p_{\text{max}}}}$: maximum p-type doping</td>
<td>$10^{16}$</td>
<td>[1/cm$^3$]</td>
</tr>
<tr>
<td>$n_i$: intrinsic impurity concentration for Si</td>
<td>$1.46(10^{10})$</td>
<td>[1/cm$^3$]</td>
</tr>
<tr>
<td>$\mu_p$: hole mobility</td>
<td>400</td>
<td>[cm$^2$/Vs]</td>
</tr>
<tr>
<td>$\mu_n$: electron mobility</td>
<td>800</td>
<td>[cm$^2$/Vs]</td>
</tr>
</tbody>
</table>
The semiconductor problem was solved by coupling together two COMSOL Multiphysics modules: an electrostatics module to solve Poisson's Equation (Equation (1.17)) for the electric scalar potential and a convection and diffusion module to describe the drift-diffusion carrier dynamics through a source continuity equation. Hole and electron flows are described with separate modules where the flow of holes is described with the following differential equation:

$$\frac{\partial p}{\partial t} + \nabla \cdot \left( -D_p \nabla p - \mu_p p \nabla \Phi \right) = R_p - G_p$$  \hspace{1cm} (2.8)

and the flow of electrons satisfies the following differential equation:

$$\frac{\partial n}{\partial t} + \nabla \cdot \left( -D_n \nabla n + \mu_n n \nabla \Phi \right) = R_n - G_n$$  \hspace{1cm} (2.9)

where $R$ and $G$ are the recombination and generation terms, respectively. For this analysis $R$ and $G$ can be set to zero—as there is no recombination/generation in the
bulk or depletion regions—and equations (2.8)—(2.9) then reduce to Equation (1.11). These drift/diffusion solvers for \( p \) and \( n \) are coupled to the Poisson's Equation solver through the free space charge density \( \rho_f \):

\[
\rho_f = q(N - n + p)
\] (2.10)

In a uniformly doped semiconductor region, the net charge in that region is zero and Equation (2.10) reduces to:

\[
(N - n + p) = 0
\] (2.11)

Additionally, \( n \) and \( p \) are related through the np product:

\[
np = n_i^2
\] (2.12)

where \( n_i^2 \) is the intrinsic impurity concentration. Equations (2.11) and (2.12) provide two equations and two unknowns. Solving these two equations allows us to provide the solver with an initial equilibrium value on \( p \) and \( n \) in the silicon region:

\[
\begin{align*}
p_{\text{init}} &= \left\{ \begin{array}{ll}
\frac{|N|}{2} + \sqrt{\left(\frac{N}{2}\right)^2 + n_i^2}, & N < 0 \\
\frac{|N|}{2} + \sqrt{\left(\frac{N}{2}\right)^2 + n_i^2}, & N \geq 0
\end{array} \right. \\
n_{\text{init}} &= \left\{ \begin{array}{ll}
\frac{|N|}{2} + \sqrt{\left(\frac{N}{2}\right)^2 + n_i^2}, & N < 0 \\
\frac{|N|}{2} + \sqrt{\left(\frac{N}{2}\right)^2 + n_i^2}, & N \geq 0
\end{array} \right.
\end{align*}
\] (2.13)

(2.14)
The initial, static equilibrium value for the built in potential in the semiconductor region is:

\[
\phi_{\text{init}} = \begin{cases} 
-kT \ln \left( \frac{p_{\text{init}}}{n_i} \right), & N < 0 \\
-kT \ln \left( \frac{n_{\text{init}}}{n_i} \right), & N \geq 0 
\end{cases}
\]  

(2.15)

Figure 2-3: Boundary conditions for COMSOL geometry #1.

The boundary conditions for both the electrostatics module and the convection and diffusion modules are shown in Figure 2-3. The insulation boundary conditions truncate the solution space by forcing the normal component of \( \vec{D} \) and \( \vec{j} \) to be zero. The boundary conditions at the top of the p-type region and the bottom of the n-type region force the electric potential and hole and electron concentrations to their initial values \( \phi_{\text{init}} \), \( p_{\text{init}} \), and \( n_{\text{init}} \), respectively. These boundaries represent
un-driven electrical contacts. The continuity boundary condition that divides the p-type and n-type regions exists solely for the purpose of mesh refinement near the active depletion region and adds no additional constraints to the solution. The electric potential boundary conditions on the EQS sensors allow us to impose a known AC voltage onto each of the sensors. Since the silicon region has a different permittivity and conductivity than that of the air-filled region, the normal component of the electric displacement vector $\vec{D}$ is discontinuous, and the relevant boundary condition is a surface charge boundary condition:

$$\hat{n} \cdot (\vec{D}_{air} - \vec{D}_{si}) = \rho_s$$

(2.16)

where $\hat{n}$ points from the silicon region into the air-filled region. Since $\rho_s$ is not known beforehand and is time-varying, the source continuity boundary condition

$$\hat{n} \cdot (\vec{j}_{air} - \vec{j}_{si}) = -\frac{\partial \rho_s}{\partial t}$$

(2.17)

is solved simultaneously. Since carriers cannot diffuse across the silicon-air interface, it is also necessary to apply COMSOL's "convective flux only" boundary conditions to the convection and diffusion solvers.

Additional details regarding the COMSOL model properties and solver settings for FEM Model #1 can be found in Appendix B.

### 2.4 FEM Model #1 Simulation Results

This section provides the results of several COMSOL simulations that were run with the parameters and settings from Section 2.3. Figure 2-4, Figure 2-5, and Figure 2-6 show the initial values for the carrier concentrations $p$ and $n$, space charge density $\rho_s$, and electric potential $\Phi$, respectively. These figures match the
description of p-n junction behavior under static equilibrium from Section 2.1. Figure 2-4 illustrates the sharp roll-off in the hole concentration from the p-type region into the n-type region and the same behavior for electrons from the n-type region into the p-type region. Figure 2-5 shows the space charge layers that are formed on each side of the junction, and Figure 2-6 shows the resulting built-in potential to be approximately 0.694V across the junction. This makes sense, because the theoretical built-in potential for an abrupt p-n step junction is [18]:

\[
V_{bi} = \frac{kT}{q} \ln \left( \frac{n_n p_p}{n_i^2} \right) = 0.695 \text{[V]}
\]  

(2.18)
The sensors were driven by an AC voltage, and the resulting current on the upper electrode was measured. The current was measured by integrating the surface charge density on the electrode's surface to get the total charge on the electrode $Q_{\text{sensor}}$ and then taking the time derivative of the total charge:
To simulate guarding—and to increase the sensitivity of the current response to the semiconductor region—only a portion of the sensor's surface was integrated. Figure 2-7 shows the integration path that was chosen along the upper sensor. Figure 2-8 shows a sensor drive scheme, with individual guard electrodes shown, that motivates this integration path approximation. The integration path on the upper electrode in Figure 2-7 represents the upper sense electrode in Figure 2-8, while the rest of the upper electrode in Figure 2-7 represents the two surrounding guards for the upper electrode in Figure 2-8. With such a configuration, guard electrodes shunt the fields from the sense electrodes toward the silicon bulk, thus increasing sensitivity.

![Figure 2-7: Integration path (shown in red) for surface charge density integration to simulate guarded electrodes in Figure 2-8.](image-url)
2.4.1 Charge Relaxation

In order for a significant portion of the sensors' fields to penetrate the semiconducting bulk, the AC excitation frequency must be on the order of the charge relaxation break frequency of the material, \( f_{\text{break}} \), where:

\[
f_{\text{break}} = \frac{\sigma}{2\pi\varepsilon}
\]  

For frequencies much lower than \( f_{\text{break}} \), the region appears as a conductor to the sensors because free charge in the bulk has ample time to migrate to the surface and terminate the electric field as a surface charge. On the other hand, for frequencies much higher than \( f_{\text{break}} \), the region appears as an insulator because the fields alternate far too quickly for a significant amount of free bulk charge to migrate to the surface. For a homogeneous semiconductor:

\[
\sigma = q(\mu_n n + \mu_p p)
\]
so the conductivities of the p-region and n-regions will vary due to the difference in hole and electron mobilities (listed in Table 2-1):

\[
\sigma_{p,\text{region}} \approx 64 \frac{S}{m} \quad ; \quad \sigma_{n,\text{region}} \approx 128 \frac{S}{m}
\]

The charge relaxation break frequencies are then:

\[
f_{\text{break},p} \approx 97.5\text{GHz} \quad ; \quad f_{\text{break},n} \approx 195\text{GHz}
\]

In order to get deep penetration of fields into the silicon region, it is then desirable to operate the sensors at a frequency comparable to \( f_{\text{break}} \).

### 2.4.2 Results

Simulations were run at 1GHz, 5GHz, 10GHz, 50GHz, and 100GHz with the upper and lower sensors excited as follows:

\[
\begin{align*}
V_{\text{upper}} &= 15 \sin(2\pi ft) \text{ [V]} \\
V_{\text{lower}} &= -15 \sin(2\pi ft) \text{ [V]}
\end{align*}
\]

For each of these cases, the upper sensor current was measured using the integration path shown in Figure 2-7. A Fast Fourier Transform (FFT) was performed to determine if the junction’s nonlinear dynamics were reflected in the sensor current’s frequency spectrum. Figure 2-9 – Figure 2-14 show the results of the FFT for each of the five different fundamental operating frequencies.
Figure 2-9: FFT of sensor current magnitude per unit depth [A/m] at 1GHz fundamental drive. In this lower frequency limit, no harmonic distortion is witnessed in the sensor current.

Figure 2-10: FFT of sensor current magnitude per unit depth [A/m] at 5GHz fundamental drive. Harmonic distortion begins to show up in the sensor current.
Figure 2-11: FFT of sensor current magnitude per unit depth [A/m] at 10GHz fundamental drive.

Figure 2-12: FFT of sensor current magnitude per unit depth [A/m] at 50GHz fundamental drive.
These results can be summarized and compared by examining the ratio of the second harmonic component of the current to the first harmonic component (as shown in Figure 2-14).

Figure 2-14: Ratio of 2nd harmonic amplitude to 1st harmonic amplitude (expressed as a percentage) vs. fundamental drive frequency [Hz].
In the low frequency limit (1GHz), it is clear that the p-n junction cannot be detected. The FFT in Figure 2-9 fails to show any noticeable harmonic distortion to the sensor current. As stated previously, this is most likely due to the fact that the excitation frequency is too low compared to the charge relaxation break frequency of the silicon regions. For visual confirmation that this is the case, Figure 2-15 shows a colormapped surface plot of the scalar potential at time $t = \frac{T}{10}$ where $T$ is the excitation period [$10^{-9}$ s]. The scale of the colormapped surface plot is truncated to $-2V \leq \Phi \leq 2V$. This is done to highlight variations in the semiconductor where the potential varies less than in the air-filled region. At 1GHz, there exists only a weak and shallow gradient in scalar potential in the semiconducting region due to the sensors; consequently, the sensors are only capable of turning the diode on and off at a very shallow depth. Moreover, a majority of the junction remains in its static equilibrium state, and the sensor current is heavily dominated by the linear air gap capacitance.

![Figure 2-15: Scalar potential [V] at t=T/10 for 1GHz drive.](image)

As the excitation frequency is raised, harmonic distortion begins to show up in the sensor current. Figure 2-14 shows approximately a 21:1 ratio in the first to
second harmonic components of the sensor current at 10GHz. Colormapped surface plots of the scalar potential and space charge density for the 10GHz excitation are provided in Figure 2-16 for several times during the first excitation period. These snapshots in time are taken every $\frac{T}{10}$ seconds for the first full excitation period. At time $t = 0$, the system is under static equilibrium. At $t = \frac{T}{10}$ there exists a large forward bias across the junction and the space charge layer begins to thin out as the diode conducts current. The imbalance in penetration depths between the p-type and n-type regions is due to the difference in conductivities (Equation (2.21)). At $t = 2\frac{T}{10}$, the sensor excitation is still on its rising edge, but free charge in the semiconducting bulk begins to resist field penetration. By $t = 4\frac{T}{10}$ a significant amount of image charges have migrated to the silicon-air interface to terminate the electric fields, forming an air-gap capacitor. It can be seen that the diode is entering a reverse bias while the sensors are still forward biased. By $t = 5\frac{T}{10}$ the space charge layer has begun to grow as the diode is increasingly reverse biased. At this point the sensors are halfway through one period and the phase difference between the sensor excitation and the semiconductor dynamics is obvious. By $t = 9\frac{T}{10}$, image charges in the bulk have caught up with the sensors to again form an air-gap capacitor as was the case at time $t = 4\frac{T}{10}$, and the space charge layer begins to diminish as the diode enters forward bias. At $t = T$ the simulation has completed one full period and the junction is forward biased.

When taking the FFT of the sensor current's steady state response, it is important to ignore this first transient period and to only consider the sensor current once it has reached sinusoidal steady state.
(a3) Potential [V]  \( t = \frac{3}{10} \)  (b3) Charge Density [C/m³]

(a4) Potential [V]  \( t = \frac{4}{10} \)  (b4) Charge Density [C/m³]

(a5) Potential [V]  \( t = \frac{5}{10} \)  (b5) Charge Density [C/m³]
Figure 2-16: Colormapped surface plots of scalar potential [V] (a1—a10) and space charge density [C/m³] (b1—b10) at intervals of length T/10 for 10GHz excitation.

The space charge density plots of Figure 2-16 show the depth to which the junction conducts. Figure 2-17 helps to illustrate this by superimposing electric field streamlines on top of the space charge density plot in the silicon region at $t = T$ when the junction is forward biased. The junction conducts to a depth of approximately 2µm. Below this depth, streamlines can be seen terminating on the space charge layer, forming a junction capacitance. Additionally, some streamlines
can be seen terminating on the upper and lower boundaries of the solution space that represent undriven electrical contacts.

In the high frequency limit (100GHz), the harmonic distortion in the sensor current begins to diminish. This makes sense as this is likely due to junction capacitance beginning to short out the nonlinear diode. Since the high frequency behavior of a capacitor is to act as a short circuit, this linear path dominates the diode current. There is then no benefit in operating the sensors at such a high frequency. For this specific geometry, there is an apparent “sweet spot” between 10GHz and 50GHz where the junction is able to be detected. In this range the second harmonic current amplitude rises to over 4% of the fundamental (as shown in Figure 2-14).
2.5 FEM Model #2 Setup

A second model was drawn in COMSOL to simulate the more realistic geometry of a p-type well doped into an n-type substrate. In this case the p-type well is not in contact with a boundary that can directly source carriers into the p-type region; rather the well is “floating” and does not extend down to the bottom of the silicon region. Consequently, for free charge carriers to exist in this region they must either be initially doped in or migrate in across the p-n junction. The COMSOL setup for this geometry is described in Sections 2.5.1 – 2.5.3, and the results of the simulation are presented in Section 2.6.

2.5.1 Geometric Properties

The geometry under evaluation is shown in Figure 2-18. An array of three coplanar sensors is centered above a p-type well that is doped into an n-type silicon substrate. The sensors reside in an air-filled region above the surface of the silicon region at a fixed height. A zoomed-in version of the geometry is provided in Figure 2-19 and important dimensions are listed in Table 2-3. For this geometry, sensors are driven by an AC voltage with the outer two electrodes driven 180° out of phase with respect to the center electrode.
Figure 2-18: COMSOL geometry #2 to be analyzed.

Figure 2-19: Zoomed-in version of COMSOL geometry #2 to show important geometric dimensions.
Table 2-3: Key geometric dimensions for geometry #2

<table>
<thead>
<tr>
<th>Dimension</th>
<th>Length [µm]</th>
</tr>
</thead>
<tbody>
<tr>
<td>p-well width</td>
<td>6</td>
</tr>
<tr>
<td>p-well depth</td>
<td>1</td>
</tr>
<tr>
<td>sensor-silicon air gap</td>
<td>0.2</td>
</tr>
<tr>
<td>sensor height</td>
<td>0.2</td>
</tr>
<tr>
<td>center sensor width</td>
<td>4</td>
</tr>
<tr>
<td>side sensor widths</td>
<td>2</td>
</tr>
<tr>
<td>sensor-sensor spacing</td>
<td>2</td>
</tr>
</tbody>
</table>

2.5.2 Physical Properties

The silicon region was doped to represent a p-type well floating in an n-type bulk. As was the case in Section 2.3.2—in the interest of achieving numerical convergence in COMSOL—an abrupt, discontinuous "step-junction" was not specified; rather, the dopant concentration function, $N$, was described using Gaussian functions with a drop-off constant $c_d$:

$$
N = N_{Dn} + N_{Dnmax}e^{-\frac{(y+y')^2}{c_d^2}} - N_{Apmax}e^{-\frac{(y-x')^2}{c_d^2}} \times \begin{cases} 
1, & -x' < x < x' \\
\frac{1}{e}, & x \geq x'
\end{cases} 
$$

(2.24)

where $N_{Dnmax}$ is the maximum donor (n-type) doping concentration, $N_{Apmax}$ is the maximum acceptor (p-type) doping concentration, and $N_{Dn}$ is the doping concentration of a majority of the n-type bulk representing an epitaxial layer. The parameter $y'$ represents the depth at which the n-type doping function begins to
smoothly transition from $N_{Dn_{\text{max}}}$ to $N_{Dn}$ and has a value of 18\,\mu m. The parameter $x'$ represents the horizontal positions at which the doping function begins to smoothly transition from $N_{Ap_{\text{max}}}$ to $N_{Dn}$ and has a value of 2\,\mu m. A summary of the physical parameters assigned to the silicon region is provided in Table 2-4.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>$N_{Dn_{\text{max}}}$: maximum n-type doping</td>
<td>$10^{16}$</td>
<td>[1/cm$^3$]</td>
</tr>
<tr>
<td>$N_{Ap_{\text{max}}}$: maximum p-type doping</td>
<td>$10^{16}$</td>
<td>[1/cm$^3$]</td>
</tr>
<tr>
<td>$N_{Dn}$: n-type epitaxial layer doping</td>
<td>$10^{15}$</td>
<td>[1/cm$^3$]</td>
</tr>
<tr>
<td>$n_i$: intrinsic impurity concentration for Si</td>
<td>$1.46(10^{10})$</td>
<td>[1/cm$^3$]</td>
</tr>
<tr>
<td>$\mu_p$: hole mobility</td>
<td>200</td>
<td>[cm$^2$/Vs]</td>
</tr>
<tr>
<td>$\mu_n$: electron mobility</td>
<td>800</td>
<td>[cm$^2$/Vs]</td>
</tr>
<tr>
<td>$k$: Boltzmann's constant</td>
<td>$1.38(10^{-23})$</td>
<td>[J/K]</td>
</tr>
<tr>
<td>$T$: temperature</td>
<td>300</td>
<td>[K]</td>
</tr>
<tr>
<td>$q$: elementary electric charge</td>
<td>$1.602(10^{-19})$</td>
<td>[C]</td>
</tr>
<tr>
<td>$\varepsilon_r$: Si relative permittivity</td>
<td>11.8</td>
<td>--</td>
</tr>
<tr>
<td>$c_d$: doping fall-off constant</td>
<td>0.659</td>
<td>[\mu m]</td>
</tr>
<tr>
<td>$\gamma_1$: doping fall-off position</td>
<td>-0.3</td>
<td>[\mu m]</td>
</tr>
</tbody>
</table>

2.5.3 Solver Properties

The COMSOL geometry is solved using the same sets of equations provided in Section 2.3.3. The relevant boundary conditions are shown in Figure 2-20.
Additional details regarding the COMSOL model properties and solver settings for FEM Model #2 can be found in Appendix C.

### 2.6 FEM Model #2 Simulation Results

This section provides the results of several COMSOL simulations that were run with the parameters and settings described in Section 2.5. Figure 2-21 and Figure 2-22 show the initial distribution of free holes and free electron in the silicon region, respectively. The Gaussian-shaped roll-off of the large concentration of free holes in the p-well to the much lower concentration in the n-type bulk is evident in Figure 2-21; the same is true for the electron distribution in Figure 2-22. Figure 2-23 shows the initial scalar potential distribution. The figure shows a built-in
equilibrium potential of approximately 0.6 V across the p-n junction. The equilibrium space charge layers (depletion region) that sets up this built-in potential bias is shown in Figure 2-24.

Figure 2-21: \( \log_{10} \) (initial concentration of holes) in \([1/m^3]\) displayed as a 3-D (left) and 2-D (right) colormap.

Figure 2-22: \( \log_{10} \) (initial concentration of electrons) in \([1/m^3]\) displayed as a 3-D (left) and 2-D (right) colormap (note: 3-D view is shown at a reverse angle of Figure 2-21).
Figure 2-23: Initial scalar potential distribution [V]. There exists a built-in equilibrium potential of approximately 0.6 V across the p-n junction.

Figure 2-24: Initial space charge density [C/m³] zoomed in near p-well to illustrate the width of the depletion region.
Sensors were driven with an AC voltage such that the center electrode was 180° out of phase from the two outer electrodes:

\[ V_{\text{center}} = 5 \sin (2\pi ft) \]  \hspace{1cm} (2.25)
\[ V_{\text{outer}} = -5 \sin (2\pi ft) \]  \hspace{1cm} (2.26)

Simulations were run at operating frequencies of 500MHz, 1GHz, 5GHz, 10GHz, and 50GHz. This range was chosen for the same reasons described in Section 2.4.1, but the range is slightly lower in frequency than those chosen for FEM Model #1 because the hole mobility was reduced from 400 [cm²/Vs] to 200 [cm²/Vs] and the n-type region doping was reduced from 10¹⁶ [1/cm³] to 10¹⁵ [1/cm³]. These frequencies should then demonstrate the lower and upper frequency limits of the sensor operation with respect to charge relaxation in the silicon regions. For each of these cases, the center electrode's current was measured using the integration path shown in Figure 2-25. This integration path simulates top-side guarding of the center electrode and increases the sensitivity of the current response to the semiconductor region. Top-side guarding shunts the electric fields from the center electrode into the bulk and prevents them from fringing through the air-filled region above the sensors. An FFT was performed to determine if the junction's nonlinear dynamics were reflected in the sensor current. Figure 2-26 – Figure 2-30 provide the FFT results.
Figure 2-25: Integration path for simulating a guarded electrode.

Figure 2-26: FFT of sensor current magnitude per unit depth [A/m] at 500MHz fundamental drive.
Figure 2-27: FFT of sensor current magnitude per unit depth [A/m] at 1GHz fundamental drive.

Figure 2-28: FFT of sensor current magnitude per unit depth [A/m] at 5GHz fundamental drive.
Figure 2-29: FFT of sensor current magnitude per unit depth [A/m] at 10GHz fundamental drive.

Figure 2-30: FFT of sensor current magnitude per unit depth [A/m] at 50GHz fundamental drive.
These results can be compared by examining the ratio of the second harmonic component of the current to the first harmonic component (as shown in Figure 2-31).

As was the case in Section 2.4.2, the junction capacitance appears to short out the diode at high frequencies, and the nonlinearity in the sensor current diminishes. In this case study, however, a low-frequency roll-off is not witnessed. This could be due to the fact that the p-well is relatively shallow and presents the sensors with a much longer junction to turn on than did the first case study. Additionally, some physical parameters were changed: the n-type region had a lower doping than the first case study ($10^{15}$ [1/cm$^3$] vs. $10^{16}$ [1/cm$^3$]), and the hole mobility $\mu_p$ was lower (200 [cm$^2$/V·s] vs. 400 [cm$^2$/V·s]). It may be the case that simulations were not run at a low enough frequency to see the low-frequency roll-off, but numerical convergence became difficult for such long time scales.

![Figure 2-31: Ratio of 2nd harmonic amplitude to 1st harmonic amplitude of center sensor current per unit depth (expressed as a percentage) vs. fundamental drive frequency [Hz].](image-url)
2.7 FEM Model #2 Sensor Scan Results

To this point, the sensors in both the FEM Model #1 and FEM Model #2 simulations have remained stationary. In both cases the sensors were positioned such that they straddled the p-n junctions and were proven to be capable of turning the junctions on and off. To demonstrate the sensors' ability to detect junctions for imaging purposes, sensors need to be scanned laterally over the surface of the silicon region while the frequency spectrum of the sensors' currents are monitored.

In this section, the sensors from FEM Model #2 are scanned laterally past the p-type well with the center sensor currents monitored at multiple positions in space. Figure 2-18 and Figure 2-19 show the geometry under evaluation when the sensors are centered over the p-type well. COMSOL Solver settings are identical to those described in Section 2.5, however, the sensor array is now free to move laterally over the surface of the silicon region at a fixed scan height of 200nm. Figure 2-32 illustrates how the array of three sensors is scanned horizontally over the surface of the silicon region. The sensor array is scanned from 8μm left-of-center to 8μm right-of-center (the position of the sensor head is taken to be the horizontal position of the center of the middle electrode relative to the center of the p-type well) in 2μm increments. For this scan, sensors are driven by an AC voltage at a fundamental frequency of 1GHz.

For each position in space, the frequency spectrum of the magnitude of the center sensor's current is monitored for harmonic distortion. To simulate a guarded electrode, only the charge on the bottom of the center electrode is considered (as shown in Figure 2-25. Again, this simulates top-side guarding of the center electrode and increases the sensitivity of the current response to the semiconductor region.
Figure 2-32: Horizontal scan of sensor array past a p-type well in an n-type bulk. The sensor array is scanned from 8μm left-of-center to 8μm right-of-center in 2μm increments (nine total positions). The sensor array is shown to be moving from its leftmost position (solid sensors) to its rightmost position (dashed sensors).

Figure 2-33: FFT of center sensor current magnitude per unit depth [A/m] when positioned 0μm left-of-center. 1GHz fundamental drive frequency.
Figure 2-34: FFT of center sensor current magnitude per unit depth [A/m] when positioned 2μm left-of-center. 1GHz fundamental drive frequency. False subharmonics are present in the FFT because the sensor current did not reach perfect sinusoidal steady state in the COMSOL simulation. This creates a periodically modulated envelope on the waveform which causes unwanted spikes in the frequency spectrum.

Figure 2-35: FFT of center sensor current magnitude per unit depth [A/m] when positioned 4μm left-of-center. 1GHz fundamental drive frequency. Again, false subharmonics are present in the FFT because the sensor current did not reach perfect sinusoidal steady state in the COMSOL simulation. This creates a periodically modulated envelope on the waveform which causes small, unwanted spikes in the frequency spectrum.
Figure 2-36: FFT of center sensor current magnitude per unit depth [A/m] when positioned 6μm left-of-center. 1GHz fundamental drive frequency.

Figure 2-37: FFT of center sensor current magnitude per unit depth [A/m] when positioned 8μm left-of-center. 1GHz fundamental drive frequency.
The FFT results for the current on the center sensor are shown in Figure 2-33 – Figure 2-37 for the sensor positioned at 0 µm, 2 µm, 4 µm, 6 µm, and, 8 µm to the left of the center of the p-well. Due to the symmetry of the sensor head, results are identical and symmetric for when the array is positioned 2 µm, 4 µm, 6 µm, and, 8 µm to the right of the center of the p-well. In Figure 2-34 and Figure 2-35 false subharmonics are present in the FFTs because the sensor current did not reach perfect sinusoidal steady state in the COMSOL simulation. Since the FFT is fed concatenated copies of the time-domain waveform from COMSOL, this creates a periodically modulated envelope on the waveform which causes small, unwanted spikes in the frequency spectrum that should be ignored.

The results of the full scan from 8µm to the left of the center of the p-well to 8µm to the right of the center are summarized in Figure 2-38. In this figure the ratio of the second harmonic current amplitude to the fundamental current
amplitude is expressed as a percentage for each of the nine positions in space. At +/- 6 µm, with there is a surprisingly low (less than 1%) second harmonic contribution to the center sensor’s current. This was initially unexpected because at these two positions, the center sensor straddles a p-n junction with one of the outer two electrodes. It is likely that the current on the center sensor is then dominated by the coupling to the other side electrode along a purely linear path. Though it is not shown, for the rightmost electrode when positioned at -6 µm (or alternatively the leftmost electrode when positioned at +6 µm), is approximately a 3.25% second-to-first-harmonic ratio. This then makes sense that for these positions, the side electrode that is straddling the junction still experiences significant harmonic distortion, but the center sensor current is dominated by the linear path to the other side electrode.

When the array is perfectly centered over the p-well at 0 µm, there is a strong spike in the harmonic distortion. This is a good quality for imaging purposes. It might then be desirable to design the sensor array to match the specific sizes and spacing of the doped wells to maximize the harmonic distortion experienced by the sensors.

Results from these case studies demonstrate how EQS sensors’ fringing fields can couple into doped semiconducting substrates and detect a p-n junction. The first case study demonstrated a clear bandpass “sweet spot” for sensor operation while the second case study only showed a high frequency roll-off in sensor performance. In both cases, it is important to take away the fact that sensors should be operated at a frequency slightly lower than the charge relaxation break frequency (Equation (2.20)) of the silicon regions to achieve significant penetration of electric fields into the material, but not so high a frequency as to short out the junctions’ nonlinear characteristics. Monitoring sensor currents for nonlinearity in this manner could potentially provide new methods for the imaging of integrated circuits.
3 Locating Surface Features and Contaminants

It was demonstrated in Chapter 2 that EQS sensors are capable of detecting features in the near-surface volume of a material. In the case that the material under evaluation is conducting (or semiconducting as was the case in Chapter 2), it is desirable for the sensors to operate at a frequency comparable to the charge relaxation break frequency (Equation (2.20)) of the material under evaluation to achieve significant penetration of electric fields into the material. In cases where the material under evaluation is highly conducting, sensors are often unable to operate at a high enough frequency to penetrate the materials bulk. For example, copper, which has an electrical conductivity of approximately $5.8 \times 10^6 [S/m]$ and a dielectric constant of $\varepsilon_r = 1$, has a charge relaxation break frequency on the order of $10^{17} [Hz]$ [20]. In this limit, EQS sensors are only able to detect a material’s surface topology or features, defects, and objects that might lie on that material’s surface. If one needed to see features beneath the surface of a good conductor, MQS sensors could be used due to enhanced field penetration depths when operated at low frequencies [4]. This chapter focuses solely on using EQS sensors for detecting features/objects that lie on the surface of a material whose charge relaxation break frequency is much higher than the sensor’s operating frequency.
3.1 Detecting Contaminants on a Photomask

One specific application which serves as the impetus for this chapter's research is locating and removing contaminant particles on photoreticles used in the mass production of integrated circuitry. Typically, photomasks are protected by a thin transparent membrane called a pellicle whose purpose is to catch contaminant particles, keeping them optically out of focus during photolithography. However, a heavily contaminated pellicle or a contaminated photomask might produce flawed devices, and it is thus desirable to know if a photomask and/or pellicle is contaminated. Figure 3-1 illustrates a contaminated photomask with a protective pellicle. As lithography methods continue to operate at smaller and smaller wavelengths, it is becoming more favorable to use pellicle-less masks thus increasing the risk of photomask contamination. As wavelengths become smaller, conventional scattering techniques for detecting contaminants becomes increasingly difficult. This chapter investigates the feasibility of using EQS sensors for detecting contaminants on pellicle-less photomasks.

![Figure 3-1: Illustration of contaminated photomask.](image-url)
3.1.1 Contaminated Photomask Simulation Setup

A geometry was drawn in COMSOL (shown in Figure 3-2) to represent an array of EQS electrodes scanning laterally over the surface of an unprotected extreme ultraviolet lithography (EUVL) photomask. The purpose of setting up this geometry was to analyze how well the array could detect a contaminant particle stuck between two absorbers in an EUVL photomask pattern. Detecting a contaminant stuck in an absorber layer gap represents a worst-case scenario since it is as far away from the sensor head as possible. Key geometric and electrical parameters used in the simulation are summarized in Table 3-1 and Table 3-2 respectively. These parameters were chosen to represent those of a real EUVL photomask [21]. Additional details regarding the COMSOL model properties and solver settings for this geometry can be found in Appendix D.

![Figure 3-2: COMSOL geometry for contaminated EUVL photomask simulation. Since simulation is performed on 2D solvers, contaminant object is cylindrical.](image)
Table 3-1: Key geometric dimensions for contaminated EUVL photomask simulation

<table>
<thead>
<tr>
<th>Dimension</th>
<th>Length [nm]</th>
</tr>
</thead>
<tbody>
<tr>
<td>air gap (sensor scan height)</td>
<td>100</td>
</tr>
<tr>
<td>absorber layer vertical thickness</td>
<td>70</td>
</tr>
<tr>
<td>individual sensor horizontal dimension</td>
<td>100</td>
</tr>
<tr>
<td>individual sensor vertical dimension</td>
<td>30</td>
</tr>
<tr>
<td>total sensor head horizontal width</td>
<td>880</td>
</tr>
<tr>
<td>absorber layer air gap horizontal width</td>
<td>100</td>
</tr>
<tr>
<td>contaminant particle radius</td>
<td>35</td>
</tr>
<tr>
<td>guard vertical thickness</td>
<td>40</td>
</tr>
<tr>
<td>sensor – sensor horizontal spacing (inner edge-to-edge)</td>
<td>50</td>
</tr>
<tr>
<td>Spacing between center two sensors (inner edge-to-edge)</td>
<td>80</td>
</tr>
<tr>
<td>sensor – guard horizontal spacing (inner edge-to-edge)</td>
<td>60</td>
</tr>
<tr>
<td>sensor – guard vertical spacing (inner edge-to-edge)</td>
<td>30</td>
</tr>
</tbody>
</table>

Table 3-2: Electrical Parameters used in contaminated EUVL photomask simulation

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>sensor head relative permittivity</td>
<td>3.9</td>
</tr>
<tr>
<td>absorber layer relative permittivity</td>
<td>2</td>
</tr>
<tr>
<td>absorber layer conductivity</td>
<td>10^6 [S/m]</td>
</tr>
<tr>
<td>photoreticle bulk conductivity</td>
<td>PEC</td>
</tr>
<tr>
<td>sensor conductivity</td>
<td>PEC</td>
</tr>
<tr>
<td>sensor frequency</td>
<td>1 [GHz]</td>
</tr>
</tbody>
</table>
Each sensor is driven by a 1GHz sinusoidally varying voltage source with a peak amplitude of 1V. The two rightmost sensors and guard shown in Figure 3-2 are driven 180° out of phase from the two leftmost sensors and guard so as to create a spatial square wave alternating in time.

Because each sensor/guard is treated as a perfect electrical conductor (PECs), we can assume there are no fields inside these regions and thus treat them as electric potential boundary conditions. The EUVL photoreticle bulk (which is a highly conducting EUV wavelength distributed Bragg reflective multilayer [21]) is also treated as a PEC. These boundaries are treated as “Port” boundary conditions in COMSOL which can be used to calculate lumped terminal parameters for the system. Since there are four voltage-driven sensors, two voltage-driven guards, and one floating potential boundary to represent the undriven photoreticle bulk, the EQS system can be represented by a 7x7 admittance matrix:

\[
\begin{pmatrix}
I_{S1} \\
I_{S2} \\
I_{S3} \\
I_{S4} \\
I_{G1} \\
I_{G2} \\
I_B
\end{pmatrix}
= 
\begin{pmatrix}
Y_{11} & Y_{12} & \cdots & Y_{16} & Y_{17} \\
Y_{21} & Y_{22} & \cdots & Y_{26} & Y_{27} \\
\vdots & \ddots & \vdots & \vdots & \vdots \\
Y_{61} & Y_{62} & \cdots & Y_{66} & Y_{67} \\
Y_{71} & Y_{72} & \cdots & Y_{76} & Y_{77}
\end{pmatrix}
\begin{pmatrix}
\hat{V}_{S1} \\
\hat{V}_{S2} \\
\hat{V}_{S3} \\
\hat{V}_{S4} \\
\hat{V}_{G1} \\
\hat{V}_{G2} \\
\hat{V}_B
\end{pmatrix}
\]  

(3.1)

where \( \hat{V}_{S1} - \hat{V}_{S4} \) are the four sensor voltages (indexed from left to right), \( \hat{V}_{G1} - \hat{V}_{G2} \) are the two guard voltages (indexed from left to right), and \( \hat{V}_B \) is the photoreticle bulk voltage. Each of the elements in the admittance matrix, \( Y_{ij} \), represent a mutual admittance coefficient between two ports in the EQS system. By reciprocity, the matrix is symmetric about its main diagonal [22, 23]. Since the bulk is an undriven, floating potential, we do not know \( \hat{V}_B \) directly, but rather that \( I_B = 0 \). We can then solve for \( \hat{V}_B \) in terms of the other six known voltages:
\[ \hat{v}_B = -\frac{(Y_{71}\hat{v}_{S1} + Y_{72}\hat{v}_{S2} + Y_{73}\hat{v}_{S3} + Y_{74}\hat{v}_{S4} + Y_{75}\hat{v}_{G1} + Y_{76}\hat{v}_{G2})}{Y_{77}} \] (3.2)

reduce \( \hat{v}_B \) from the system, and solve for the six unknown currents: \( I_{S1} \), \( I_{S2} \), \( I_{S3} \), \( I_{S4} \), \( I_{G1} \), and \( I_{G2} \).

### 3.1.2 Contaminated Photomask Results

The sensor head shown in Figure 3-2 was scanned laterally past the absorber layer gap at a fixed height of 100nm over the absorber layer’s upper surface. Contaminant particles of various different conductivity and permittivity were placed in the absorber layer gap. The magnitude of each of the four sensor currents as a function of sensor head position were determined using the method described in Equations (3.1)—(3.2). The sensor head position is taken to be its horizontal position relative the center of the gap in the absorber layer.

![Two-dimensional COMSOL simulation results with cylindrical contaminant particle positioned 200nm right of center. In this case, the contaminant particle is characterized by a dielectric constant of \( \varepsilon_r = 4 \). Purple streamlines are electric field lines and the color-mapped contours represent equipotentials (lines of constant voltage [V]).](image.png)
Figure 3-3 shows an electric field plot from COMSOL. In this case a dielectric contaminant with $\varepsilon_r = 4$ is positioned in the absorber layer gap 200 nm to the right of the sensor head center, representing an insulating particle stuck in the gap. The electric field lines from sensor 1 are primarily vertical and terminate on the surface of the absorber layer; this is due to guarding effects caused by sensor 2 and the dedicated guard electrode which are driven at the same magnitude and phase as sensor 1. The high density of equipotentials located between sensor 2 and sensor 3 show they are strongly coupled to each other in this region. Consequently, we can expect these two sensors to be poor at detecting the contaminant particle when stuck in the absorber layer gap. Only a small portion of these sensors' fringing fields will couple to the contaminant particle; this should manifest itself as only a weak change in current when these two sensors scan past the contaminant. Some of the fields from sensor 4 are shown to pass through the dielectric contaminant, while others bend and terminate on the sidewalls of the absorber.

Each of the sensor current magnitude responses are plotted (Figure 3-4) for contaminants of various $\varepsilon_r$ and $\sigma$. Because of the symmetry of the sensor head geometry, the results for sensor 1 and sensor 2 will be identical (but mirror images) of the results for sensor 4 and sensor 3, respectively.

As expected, sensors 1 and 4 react more strongly to the absorber layer gap than sensors 2 and 3. With no contaminant present sensor 1 sees about a 7% change in signal magnitude from the baseline value of 0.083 [A/m] while sensor 2 yields only about a 1.5% change in signal magnitude. In cases where the contaminant particle is a strong dielectric ($\varepsilon_r = 10$) or highly conducting ($\sigma = 1e6$ [S/m]) the sensors can distinguish between a contaminated and clean gap with a difference in signal magnitude of 4% or more from what is expected for a clean gap. In the cases where the contaminant is a poor dielectric or weakly conducting, it becomes increasingly more difficult for the sensors to distinguish between a contaminated and clean photomask.
The widths of the sensors were reduced to 50 nm in attempt to improve sensitivity in detecting contaminant particles. Figure 3-5 shows an electric field plot from COMSOL for the reduced sensor size with a dielectric contaminant particle of $\varepsilon_r = 4$ in the absorber layer gap. Some field lines from sensor 4 can still be seen terminating on the sidewalls and sharp corners of the absorber layer; however, the decrease in sensor size should increase lateral resolution and possibly increase sensitivity to the presence of a contaminant.
Figure 3-5: COMSOL simulation results for reduced sensor size (50nm width) with contaminant particle positioned 130nm right-of-center. Contaminant particle is characterized by dielectric constant of $\varepsilon_r = 4$. Purple streamlines are electric field lines and the colormapped contours represent equipotentials (lines of constant voltage [V]).

The magnitude of current per-unit-depth for sensor 3 and sensor 4 are plotted in Figure 3-6 (again, sensor 1 and sensor 2 have identical, mirror-image responses to sensor 4 and sensor 3, respectively). As expected the sensor 3 current changes very weakly (less than 1%) as it scans past the absorber layer gap. Sensitivity for sensor 4 remains relatively constant compared to the previous case when sensors were 100 nm wide; however, there does exist an improvement in lateral resolution. There is approximately a 7% change in signal magnitude from the baseline value for the case that the gap is clean. In cases where the contaminant particle is a strong dielectric ($\varepsilon_r = 10$) or highly conducting ($\sigma = 1e6$ [S/m]), the sensors can distinguish between a contaminated and clean gap with a difference in signal magnitude of 4% or more from what is expected for a clean gap.
Unlike what was presented in Chapter 2, the contaminant EUVL photomask COMSOL simulations demonstrated that direct fringing field coupling between sensors was not the mechanism for detecting contaminant objects stuck in the absorber layer gap. Rather, it was the variations in the vertically dominant fields from guarded sensors coupling to the highly conducting photomask showing up in the individual sensor currents that made detection possible. For the specific differential drive scheme used in this example, highly conducting bulk floats near zero potential and the circuit essentially reduces to two “half-circuits” separated by an approximate virtual ground. This is again due to EQS sensors’ inherent lack of ability to penetrate the surface of a good conductor due to charge relaxation.

An array of MQS sensors operated at a low excitation frequency would indeed be able to penetrate the surface of the highly conducting absorber layer, which may prove advantageous in features detection; however, the MQS sensor array would not be able to detect dielectric contaminants.
3.2 Laboratory Experiment

A macro-scale laboratory experiment was set up to further investigate the performance of the EQS sensors in detecting contaminants stuck in an absorber layer trench. Sensors and samples were fabricated with material properties and aspect ratios so as to mimic those sensors simulated in the Section 3.1. The goal of the experiment is to confirm simulation results. Due to the scalability of Maxwell’s Equations, it is expected that sensors fabricated at the millimeter size scale will be able to detect and distinguish objects with the same ability as those simulated at submicron sizes assuming dimensions are scaled equally.

Unlike the simulation shown in Figure 3-2 which did not have any direct electrical contact with the sample, the experiments in this section utilize a ground plane beneath conducting samples. As stated previously, this type of configuration is an excellent “half-circuit” approximation to the differentially driven sensor array show in Figure 3-2. Again, this is because the highly conducting sample floats near zero potential in the previous simulation.
3.2.1 Laboratory Setup

The experimental setup is summarized by the block diagram in Figure 3-7. Capacitive sensors were fabricated on a printed circuit board (PCB). These sensors interface with an Analog Devices AD7747 24-bit capacitance-to-digital converter [24]. The AD7747 has a dynamic input range of ±8pF with 10fF precision and can measure a static capacitance of up to 17pF. The AD7747 interfaces with a computer through a USB port. Figure 3-8 is a photograph of the PCB capacitive sensors with one of the sensors connected to the AD7747 (shown to the left) through a SubMiniature Version C (SMC) cable. Shown in the figure are the top sides of six difference capacitive sensors. The bottom of the sensor board is shown in Figure 3-9.
Each capacitive sensor is comprised of three electrodes: a sensor plate, a guard ring, and a top-side guard plate. The top-side guard plate is electrically connected to the guard ring by plated vias. The guard electrodes are driven at the
same voltage as the sensor plate to block stray fields from fringing off the top or sides of the sensor plate and to shunt the fields down toward the sample under evaluation. Figure 3-10 illustrates a side view of a capacitive sensor over a sample; plated vias are shown connecting the guard electrodes on the top and bottom layers of the FR-4 PCB substrate. The AD7747 measures changes in capacitance between the A—B terminal pair show in Figure 3-10 below as the sensor board is scanned laterally over the surface of the sample.

![Figure 3-10: Capacitive sensor (side view).](image)

Referring back to Figure 3-7, the grounded sample rests on an X-Y-Z stage. A milling machine stage with a motor-driven X-axis table feed and an absolute digital X-Y positioner accurate to 0.01mm was used to maintain X-Y precision. A fixed scan height was maintained by a manually-tuned Z-axis jack and set of digital Vernier calipers accurate to 0.01mm.

Samples were prepared to mimic the absorber layer trenches from the photomask that was simulated in the previous section. Aluminum was chosen as the sample material’s substrate because it has an excellent electrical conductivity (approximately $10^7$ [S/m]), it is low cost, and it is easily milled. Trenches of various
cross-sections were milled out of an aluminum bar with a cross-section of 13mm×102mm. Figure 3-11 shows photographs of the milled trench samples.

![Figure 3-11: Trenches milled out of aluminum bar to represent absorber layer gaps of various depths and widths.](image)

Sensors were mounted above the sample by clamping a PCB holder onto a vertical rod extending down from the mill spindle. Photographs of the entire experimental setup are shown in Figure 3-12 and Figure 3-13.
Figure 3-12: Laboratory setup (top view).

Figure 3-13: Laboratory setup (side view).
3.2.2 Experimental Results

Objects of various sizes, cross-sections, and material properties were placed in the trenches to see if a capacitive sensor would be capable of detecting the presence of the objects. These objects ran the length of the trench, and the sensor board was scanned at a fixed height over the surface of the aluminum in a direction perpendicular to the trench. Figure 3-14 illustrates a capacitive sensor scanning over a contaminant filled trench. Figure 3-15 shows photographs of the trench containing six different “contaminant” objects tested in the lab. The six objects that were tested included: a copper rod with square cross-section, a copper cylindrical rod, a stainless steel cylindrical rod, an aluminum cylindrical rod, a styrene plastic cylindrical rod, and polymer modeling clay rolled into a cylindrical rod. The trench, object, and sensor dimensions are summarized in Table 3-3.

Figure 3-14: Capacitive sensor over contaminant filled trench. Contaminants of various shapes, sizes, and material properties were used.
Figure 3-15: Cross-sections of various "contaminant" objects in 5.15mm×9.13mm trench. An empty trench is shown in (a) and the six objects that were tested include: (b) copper rod with square cross-section, (c) copper cylindrical rod, (d) stainless steel cylindrical rod, (e) aluminum cylindrical rod, (f) styrene plastic cylindrical rod, and (g) polymer modeling clay rolled into a cylindrical rod.
Table 3-3: Key geometric dimensions for laboratory experiment

<table>
<thead>
<tr>
<th>Dimension</th>
<th>Length [mm]</th>
</tr>
</thead>
<tbody>
<tr>
<td>trench depth</td>
<td>5.15</td>
</tr>
<tr>
<td>trench width</td>
<td>9.13</td>
</tr>
<tr>
<td>copper square rod side length</td>
<td>3.20</td>
</tr>
<tr>
<td>copper rod diameter</td>
<td>4.76</td>
</tr>
<tr>
<td>stainless steel rod diameter</td>
<td>5.57</td>
</tr>
<tr>
<td>aluminum rod diameter</td>
<td>6.36</td>
</tr>
<tr>
<td>plastic rod diameter</td>
<td>6.36</td>
</tr>
<tr>
<td>polymer clay rod diameter</td>
<td>6.90</td>
</tr>
<tr>
<td>sensor width</td>
<td>5.75</td>
</tr>
<tr>
<td>sensor length</td>
<td>50.5</td>
</tr>
<tr>
<td>sensor - guard ring spacing</td>
<td>3.15</td>
</tr>
<tr>
<td>guard ring width</td>
<td>5.25</td>
</tr>
</tbody>
</table>

The sensor board was scanned at two different fixed scan heights: 5.75mm and 7.75mm. The capacitance between the sensor and grounded aluminum sample vs. the sensor’s horizontal position for each type of contaminant is shown in Figure 3-16 and Figure 3-17. For the highly conducting objects (copper, stainless steel, and aluminum), the family of curves clearly show that the larger the object is, the easier it is to detect. For the case that the sensor scans over the aluminum rod sample, the rod diameter is larger than the trench depth and the capacitance actually rises above its baseline values. For the insulating objects (styrene plastic and polymer modeling clay), both size and dielectric strength determine the sensor’s ability to detect the object. The styrene plastic rod (whose dielectric constant is approximately 2.4) is the same diameter as the aluminum rod, but is much more
difficult for the sensor to detect. The polymer clay rod is only slightly larger than the plastic rod and is well-detected by the sensor. It is likely that the polymer modeling clay has a higher dielectric constant than the styrene plastic.

Comparing Figure 3-16 to Figure 3-17 shows how the sensor's ability to detect the objects degrades when the scan height is increased. For example, for the case that the trench is clean, and the sensors are scanned at a height of 5.75mm, there is a maximum change in the capacitance signal magnitude of 24% of the baseline value; however, when the scan height is increased to 7.75mm, the maximum change in capacitance signal magnitude drops to only 11% of the baseline value.

![Figure 3-16: Sensor-Sample capacitance [pF] vs. horizontal position [mm] for 5.75mm scan height.](image)

Figure 3-16: Sensor-Sample capacitance [pF] vs. horizontal position [mm] for 5.75mm scan height.
The same set of six different “contaminant” objects were then placed in a different trench with dimensions 9.1mm×8.8mm (depth × width). This deeper, narrower trench is expected to make it more difficult for the capacitive sensor to detect and distinguish the objects since a large portion of the electric field lines from the sensor will couple to the corners and upper sidewalls of the trench without detecting the objects; moreover, a much smaller fraction of the field lines will couple to ground through the object sitting in the bottom of the trench. Figure 3-18 provides photographs of the new set of samples. It is shown how the objects reside much deeper in the trench than in the previous case shown in Figure 3-15.
For the same fixed scan heights as before (5.75mm and 7.75mm), the capacitance between the sensor and grounded aluminum sample vs. the sensor's horizontal position is plotted for each type of contaminant; results are summarized in Figure 3-19 and Figure 3-20. As expected, it is much more difficult for the sensor to locate and distinguish the contaminant objects in the deep trench. For example,
for the case that the object is a 6.36mm aluminum rod and the scan height is 5.75mm (shown in Figure 3-19(b)), the capacitance signal magnitude is only approximately 2.4% different than that of the clean trench; increasing the scan height to 7.75mm (Figure 3-20(b)) reduces this same percent difference in signal to about 1.2%.

![Figure 3-19: Sensor-Sample capacitance [pF] vs. horizontal position [mm] for 5.75mm scan height. Figure (b) is a zoomed-in version of the trough in Figure (a).](image1)

![Figure 3-20: Sensor-Sample capacitance [pF] vs. horizontal position [mm] for 7.75mm scan height. Figure (b) is a zoomed-in version of the trough in Figure (a).](image2)
While the experiments in this section were not perfectly scaled replicas of the simulations from Section 3.1, they served to qualitatively confirm the results quite well. For example, in the COMSOL simulation shown in Figure 3-5, sensors are 50 nm wide and scanned at a fixed height of 100 nm over a gap that is 70nm×100 nm (depth × width). In the case where the sensors scan past an empty trench, the signal magnitude on sensor 1 drops to approximately 7% of its baseline value. The experiment that is most similar to this simulation is the case where the 5.75 mm wide sensor is scanned at a fixed scan height of 7.75 mm past a trench that is 5.15 mm×9.13 mm. For the case where the trench is empty, the signal magnitude on the sensor drops to approximately 11% of its baseline value. This is confirmation that when the simulation and experiment are run with similar aspect ratios, the changes in signal magnitudes are likely to be very similar.

The experiment is also capable of quickly providing insights to the limitations of EQS sensors for detecting objects in a deep trench. It was shown that when the six different contaminant objects were placed in a 9.1 mm×8.8 mm (depth × width) trench the sensors’ ability to detect and distinguish the objects degraded severely compared to the case when the trench was 5.15 mm×9.13 mm. This is because a large portion of the electric field lines from the sensor couple to the corners and upper sidewalls of the deeper trench without passing through the contaminant objects. With a much smaller fraction of the field lines coupling to ground through the object in the bottom of the trench, it becomes very difficult to distinguish between different objects.
3.3 Low-Noise Pickup Circuitry

The results from the previous two sections demonstrate a clear need for low-noise circuitry to interface with the sensors. If a typical capacitive current signal fluctuates in response to features at a level that is smaller than the inherent noise levels present in the detection system, then detecting a feature through these signal variations is a lost cause. It is the goal of this section to demonstrate the need for low-noise pickup circuitry through a simple numerical example. The results of this chapter should provide the reader with a basic understanding of thermal noise issues when attempting to detect and amplify weak sensor signals.

Until this point, the COMSOL simulations for the detection of a contaminant particle stuck in an absorber layer gap (Section 3.1) have not considered noise of any sort. This section takes a look at the noise levels that might be encountered from two distinct sources:

1.) Noise due to the absorber layer resistance
2.) Noise due to the pickup circuitry required to monitor variations in sensor currents

This analysis is based on the same geometry that was evaluated in Section 3.1. The geometry is repeated below in Figure 3-21 for the reader's convenience, and key geometric and electrical properties are listed in Table 3-1 and Table 3-2.
The previous figure shows the sensor array at a height of 100nm above the absorber layer of the photomask. In this section, we will only consider the leftmost sensor (referred to as “sensor 1” in Section 3.1). As a reminder, each sensor is driven by a 1GHz sinusoidally varying voltage source with a peak amplitude of 1V. The two rightmost sensors and guard are driven 180° out of phase from the two leftmost sensors and guard so as to create a spatial square wave alternating in time. Since the sensor we are considering is guarded on the top and both sides by electrodes that are driven by a voltage at the same magnitude and phase, its electric field lines will be primarily vertical and couple to the absorber surface directly below it. This is illustrated in Figure 3-3.

We can then assume that the sensor-substrate interaction can be accurately modeled as a lumped air-gap capacitance, $C_{air}$, in series with an absorber layer resistance, $R_{absorb}$. In order to determine values for these parameters we first plot
the electric potential along the upper surface of the absorber layer. As shown in Figure 3-23, the magnitude of the potential at the absorber layer's upper surface under the sensor we are considering is approximately $0.6 \times 10^{-14}$ [V]. Additionally, Figure 3-4 shows that the magnitude of the steady-state current per-unit-depth on sensor 1 is approximately 0.082 [A/m]

![Figure 3-22: Lumped circuit model of EQS sensor-substrate interaction.](image)

![Figure 3-23: Electric potential [V] along absorber layer surface vs. horizontal position [nm] with sensor head centered over absorber layer gap.](image)
Using lumped Port boundary conditions in COMSOL, we can get a value for the air-gap capacitance per-unit-depth $C'_\text{air}$:

\[
Z'_\text{air} = -j12.3 \, [\Omega \cdot m] \tag{3.3}
\]

\[
C'_\text{air} = \frac{1}{j2\pi f Z'_\text{air}} = 1.29 \times 10^{-11} \, [\text{F/m}] \tag{3.4}
\]

We can confirm this with:

\[
\frac{\hat{V}_\text{sensor} - \hat{V}_\text{absorb}}{\hat{I}_\text{sensor}} = Z'_\text{air} = -j12.3 \, [\Omega \cdot m] \tag{3.5}
\]

We then approximate the substrate resistivity as:

\[
R'_\text{absorb} \approx \frac{\hat{V}_\text{absorb}}{\hat{I}_\text{sensor}} = 7.35 \times 10^{-14} \, [\Omega \cdot m] \tag{3.6}
\]

The “primed” variables above represent parameters that are per-unit-depth. From this point on, a depth of 100nm is assumed to eliminate the “per-unit-depth” units from the parameters so that one can get realistic noise levels for the sensors. The sensor-substrate interaction then has the following numerical values:
At 1GHz, the absorber layer resistance is extremely small compared to the capacitive air-gap impedance; consequently, the sensor current leads the sensor voltage by approximately 90°. Given this extremely small value for $R_{\text{absorb}}$, it can be considered negligible and is not likely to contribute an appreciable amount of thermal noise. For completeness, though, analysis will be carried out with $R_{\text{absorb}}$, included, and it will be shown that thermal noise from the absorber layer losses are negligible.

From this point on we will consider only the magnitudes of the complex current and voltage when compared to RMS noise levels. Therefore, the complex "hats" will be dropped off the current and voltage variables, and it will be assumed that we're dealing strictly with the magnitudes of these complex quantities.

As it stands in the circuit of Figure 3-24, we have no mechanism for detecting changes in the sensor current magnitude, $\Delta I_{\text{sensor}}$, as it scans past a feature. One possible solution is to couple to the sensor current with a current-step-up transformer ($\# \text{ primary windings} > \# \text{ secondary windings}$) and then feed this into some type of current-to-voltage amplifier. We ultimately want to detect changes in the magnitude, or envelope, of our sensor current. Since our sensor excitation is at 1GHz, we need to demodulate our waveform by this carrier frequency and then low-
pass filter the signal over some bandwidth, \( \Delta f \) [14]. By low-pass filtering, we allow ourselves to scan the sensors as slowly as we'd like, and as quickly as the corner frequency of the LPF passband will permit. In this analysis, we'll assume a bandwidth of 1MHz. Figure 3-25 provides a schematic view of this sensor current detection circuit.

![Sensor signal detection circuit](image)

**Figure 3-25: Sensor signal detection circuit.**

We are now in a position to begin evaluating the noise in our circuit. Rather than considering the noise at the output of the LPF stage, we should first consider the signal-to-noise ratio (SNR) at \( V_{OUT} \). We need a reasonable SNR at \( V_{OUT} \) if we are ever going to detect signal fluctuations at the output of the LPF.

As a first step in the noise analysis, it is assumed that the transformer and op-amp are both ideal. This allows for a "best case" SNR at the output, where the noise considered is only the thermal noise due to resistors in the circuit. The thermal noise due to a resistor is white, meaning its power spectrum is flat over all frequencies [25, 26]. When performing noise analysis we can replace the ideal...
resistors in Figure 3-25 with ones that contain thermal noise generators, as seen in Figure 3-26,

\[
\begin{align*}
R & \quad \rightarrow \quad \begin{array}{c}
\text{\textbullet} \\
\text{\textbullet} \\
\text{\textbullet}
\end{array} \\
\text{\textbullet} & = \frac{4kTG}{\Delta f} \\
\text{\textbullet} & = 4kTR\Delta f
\end{align*}
\]

Figure 3-26: Resistor thermal noise model [26].

where \( G = 1/R \). \( \frac{\Delta i^2}{\Delta f} \) and \( \frac{\Delta v^2}{\Delta f} \) are the current and voltage variances (mean square) per hertz bandwidth representing the power spectral density (PSD) of the noise (4kTG and 4kTR have units of \([A^2/Hz]\) and \([V^2/Hz]\), respectively). All noise analysis in this document is performed at a temperature of 300K.

We can get a total RMS noise level at \( V_{\text{OUT}} \) by the linear superposition of the two uncorrelated noise generators due to \( R_{\text{absorb}} \) and \( R_f \). We'll first turn off the \( R_f \) noise generator and find \( \overline{v_{\text{OUT}^1}}^2 \), the contribution to the output noise from \( R_{\text{absorb}} \). The schematic for this circuit is shown in Figure 3-27.
In this case, the output is given by:

\[
\bar{v}_{OUT1}^2 = \left| -N(i_{n1}) \left( \frac{R_{absorb}}{R_{absorb} + \frac{1}{j\omega C_{air}}} \right) R_f \right|^2 \tag{3.7}
\]

\[
\bar{v}_{OUT1}^2 = \left| -N^2(4kT_{air}A_f) \left( \frac{j\omega C_{air}}{1 + j\omega C_{air} R_{absorb}} \right)^2 \right| R_f^2 \tag{3.8}
\]

Next, we turn off the $R_{absorb}$ noise generator and find $\bar{v}_{OUT2}^2$, the contribution to the output noise from $R_f$. This is shown in Figure 3-28. Here, $R_{absorb}$ and $C_{air}$ get reflected across the transformer by the square of the turns ratio into a lumped impedance $Z_{in}$. This is shown in Figure 3-29.
Figure 3-28: Circuit for evaluating output noise due to $R_f$ only.

\[ i_{n2}^2 = 4kT G_f \Delta f \]

Figure 3-29: $R_{\text{absorb}}$ and $C_{\text{air}}$ transformed into impedance $Z_{\text{in}}$.

\[ i_{n2}^2 = 4kT G_f \Delta f \]
In this case the equivalent transformed impedance is given by:

\[ Z_{in} = N^2 \left( \frac{1 + j\omega C_{air} R_{absorb}}{j\omega C_{air}} \right) \]  \hspace{1cm} (3.9)

Assuming the op-amp is ideal:

\[ i_{n2} = -\frac{v_-}{Z_{in}} + \frac{-A v_- - v_-}{R_f} \approx \frac{\overline{v}_{OUT2}}{A} \left( \frac{1}{Z_{in}} + \frac{A}{R_f} \right) \]  \hspace{1cm} (3.10)

In this limit we can assume \( A \to \infty \) and thus:

\[ \frac{A}{R_f} \gg \frac{1}{Z_{in}} \]  \hspace{1cm} (3.11)

In this limit then:

\[ \overline{v}_{OUT2} = i_{n2} R_f \]  \hspace{1cm} (3.12)

\[ \overline{v}_{OUT2}^2 = |4kT \Delta f R_f^2| \]  \hspace{1cm} (3.13)

\[ \tilde{v}_{OUT2}^2 = |4kT R_f \Delta f| \]  \hspace{1cm} (3.14)

Applying superposition to the two uncorrelated noise sources:

\[ \frac{\overline{v}_{OUT-NOISE}^2}{\Delta f} = \frac{\overline{v}_{OUT1}^2}{\Delta f} + \frac{\overline{v}_{OUT2}^2}{\Delta f} \]  \hspace{1cm} (3.15)

\[ \frac{\overline{v}_{OUT-NOISE}^2}{\Delta f} = \left| -N^2 (4kT R_{absorb}) \left( \frac{j\omega C_{air}}{1 + j\omega C_{air} R_{absorb}} \right)^2 R_f^2 \right| + |4kT R_f| \]  \hspace{1cm} (3.16)

Let's assume that \( R_f = 10k\Omega \) so that we can plot and compare the output noise PSDs due to \( R_{absorb} \) and \( R_f \).
As shown previously, the noise contribution from the feedback resistor is independent of $N$.

Figure 3-31: Output voltage noise PSD due to $R_f$ vs. $\omega$ (independent of $N$).
As was expected, it is clear that the output noise comes primarily from the feedback resistor, and the noise due to $R_{\text{absorb}}$ is negligible by several orders of magnitude. This makes sense because $R_{\text{absorb}}$ is extremely small compared to $R_f$. There is then no inherent battle with noise from the absorber layer resistance. If we considered the voltage noise due to $R_{\text{absorb}}$ over 1MHz bandwidth \textit{in the drive circuit alone}, we would get an RMS voltage noise level of $1.38 \times 10^{-10}$ [V]. With a voltage drive level of 1V, the signal would be approximately $7 \times 10^9$ times larger than the noise.

We are now in a position to evaluate a SNR at $V_{\text{out}}$. Integrating the total noise PSD at $V_{\text{out}}$ over 1MHz bandwidth (assuming first-order roll off after the 1MHz corner) gives a total RMS voltage noise level of:

$$
\bar{v}_{\text{OUT-Noise}} = \sqrt{4kT_R f \cdot 1\text{MHz} \cdot \frac{\pi}{2}} = 16.1 \text{ [\mu V]} \quad (3.17)
$$

We know that variations in the output signal $\Delta V_{\text{OUT}}$ go as follows:

$$
|\Delta V_{\text{OUT}}| = \left| -N(\Delta I_{\text{sensor}})R_f \right| \quad (3.18)
$$

where $\Delta I_{\text{sensor}}$ is the magnitude of the fluctuation in the sensor current magnitude as it scans past a feature. Looking back at the current response for $s$ (Figure 3-4)—in the event that it scans over an empty trench in the absorber pattern—the signal will fluctuate on the order of $\Delta I_{\text{sensor}} \approx 0.6$ [pA]. Consequently the signal magnitude at $V_{\text{out}}$ is:

$$
|\Delta V_{\text{OUT}}| = 6 \cdot N \text{ [\mu V]} \quad (3.19)
$$

We express a signal-to-noise ratio in the 1MHz passband as:
It is clear from Figure 3-32 that we need an appreciable amount of turns on the transformer primary to overcome the thermal noise caused by $R_f$ ($N = 10$ turns gives an SNR of approximately 4:1). It should be noted that driving the sensors at 1V zero-to-peak amplitude can be considered conservative with regards to breakdown and field emissions. For a 100nm air gap, it is likely that field emissions will occur far before electric breakdown [27, 28]. Electron field emissions in pure metals occur at $10^9$ [V/m], whereas our sensors are driven at 1V across a 100nm gap [27, 28]. It should be possible to drive the sensors at 10V across this 100nm gap and still be a factor of 10 away from FE. Increasing the drive level will increase the signal magnitude linearly without affecting the noise level (again,
assuming the transformer is ideal). Figure 3-33 shows SNR vs. turns ratio for various drive levels.

![Graph showing SNR vs. turns ratio for various drive levels.](image)

**Figure 3-33:** SNR at output for various turns ratios for 1V, 5V, and 10V sensor drive at 1GHz drive frequency.

Another way to increase the SNR linearly is to increase the drive frequency. Since the sensor current is dominated by the air-gap capacitance, $C_{air}$, the sensor current is approximately:

$$i_{sensor} \approx j \omega C_{air} \hat{V}_{sensor} \quad (3.21)$$

Figure 3-34 is the same plot as Figure 3-33 but at an increased drive frequency of 5GHz. As expected, a 5x increase in SNR is observed.
Figure 3-34: SNR at output for various turns ratios for 1V, 5V, and 10V sensor drive at 5GHz drive frequency.

It is important to reiterate that this analysis only takes into account the thermal noise due to $R_{\text{absorb}}$ and $R_f$. A more complete analysis of this topology would take into account a non-ideal transformer and a non-ideal op-amp. This analysis does not take into account the noise in the demodulation and filtering circuitry. Such an analysis should indeed be performed when more quantitative details are known about the transformer and low-noise amplifier to be implemented. One should also realize this is only one possible (and rather unlikely due to its wideband nature) circuit topology for detecting the sensor current response. Nonetheless, it demonstrates the extreme importance of having low-noise pickup circuitry to interface with the sensor array. An investigation into other possible low-noise pickup circuits could serve as a topic of future research for this research project. In the example presented in the chapter, variations in the sensor current in response to features were on the order of less than 1 nA. Detecting such a small current
require a very narrowband, ultra-low-noise amplification circuit interfacing with the sensors. For a deeper understanding of the operation of narrowband low-noise amplifiers, [29] is a suggested reading.

Additionally, this analysis assumes that the sensor head scans at a fixed height of 100 nm. One should consider the noise that is introduced by mechanical vibrations that might cause the sensor's scan height to fluctuate relative to the sample. Such vibrations need to be bounded to enable good imaging.
4 Sensor Signal Inversion through a Radial Basis Function Artificial Neural Network

This chapter concerns the inversion of EQS sensor signal response data for the purpose of predicting feature/defect profiles. To this point, only the forward problem of determining sensor signal responses for a given feature/defect have been considered. These forward problems are well-posed in that for a given geometry there exists a unique EQS solution that depends continuously on the physical and electrical properties of the geometry. The inverse problem is then to infer information about a geometry (material properties, feature sizes/locations, etc.) that caused a measured sensor signal[12]. Inverse problems are in general ill-posed in that, for a given measured sensor signal, there does not necessarily exist a unique solution that depends continuously on the physical and electrical properties of the network.

The goal of this chapter is to predict the dimensions (depth and width) of a sub-micrometer scale trench in doped silicon based upon a measured transimpedance between two sensors in a coplanar array that is scanned laterally over the surface of the silicon. This is an example of the type of inverse problem that might be encountered in an EQS array microscope and one possible approach to its solution. To solve the inverse problem, a radial basis function artificial neural network is trained with a small database of COMSOL simulation results to perform
the forward function of mapping trench dimensions into a measureable transimpedance between two sensors in the array. Once the artificial neural network is trained, it can be used in an iterative error-minimizing inversion routine. The chapter describes how the inverse EQS problem is solved in this manner.

4.1 Simulating the Forward Problem

The evaluated geometry is shown in Figure 4-1 with key geometric and electrical parameters provided in Table 4-1 and Table 4-2. Figure 4-1 shows a sensor head containing six sensors and two guards at a fixed height of 50 nm over a doped silicon bulk. In the doped silicon bulk there exists an air-filled trench that can take on a variety of widths and depths.

Figure 4-1: COMSOL geometry for locating trenches of various dimensions (depth and width) in doped silicon with an array of coplanar EQS electrodes.
Table 4-1: Key geometric dimensions for trench simulations

<table>
<thead>
<tr>
<th>Dimension</th>
<th>Length [nm]</th>
</tr>
</thead>
<tbody>
<tr>
<td>air gap (sensor scan height)</td>
<td>50</td>
</tr>
<tr>
<td>sensor width</td>
<td>100</td>
</tr>
<tr>
<td>sensor height</td>
<td>50</td>
</tr>
<tr>
<td>total sensor head width</td>
<td>1100</td>
</tr>
<tr>
<td>trench depth</td>
<td>50 – 200</td>
</tr>
<tr>
<td>trench width</td>
<td>40 – 120</td>
</tr>
</tbody>
</table>

Table 4-2: Electrical parameters used in FEM simulation

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>sensor head relative permittivity (SiO₂)</td>
<td>3.9</td>
</tr>
<tr>
<td>silicon relative permittivity</td>
<td>11.8</td>
</tr>
<tr>
<td>silicon conductivity</td>
<td>0.005 [S/m]</td>
</tr>
<tr>
<td>sensor conductivity</td>
<td>PEC</td>
</tr>
<tr>
<td>sensor frequency</td>
<td>7.62 [MHz]</td>
</tr>
</tbody>
</table>

Electrodes on the left half of the sensor head are driven by a 7.62MHz sinusoidal voltage source with peak amplitude of 1V. This frequency was chosen because it is on the order of the charge relaxation break frequency of the semiconducting silicon bulk. Although this analysis only considers the magnitude of the impedance between sensors in the array, choosing a drive frequency on the order of the charge relaxation time of the bulk can provide interesting phase information as well. With the intrinsic conductivity of silicon being approximately
4.3 \times 10^{-4} \text{ [S/m]}, the silicon in the simulation with conductivity of 5 \times 10^{-3} \text{ [S/m]} represents a weakly doped substrate. Electrodes on the right half of the sensor head are short-circuited to ground. Because each sensor/guard is treated as a perfect electrical conductor (PEC), we can assume there are no fields inside these regions and thus treat them as electric potential boundary conditions. "Port" boundary conditions are used in COMSOL to calculate lumped terminal parameters for the system. The particular parameter of interest is the mutual transimpedance between sensor 2 and sensor 5 (sensor indices shown in Figure 4-1).

Figure 4-2: COMSOL simulation results with 300nm\times25nm trench positioned 100nm right of center. Red streamlines are electric field lines and the blue contours represent equipotentials (lines of constant voltage). For simplicity, fields from guard electrodes are not shown.

Figure 4-2 shows an electric field streamline plot from COMSOL reacting to a high aspect ratio trench (300nm\times25nm) in the silicon bulk. Electric fields from
sensor 2 are shunted into the silicon bulk by guarding effects from sensor 1, sensor 3, and the top-side guard. These field lines can be seen bending and reacting to the presence of the air-filled trench. The presence of the air-filled trench shows up as variations in both the magnitude and phase of the mutual transimpedance between sensor 2 and sensor 5 as the sensor head scans past the trench. Figure 4-3 provides families of transimpedance responses vs. sensor head position for trenches of various depths and widths. Figure 4-3(a) shows a family of responses for trenches of varying depths with width fixed at 50nm, and Figure 3-4(b) shows a family of responses for trenches of varying widths with depth fixed at 100nm.

Figure 4-3: Sensor 2 - Sensor 5 transimpedance [Ω-m] vs. sensor head position [nm] for trenches of various depths and widths. In this case impedance has units of [Ω-m] because the simulation is performed on a 2D solver. Figure (a) shows a family of responses for trenches of varying depths with width fixed at 50nm, Figure (b) shows a family of responses for trenches of varying widths with depth fixed at 100nm.

4.2 Solving the Inverse Problem

Looking at the curves in Figure 4-3, one can see that there exists some monotonic dependencies of impedance on trench depth and impedance on trench width. For example, qualitatively speaking, it's clear in Figure 4-3(a) that the impedance
increases with trench depth and that the trenches are most easily distinguished from one another when they are nearly centered under the sensor head.

To solve the inverse problem of predicting trench depth and width based on a given impedance curve like those shown in Figure 4-3, one can imagine building a giant database of the results for many different trenches and traversing that database for a match based on some error minimization function. A more efficient method would be to train a function-approximation device to predict the forward model through some type of functional mapping from input space (trench dimensions) to output space (impedance response) [30, 31]. This device can then be used to replace the large database of results. This is the method that will be used in this chapter to solve the inverse trench problem.

The specific algorithm that was chosen to invert the measured sensor data into predicted trench dimensions is illustrated in the block diagram in Figure 4-4. A radial basis function artificial neural network (RBF-ANN) is trained to accurately predict the forward function of mapping trench dimensions into a measurable sensor transimpedance [31]. This RBF-ANN is then fed an initial guess for the trench dimensions, compares the results to the measured transimpedance response, and then iterates through a sum of squares error minimization routine. This iterative routine then converges to a value for trench dimensions that minimizes the error between the RBF-ANN forward model and the measured data. The training database is built using COMSOL simulation results.

![Figure 4-4: Iterative signal inversion block diagram][31].
4.2.1 Artificial Neural Networks (ANNs): Training and Operation

An artificial neural network is a mathematical model consisting of an interconnected cluster of "neurons," or nodes, that attempt to approximate a function through weighted combinations of the neurons’ activation functions. In the case of an RBF-ANN, the neuron activation function is a radial basis function, or a function whose value depends only on distance from some center point. The classic example of an RBF is the zero-centered Gaussian function, which takes the form:

\[ f(x) = ae^{-bx^2}; \quad a, b > 0 \]  

(4.1)

The general structure of an RBF-ANN is below. The input layer contains “R” inputs that interface with a hidden layer of “S’” neurons through an “S1 x R” matrix of weighted connections “W_{S1,R}”. These weights determine the level to which each of the neurons “fire,” or contribute, to the output for a given input. The output vector has a length “S2” whose elements are formed through a weighted, linear summation of each neuron’s basis function (via the “L_{S2,S1}” branches).

Figure 4-5: RBF-ANN basic architecture.
The MATLAB Neural Network Toolbox has built-in capabilities for quickly training and implementing an RBF-ANN with the architecture shown above [32]. The detailed inner working of each layer is shown in Figure 4-6. In this case, the network is described as having “R” inputs, “S1” RBF neurons in the hidden layer, and the output vector has length “S2.”

![Figure 4-6: MATLAB RBF-ANN architecture details](image)

The above network is best understood by tracing the flow of an input vector through the network of Figure 4-6. Each input element in “R” is compared to an “S1 × R” matrix of weights “IW1,1” producing an “S1 × 1” vector of Euclidean distances between the input vector and each row of the weight matrix. The Euclidean distance is taken to be the square root of the sum of the individual distances squared. For example if an input vector is \([1, 2]\) and weight matrix “IW1,1” is \([3, 3; 1, 2]\), then the 2 × 1 vector of Euclidean distances would be \([\sqrt{5}; 0]\). The vector “b1” is a vector of spread biases for each neuron’s Gaussian basis function corresponding to the distance from the origin at which the amplitude of the Gaussian drops to one-half its center amplitude. If the distance between “R” and a neuron’s weight is
relatively small, that neuron will “fire” or activate, while if the distance is relatively large it will not. The larger the spread bias the more likely the neuron is to fire for inputs that are not very close to the weights. On the other hand, a small spread bias means that the neuron is extremely selective [32]. The output of the Radial Basis Layer “a1” is then an “$S^1 \times 1$” vector of values determined by the MATLAB function $\text{radbas}()$, where:

$$\text{radbas}(n) = e^{-n^2}$$  \hspace{1cm} (4.2)

Where $n$ is the spread bias times the distance. Continuing along with the same numerical example, with the Euclidian distance vector $\begin{bmatrix} \sqrt{5} \\ 0 \end{bmatrix}$, and a spread bias constant of 0.8326 (corresponding to the standard unit Gaussian), then the “a1” vector would be $\begin{bmatrix} 0.0312 \\ 1.0000 \end{bmatrix}$. This means that lower neuron in the vector is fully firing, while the upper neuron is only weakly firing due to its relatively large Euclidean distance for the given spread. The values in “a1” are then weighted by “$\text{LW}_{2,1}$” and level-shifted by “$\text{b}^{2}$” in the Linear Layer. The resultant output “a2” is an “$S^2 \times 1$” vector of values which represents the RBF-ANN’s predicted output for an input “R.”

MATLAB has two built in algorithms for instantiating and training an RBF-ANN [32]. One method uses exact design and produces a network with zero error on the training data. This method takes in a matrix of input vectors, a matrix of output vectors, and a spread constant then sets the weight matrices such that the function has zero error for any of these training inputs. Consequently, this method produces a network with as many neurons in the hidden layer as there are input vectors in the training matrix. A second, potentially more efficient, design iteratively adds neurons one at a time and adjusts weights until a sum-squared error goal is met. This training algorithm can result in a network that accurately performs its function with fewer neurons than the exact design training algorithm. In this chapter, RBF-ANNs implementing both training algorithms are used and compared.
4.2.2 Training Results

A training database of 30 input-output relations was created using COMSOL simulation. The 30 inputs (trench dimensions) used for training are listed in Figure 4-7 (the 100nm×80nm case was excluded from the training database and is used later as one of the test cases).

![Training data inputs](image)

Networks were trained using both the exact and iterative methods described earlier. In each case a spread constant of 100 is specified [32]. Figure 4-8 provides a screenshot of the progress of the iterative training method. The network reaches a sum-squared error goal of $1 \times 10^{-6}$ after adding 29 RBF neurons to the hidden layer. Because there are 30 sets of training data, the exact network has 30 RBF neurons in the hidden layer, and the iteratively-trained network ended up with one less neuron; however, the iteratively-trained network ended up converging to a network that is almost identical to the exact-trained network. The 29 neurons in the iteratively-trained network were nearly the same as 29 out of 30 of the neurons in the exact-trained network with differences in the “LW_{2,1}” matrix of less than 1%. For this reason, we can expect the two networks to perform nearly the same.
Several test cases were used to evaluate the performance of each network in predicting the forward model. The networks output prediction is compared against COMSOL simulation results. Sample results for a 100nm × 80nm trench and a 120nm × 60nm trench (depth × width) are shown in Figure 4-9 and Figure 4-10, respectively. These trenches were not part of the training database. With only 30 sets of training data, it’s clear that the RBF-ANN is excellent at mapping the forward model for trenches whose dimensions are on the order of those used in the training database. The performance of the iteratively-trained network is further demonstrated in Figure 4-11.
Figure 4-9: Forward model prediction performance for exact-trained and iteratively-trained RBF networks. Results are for a trench that is 100nm deep and 80nm wide.

Figure 4-10: Forward model prediction performance for exact-trained and iteratively-trained RBF networks. Results are for a trench that is 120nm deep and 60nm wide.
Figure 4-11: Demonstration of iteratively-trained RBF network performance. For a fixed trench width of 50nm, both network-predicted and actual outputs are plotted for various trench depths. The family of curves shows the accuracy of the RBF network compared to actual COMSOL results.

4.2.3 Signal Inversion Results

With confidence that the RBF network is well-trained for predicting the forward model through function approximation, it can now be used in an iterative signal inversion routine. The routine illustrated in Figure 4-4 is repeated below for the reader’s convenience [31].
The iterative error minimization routine is implemented using MATLAB's built-in function `fminsearch()`. This multivariable, nonlinear error minimization function takes in an initial guess for the trench dimensions and attempts to converge to a local minimum in this input space. MATLAB code for the signal inversion routine can be found in Appendix A.

The signal inversion routine was tested using measured trench data that did not belong to the network training database. Both the exact-trained and iteratively-trained networks were used in the routine. The performance of the routine is demonstrated in Figure 4-13 – Figure 4-16 for two different test cases implementing each of the two networks. The first two figures show the results for a 120nm×60nm trench—which is not part of the training database—using an exact-trained network and an iteratively-trained network, respectively. In each case an initial guess of 50nm×50nm is used. Figure 4-13 and Figure 4-14 indicate that each network type converges with almost identical performance (as expected) to predicted trench dimensions of 119.9nm×59.61nm—well within 1% of the actual values. Figure 4-15 and Figure 4-16 show the results for a 100nm×80nm trench with an initial guess of 200nm×200nm. The predicted dimensions are again within approximately 1% of the actual dimensions.
Figure 4-13: Signal inversion routine convergence for 120nm×60nm trench with initial guess of 50nm×50nm for exact-trained ANN.

Figure 4-14: Signal inversion routine convergence for 120nm×60nm trench with initial guess of 50nm×50nm for iteratively-trained ANN.
Figure 4-15: Signal inversion routine convergence for 100nm×80nm trench with initial
guess of 200nm×200nm for exact-trained ANN.

Figure 4-16: Signal inversion routine convergence for 100nm×80nm trench with initial
guess of 200nm×200nm for iteratively-trained ANN.

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It's clear that the networks are capable of accurately predicting the forward model, given a relatively small set of training data. It was demonstrated that these networks can be plugged into an iterative signal inversion routine to accurately predict an unknown trench's dimensions (within 1%), given a measured output signal. These specific networks were capable of performing forward functional mapping for two input parameters: trench depth and trench width. One can imagine extending the networks capabilities to more geometric and/or material input parameters (e.g. depth, width, length, conductivity, permittivity, pitch, radius, etc.) As one increases the number of inputs, though, the complexity of the network grows and a larger training database is required to achieve accurate forward functional mapping.
5 Conclusions and Suggestions for Future Work

The work presented in this thesis summarizes the results of several different case studies solving both forward and inverse electromagnetic sensor problems with a focus on capacitive sensors that operate in the electroquasistatic approximate. The capabilities and limitations of EQS sensors in detecting both surface features/objects and subsurface features were demonstrated. One of the largest limiting factors for EQS sensors in detecting subsurface features is charge relaxation. It was shown in this thesis how the charge relaxation (Equation (2.20)) determines whether a material will appear insulating or conducting to the sensors, depending on their operating frequency. For detecting subsurface features in relatively highly conducting materials, sensors operating in the magnetoquasistatic regime often prove to be a more effective solution due to induced eddy currents and enhanced field penetration depth when operated at low frequencies [1, 3-5, 16]. One possible area for future research in the field of sub-micron-scale imaging and detection via quasistatic sensors is an investigation into the scalability of EQS sensors vs. MQS sensors and the difficulties of fabricating nano-scale MQS sensor coils.

Chapter 2 presented a promising new method for mapping out the semiconducting layers of an integrated circuit. It was demonstrated through finite element method simulations how p-n junctions in a substrate can be located by monitoring steady-state sensor currents for harmonic distortion. With sensors located over a p-n junction at a scan height of 200 nm and driven at 1GHz, the ratio
of the second harmonic current to the fundamental current on a sensor was shown exceed 9%. By coupling into p-n junctions through an air gap, non-contact, non-destructive methods for quickly imaging integrated circuits may be possible. Such an IC imaging technique could prove to be useful for verification and detection of fabrication errors as well as detecting hidden Trojan circuits that might be present on die. Advanced 3D FEM simulations of sensor scans over wells of various dimensions are suggested to extend the simulation work presented in this thesis. In addition to more simulation-based analysis, laboratory experiments would prove invaluable in confirming simulation results.

Chapter 3 demonstrated the sensitivity of EQS sensors to contaminant objects on the surface of a photomask. FEM simulation results showed the capability of capacitive EQS sensors in detecting various contaminant particles located in a 100nm wide by 70nm deep gap in the absorber layer of an EUVL photomask. With variations in the sensor currents on the order of 1 nA, these results motivate the need for the development of low-noise pickup circuitry to interface with the sensors. A brief discussion of thermal noise considerations was presented. An investigation into possible narrow band, low-noise circuits could serve as a topic of future research.

Chapter 4 solved an inverse electromagnetic sensor problem by training a radial basis function artificial neural network to accurately approximate the forward mapping of a feature's physical dimensions into a sensor's impedance response as it scans past the feature. This function-approximation network was then inserted into an iterative signal inversion routine. The RBF-ANN was capable of accurately predicting an unknown trench's dimensions to within 1%, given a measured output signal. These specific networks were capable of performing forward functional mapping for two input parameters: trench depth and trench width. Extending the network capabilities to more geometric and/or material input parameters (e.g. conductivity, permittivity, pitch, radius, etc.) could serve as a topic of future research on this project. Furthermore, while this specific algorithm proved
to solve the inverse problem quite successfully, it was performed strictly as a post-processing exercise. A suggested area for future research would be the integration of the signal inversion routine into the real-time operation of the sensor array. It would indeed be an interesting case-study to investigate the operation of the signal inverter in real-time and its potential limitations on scan speed.

One final suggestion for future work is rooted in the idea of massive parallelism. Present-day scanning imaging techniques (SCM, AFM, SMM, etc.) rely on the raster-scanning of a single probe/electrode [13-15, 33]. Large arrays of EQS/MQS electrodes could potentially provide the integrated circuit industry with inspection tools that can quickly scan photolithography equipment, ICs, and other IC fabrication equipment for features, defects, and contaminants at speeds far above the capabilities of current, single-probe technologies.
Bibliography


Appendix A: MATLAB Code for Iterative Signal Inversion Routine

The following code corresponds to the iterative signal inversion routine described in Section 4.2.

```matlab
%Function RBF_Input_Predictor takes in three parameters:
% initial_guess - An initial guess at the trench dimensions: [depth; width]
% measured_output_data - measured impedance signal for the unknown trench
% network - A trained artificial neural network to approximate forward model
%Attempts to converge to a set of predicted trench dimensions [depth; width] that might have caused measured_output_data. Implements fminsearch() to minimize a sum of squares error between RBF-ANN output and measured output data.

function Inputs = RBF_Input_Predictor( initial_guess, measured_output_data, network )

    iter = 0;
    net = network;

    %Function errorfun calculates a sum-of-squares error between the current iteration's predicted output and the measured output data.
    %Takes in two parameters:
    % currentInputValues - current iteration's guess at the trench dimensions [depth; width]
    % measured_output_data - measured impedance signal for the unknown trench
    function Error = errorfun( currentInputValues, measured_output_data )

        hold on;

        %run the RBFANN forward model for the current iteration's input values
        CurrentOutput = sim(net, currentInputValues);
```

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%determine the sum of squares error for the current output vs the measured output data
Difference = CurrentOutput - measured_output_data;
SqDifference = Difference.^2;
Error = sqrt(sum(SqDifference));

%plotting details
disp([currentInputValues', Error]);
curdepth = currentInputValues(1);
curwidth = currentInputValues(2);
iter = iter + 1;
handlevec(:,1)=plot(iter, curdepth, 'b+');
handlevec(:,2)=plot(iter, curwidth, 'ro');
pause(0.01);
end

%Termination tolerance on error
Options = optimset('TolFun', 0.05);
%Iterative error minimization search function. Attempts to minimize function errorfun() for measured_output_data with initial_guess.
Inputs = fminsearch(@(currentInputValues) errorfun(currentInputValues, measured_output_data ), initial_guess, Options );

%plotting details
legend(handlevec);
end
Appendix B: COMSOL Settings for p-n Junction Geometry #1

The following is a COMSOL auto-generated report that corresponds to the FEM simulation results that were presented in Section 2.3 and Section 2.4. The report provides information about FEM model properties, meshing settings, boundary conditions, solver settings, solver variables, constants used, etc.
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<td>Company</td>
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<td>Department</td>
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<td>Reference</td>
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Application modes and modules used in this model:

- Geom1 (2D)
  - Electrostatics
  - Convection and Diffusion
  - Convection and Diffusion
  - Weak Form, Boundary

1.1. Model description

Semiconductor Diode

A semiconductor device model featuring a diode with p- and n-type regions. The image shows the hole concentration for 0.5V forward bias.

2. Constants

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### 3. Geom1

Space dimensions: 2D

Independent variables: x, y, z

#### 3.1. Scalar Expressions

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#### 3.2. Mesh

##### 3.2.1. Mesh Statistics

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Application mode name: es

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file://C:\Documents and Settings\BCANNON\Desktop\PN Junction Air Cases\Segmented ... 4/20/2010
3.3.3. Variables

Dependent variables: \( \psi \)

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Interior boundaries active

3.3.4. Boundary Settings

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3.3.5. Subdomain Settings

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3.4. Application Mode: Convection and Diffusion (cd)

Application mode type: Convection and Diffusion

Application mode name: cd

3.4.1. Application Mode Properties

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3.4.2. Variables

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p-n junction Geometry

Shape functions: shlag(2,'lm2'), shlag(2,'cn')

Interior boundaries active

### 3.4.3. Boundary Settings

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<tr>
<th>Boundary</th>
<th>1, 3</th>
<th>2, 5</th>
<th>4, 7, 9-20</th>
</tr>
</thead>
<tbody>
<tr>
<td>Type</td>
<td>Insulation/Symmetry</td>
<td>Concentration</td>
<td>Continuity</td>
</tr>
<tr>
<td>Concentration (c0)</td>
<td>mol/m³</td>
<td>n_init</td>
<td>0</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Boundary</th>
<th>6, 8</th>
</tr>
</thead>
<tbody>
<tr>
<td>Type</td>
<td>Convective flux</td>
</tr>
<tr>
<td>Concentration (c0)</td>
<td>mol/m³</td>
</tr>
</tbody>
</table>

### 3.4.4. Subdomain Settings

<table>
<thead>
<tr>
<th>Subdomain</th>
<th>1-2</th>
</tr>
</thead>
<tbody>
<tr>
<td>Shape functions (shape)</td>
<td>shlag(2,'lm2'), shlag(2,'cn')</td>
</tr>
<tr>
<td>Integration order (gorder)</td>
<td>4</td>
</tr>
<tr>
<td>Diffusion coefficient (D)</td>
<td>m²/s, On</td>
</tr>
<tr>
<td>x-velocity (u)</td>
<td>m/s, mun*psix</td>
</tr>
<tr>
<td>y-velocity (v)</td>
<td>m/s, mun*psiy</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Subdomain initial value</th>
<th>1-2</th>
</tr>
</thead>
<tbody>
<tr>
<td>Concentration, on (cn)</td>
<td>mol/m³, n_init</td>
</tr>
</tbody>
</table>

### 3.5. Application Mode: Convection and Diffusion (cd2)

Application mode type: Convection and Diffusion

Application mode name: cd2

#### 3.5.1. Application Mode Properties

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Default element type</td>
<td>Lagrange - Quadratic</td>
</tr>
<tr>
<td>Analysis type</td>
<td>Transient</td>
</tr>
<tr>
<td>Equation form</td>
<td>Conservative</td>
</tr>
<tr>
<td>Frame</td>
<td>Frame (ref)</td>
</tr>
<tr>
<td>Weak constraints</td>
<td>On</td>
</tr>
<tr>
<td>Constraint type</td>
<td>Ideal</td>
</tr>
</tbody>
</table>

#### 3.5.2. Variables

Dependent variables: cp

Shape functions: shlag(2,'lm3'), shlag(2,'cp')

Interior boundaries active

#### 3.5.3. Boundary Settings
p-n junction Geometry

<table>
<thead>
<tr>
<th>Boundary</th>
<th>1.3</th>
<th>2.5</th>
<th>4.7, 9-20</th>
</tr>
</thead>
<tbody>
<tr>
<td>Type</td>
<td>Insulation/Symmetry</td>
<td>Concentration</td>
<td>Continuity</td>
</tr>
<tr>
<td>Concentration (c0)</td>
<td>mol/m³</td>
<td>0</td>
<td>( p_{init} )</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Boundary</th>
<th>6, 8</th>
</tr>
</thead>
<tbody>
<tr>
<td>Type</td>
<td>Convective flux</td>
</tr>
<tr>
<td>Concentration (c0)</td>
<td>mol/m³</td>
</tr>
</tbody>
</table>

### 3.5.4. Subdomain Settings

<table>
<thead>
<tr>
<th>Subdomain</th>
<th>1-2</th>
</tr>
</thead>
<tbody>
<tr>
<td>Shape functions (shape)</td>
<td>shlag(2, 'lm3') shlag(2, 'cp')</td>
</tr>
<tr>
<td>Integration order (gporder)</td>
<td>4</td>
</tr>
<tr>
<td>Diffusion coefficient (D)</td>
<td>( m^2/s ) ( D_p )</td>
</tr>
<tr>
<td>x-velocity (u)</td>
<td>m/s</td>
</tr>
<tr>
<td>y-velocity (v)</td>
<td>m/s</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Subdomain initial value</th>
<th>1-2</th>
</tr>
</thead>
<tbody>
<tr>
<td>Concentration, cp (cp)</td>
<td>mol/m³</td>
</tr>
</tbody>
</table>

### 3.6. Application Mode: Weak Form, Boundary (wb)

Application mode type: Weak Form, Boundary

Application mode name: wb

#### 3.6.1. Application Mode Properties

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Default element type</td>
<td>Lagrange - Quadratic</td>
</tr>
<tr>
<td>Wave extension</td>
<td>Off</td>
</tr>
<tr>
<td>Frame</td>
<td>Frame (ref)</td>
</tr>
<tr>
<td>Weak constraints</td>
<td>Off</td>
</tr>
</tbody>
</table>

#### 3.6.2. Variables

Dependent variables: rhoS, rhoS_t

Shape functions: shlag(2, 'rhoS')

Interior boundaries not active

#### 3.6.3. Boundary Settings

<table>
<thead>
<tr>
<th>Boundary</th>
<th>6, 8</th>
</tr>
</thead>
<tbody>
<tr>
<td>Weak term (weak)</td>
<td>rhoS_test*('q'ntflux_cn_cd+q'ntflux_cp_cd2)</td>
</tr>
<tr>
<td>Time-dependent weak term (dweak)</td>
<td>rhoS_test*rhoS_time</td>
</tr>
</tbody>
</table>

### 4. Materials/Coefficients Library

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4.1. Air

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Heat capacity at constant pressure (C)</td>
<td>( C_p(T[K])/(J/(kg*K)) )</td>
</tr>
<tr>
<td>Speed of sound (cs)</td>
<td>( cs(T[K])/m/s )</td>
</tr>
<tr>
<td>Dynamic viscosity (eta)</td>
<td>( \eta(T[K])/Pa*s )</td>
</tr>
<tr>
<td>Ratio of specific heats (gamma)</td>
<td>1.4</td>
</tr>
<tr>
<td>Thermal conductivity (k)</td>
<td>( k(T[K])/W/(m*K) )</td>
</tr>
<tr>
<td>Kinematic viscosity (nuO)</td>
<td>( \nu_0(T[K])/m^2/s )</td>
</tr>
<tr>
<td>Density (rho)</td>
<td>( \rho(p[1/Pa],T[K])/kg/m^3 )</td>
</tr>
<tr>
<td>Electric conductivity (sigma)</td>
<td>( \sigma[Ohm^{-1}m] )</td>
</tr>
</tbody>
</table>

4.1.1. Functions

<table>
<thead>
<tr>
<th>Function</th>
<th>Expression</th>
<th>Derivatives</th>
<th>Complex output</th>
</tr>
</thead>
<tbody>
<tr>
<td>( cs(T) )</td>
<td>( \sqrt{.4<em>287</em>T} )</td>
<td>( d(\sqrt{1.4<em>287</em>T},T) )</td>
<td>false</td>
</tr>
<tr>
<td>( \rho(p,T) )</td>
<td>( p*0.02897/8.314/T )</td>
<td>( d(p*0.02897/8.314/T,T) )</td>
<td>false</td>
</tr>
</tbody>
</table>

4.1.2. Piecewise Analytic Functions

4.1.2.1. Function: \( C_p(T) \)

Type: Polynomial

<table>
<thead>
<tr>
<th>( x_{\text{start}} )</th>
<th>( x_{\text{end}} )</th>
<th>( f(x) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>200</td>
<td>1600</td>
<td>0.104763657E+03</td>
</tr>
</tbody>
</table>
| 4.1.2.2. Function: \( \eta(T) \)

Type: Polynomial

<table>
<thead>
<tr>
<th>( x_{\text{start}} )</th>
<th>( x_{\text{end}} )</th>
<th>( f(x) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>200</td>
<td>1600</td>
<td>-8.38278000E-07</td>
</tr>
</tbody>
</table>
| 4.1.2.3. Function: \( \nu_0(T) \)

Type: Polynomial

<table>
<thead>
<tr>
<th>( x_{\text{start}} )</th>
<th>( x_{\text{end}} )</th>
<th>( f(x) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>200</td>
<td>1600</td>
<td>-5.86912845E-06</td>
</tr>
</tbody>
</table>
| 4.1.2.4. Function: \( k(T) \)

Type: Polynomial

<table>
<thead>
<tr>
<th>( x_{\text{start}} )</th>
<th>( x_{\text{end}} )</th>
<th>( f(x) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>200</td>
<td>1600</td>
<td>-2.27583562E-03</td>
</tr>
</tbody>
</table>

5. Integration Coupling Variables
5.1. Geom1

6. Solver Settings

Solve using a script: off

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Auto select solver</td>
<td>On</td>
</tr>
<tr>
<td>Solver</td>
<td>Time dependent</td>
</tr>
<tr>
<td>Solution form</td>
<td>Automatic</td>
</tr>
<tr>
<td>Symmetric</td>
<td>Off</td>
</tr>
<tr>
<td>Adaptive mesh refinement</td>
<td>Off</td>
</tr>
<tr>
<td>Optimization/Sensitivity</td>
<td>Off</td>
</tr>
<tr>
<td>Plot while solving</td>
<td>Off</td>
</tr>
</tbody>
</table>

6.1. Direct (PARDISO)

Solver type: Linear system solver

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Preordering algorithm</td>
<td>Nested dissection</td>
</tr>
<tr>
<td>Row preordering</td>
<td>On</td>
</tr>
<tr>
<td>Bunch-Kaufmann</td>
<td>Off</td>
</tr>
<tr>
<td>Pivoting perturbation</td>
<td>1.0E-8</td>
</tr>
<tr>
<td>Relative tolerance</td>
<td>1.0E-6</td>
</tr>
<tr>
<td>Factor in error estimate</td>
<td>400.0</td>
</tr>
<tr>
<td>Check tolerances</td>
<td>On</td>
</tr>
</tbody>
</table>

6.2. Time Stepping

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Times</td>
<td>range(0, 0.0000001, 0.0000004)</td>
</tr>
<tr>
<td>Relative tolerance</td>
<td>0.0005</td>
</tr>
<tr>
<td>Absolute tolerance</td>
<td>0.000005</td>
</tr>
<tr>
<td>Times to store in output</td>
<td>Specified times</td>
</tr>
<tr>
<td>Time steps taken by solver</td>
<td>Strict</td>
</tr>
<tr>
<td>Maximum BDF order</td>
<td>5</td>
</tr>
<tr>
<td>Singular mass matrix</td>
<td>Maybe</td>
</tr>
<tr>
<td>Consistent initialization of DAE systems</td>
<td>Backward Euler</td>
</tr>
<tr>
<td>Error estimation strategy</td>
<td>Include algebraic</td>
</tr>
<tr>
<td>Allow complex numbers</td>
<td>Off</td>
</tr>
</tbody>
</table>

6.3. Advanced

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Constraint handling method</td>
<td>Elimination</td>
</tr>
<tr>
<td>Null-space function</td>
<td>Automatic</td>
</tr>
<tr>
<td>Automatic assembly block size</td>
<td>On</td>
</tr>
<tr>
<td>Assembly block size</td>
<td>1000</td>
</tr>
<tr>
<td>Use Hermitian transpose of constraint matrix and in symmetry detection</td>
<td>Off</td>
</tr>
<tr>
<td>Use complex functions with real input</td>
<td>Off</td>
</tr>
</tbody>
</table>

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7. Variables

7.1. Boundary

7.1.1. Boundary 1-6, 8

<table>
<thead>
<tr>
<th>Name</th>
<th>Description</th>
<th>Unit</th>
<th>Expression</th>
</tr>
</thead>
<tbody>
<tr>
<td>unTEx_es</td>
<td>Maxwell surface stress tensor (x)</td>
<td>Pa</td>
<td>$-0.5 \times (\text{up}(\text{Dx}<em>{es}) * \text{up}(\text{Ex}</em>{es}) + \text{up}(\text{Dy}<em>{es}) * \text{up}(\text{Ey}</em>{es})) \times \text{dx} + (\text{dx} * \text{up}(\text{Dx}<em>{es}) + \text{dy} * \text{up}(\text{Dy}</em>{es})) * \text{up}(\text{Ex}_{es})$</td>
</tr>
<tr>
<td>unTEy_es</td>
<td>Maxwell surface stress tensor (y)</td>
<td>Pa</td>
<td>$-0.5 \times (\text{up}(\text{Dx}<em>{es}) * \text{up}(\text{Ex}</em>{es}) + \text{up}(\text{Dy}<em>{es}) * \text{up}(\text{Ey}</em>{es})) \times \text{dy} + (\text{dx} * \text{up}(\text{Dx}<em>{es}) + \text{dy} * \text{up}(\text{Dy}</em>{es})) * \text{up}(\text{Ey}_{es})$</td>
</tr>
<tr>
<td>dnTEx_es</td>
<td>Maxwell surface stress tensor (x)</td>
<td>Pa</td>
<td>$-0.5 \times (\text{down}(\text{Dx}<em>{es}) * \text{down}(\text{Ex}</em>{es}) + \text{down}(\text{Dy}<em>{es}) * \text{down}(\text{Ey}</em>{es})) \times \text{dx} + (\text{dx} * \text{down}(\text{Dx}<em>{es}) + \text{dy} * \text{down}(\text{Dy}</em>{es})) \times \text{down}(\text{Ex}_{es})$</td>
</tr>
<tr>
<td>dnTEy_es</td>
<td>Maxwell surface stress tensor (y)</td>
<td>Pa</td>
<td>$-0.5 \times (\text{down}(\text{Dx}<em>{es}) * \text{down}(\text{Ex}</em>{es}) + \text{down}(\text{Dy}<em>{es}) * \text{down}(\text{Ey}</em>{es})) \times \text{dy} + (\text{dx} * \text{down}(\text{Dx}<em>{es}) + \text{dy} * \text{down}(\text{Dy}</em>{es})) \times \text{down}(\text{Ey}_{es})$</td>
</tr>
<tr>
<td>unTx_es</td>
<td>Exterior Maxwell stress tensor (u), x component</td>
<td>Pa</td>
<td>$\text{unTEx}<em>{es} + \text{unTM}</em>{x es}$</td>
</tr>
<tr>
<td>unTMx_es</td>
<td>Exterior magnetic Maxwell stress tensor (u), x component</td>
<td>Pa</td>
<td>0</td>
</tr>
<tr>
<td>unTy_es</td>
<td>Exterior Maxwell stress tensor (u), y component</td>
<td>Pa</td>
<td>$\text{unTEy}<em>{es} + \text{unTY}</em>{es}$</td>
</tr>
<tr>
<td>unTMy_es</td>
<td>Exterior magnetic Maxwell stress tensor (u), y component</td>
<td>Pa</td>
<td>0</td>
</tr>
<tr>
<td>dnTx_es</td>
<td>Exterior Maxwell stress tensor (d), x component</td>
<td>Pa</td>
<td>$\text{dnTEx}<em>{es} + \text{dnTM}</em>{x es}$</td>
</tr>
<tr>
<td>dnTMx_es</td>
<td>Exterior magnetic Maxwell stress tensor (d), x component</td>
<td>Pa</td>
<td>0</td>
</tr>
<tr>
<td>dnTy_es</td>
<td>Exterior Maxwell stress tensor (d), y component</td>
<td>Pa</td>
<td>$\text{dnTEy}<em>{es} + \text{dnTY}</em>{es}$</td>
</tr>
<tr>
<td>dnTMy_es</td>
<td>Exterior magnetic Maxwell stress tensor (d), y component</td>
<td>Pa</td>
<td>0</td>
</tr>
<tr>
<td>dVolbnd_es</td>
<td>Volume integration contribution</td>
<td>m</td>
<td>$\text{d}_{es}$</td>
</tr>
<tr>
<td>nD_es</td>
<td>Surface charge density</td>
<td>C/m²</td>
<td>$\text{unx} \times (\text{down}(\text{Dx}<em>{es}) - \text{up}(\text{Dx}</em>{es})) + \text{uny} \times (\text{down}(\text{Dy}<em>{es}) - \text{up}(\text{Dy}</em>{es}))$</td>
</tr>
</tbody>
</table>
### 7.1.2. Boundary 7, 9-20

<table>
<thead>
<tr>
<th>Name</th>
<th>Description</th>
<th>Unit</th>
<th>Expression</th>
</tr>
</thead>
<tbody>
<tr>
<td>unTEx_es</td>
<td>Maxwell surface stress tensor (x)</td>
<td>Pa</td>
<td>(-0.5 \times (\text{up}(Dx_{es}) \times \text{up}(Ex_{es}) + \text{up}(Dy_{es}) \times \text{up}(Ey_{es}))) - (\text{dnx}(\text{dnx} \times \text{up}(Dx_{es}) + \text{dny} \times \text{up}(Dy_{es})) \times \text{up}(Ex_{es}))</td>
</tr>
<tr>
<td>unTEy_es</td>
<td>Maxwell surface stress tensor (y)</td>
<td>Pa</td>
<td>(-0.5 \times (\text{up}(Dx_{es}) \times \text{up}(Ex_{es}) + \text{up}(Dy_{es}) \times \text{up}(Ey_{es}))) - (\text{dny}(\text{dnx} \times \text{up}(Dx_{es}) + \text{dny} \times \text{up}(Dy_{es})) \times \text{up}(Ey_{es}))</td>
</tr>
<tr>
<td>dnTEx_es</td>
<td>Maxwell surface stress tensor (x)</td>
<td>Pa</td>
<td>(-0.5 \times (\text{down}(Dx_{es}) \times \text{down}(Ex_{es}) + \text{down}(Dy_{es}) \times \text{down}(Ey_{es}))) + (\text{unx}(\text{unx} \times \text{down}(Dx_{es}) + \text{uny} \times \text{down}(Dy_{es})) \times \text{down}(Ey_{es}))</td>
</tr>
<tr>
<td>dnTEy_es</td>
<td>Maxwell surface stress tensor (y)</td>
<td>Pa</td>
<td>(-0.5 \times (\text{down}(Dx_{es}) \times \text{down}(Ex_{es}) + \text{down}(Dy_{es}) \times \text{down}(Ey_{es}))) + (\text{uny}(\text{unx} \times \text{down}(Dx_{es}) + \text{uny} \times \text{down}(Dy_{es})) \times \text{down}(Ey_{es}))</td>
</tr>
<tr>
<td>unTx_es</td>
<td>Exterior Maxwell stress tensor (u), x component</td>
<td>Pa</td>
<td>unTEx_es + unTMx_es</td>
</tr>
<tr>
<td>unTMx_es</td>
<td>Exterior magnetic Maxwell stress tensor (u), x component</td>
<td>Pa</td>
<td>0</td>
</tr>
<tr>
<td>unTy_es</td>
<td>Exterior magnetic Maxwell stress tensor (u), y component</td>
<td>Pa</td>
<td>unTEy_es + unTMy_es</td>
</tr>
<tr>
<td>unTMy_es</td>
<td>Exterior magnetic Maxwell stress tensor (u), y component</td>
<td>Pa</td>
<td>0</td>
</tr>
<tr>
<td>dnTx_es</td>
<td>Exterior Maxwell stress tensor (d), x component</td>
<td>Pa</td>
<td>dnTEx_es + dnTMx_es</td>
</tr>
<tr>
<td>dnTMx_es</td>
<td>Exterior magnetic Maxwell stress tensor (d), x component</td>
<td>Pa</td>
<td>0</td>
</tr>
<tr>
<td>dnTy_es</td>
<td>Exterior magnetic Maxwell stress tensor (d), y component</td>
<td>Pa</td>
<td>dnTEy_es + dnTMy_es</td>
</tr>
<tr>
<td>dnTMy_es</td>
<td>Exterior magnetic Maxwell stress tensor (d), y component</td>
<td>Pa</td>
<td>0</td>
</tr>
<tr>
<td>dVolbnd es</td>
<td>Volume integration contribution</td>
<td>m</td>
<td>(d_{es})</td>
</tr>
<tr>
<td>nD_es</td>
<td>Surface charge density</td>
<td>C/m^2</td>
<td>(\text{unx}(\text{down}(Dx_{es}) - \text{up}(Dx_{es})) + \text{uny}(\text{down}(Dy_{es}) - \text{up}(Dy_{es})))</td>
</tr>
<tr>
<td>ndflux_cn_cd</td>
<td>Normal diffusive flux, cn</td>
<td>mol/ (m^2*s)</td>
<td>(\text{rn}<em>{cd} \times \text{dflux}</em>{cn}_x_{cd} + \text{ny}<em>{cd} \times \text{dflux}</em>{cn}_y_{cd})</td>
</tr>
<tr>
<td>ncflux_cn_cd</td>
<td>Normal convective flux, cn</td>
<td>mol/ (m^2*s)</td>
<td>(\text{rn}<em>{cd} \times \text{cflux}</em>{cn}_x_{cd} + \text{ny}<em>{cd} \times \text{cflux}</em>{cn}_y_{cd})</td>
</tr>
</tbody>
</table>

---

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<table>
<thead>
<tr>
<th>Name</th>
<th>Description</th>
<th>Unit</th>
<th>Expression</th>
</tr>
</thead>
<tbody>
<tr>
<td>dVols</td>
<td>Volume integration contribution</td>
<td>m</td>
<td>d_es</td>
</tr>
<tr>
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### 7.2.2. Subdomain 3-5

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Appendix C: COMSOL Settings for p-n Junction Geometry #2

The following is a COMSOL auto-generated report that corresponds to the FEM simulation results that were presented in Section 2.5 and Section 2.6. The report provides information about FEM model properties, meshing settings, boundary conditions, solver settings, solver variables, constants used, etc.
1. Model Properties

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</tr>
<tr>
<td>Company</td>
<td>COMSOL</td>
</tr>
<tr>
<td>Department</td>
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</tr>
<tr>
<td>Reference</td>
<td>Copyright (c) 1998-2008 by COMSOL AB</td>
</tr>
<tr>
<td>URL</td>
<td><a href="http://www.comsol.com">www.comsol.com</a></td>
</tr>
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<td>Creation date</td>
<td>Nov 17, 2008 7:33:45 PM</td>
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<tr>
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1.1. Model description

Semiconductor Diode

A semiconductor device model featuring a diode with p- and n-type regions. The image shows the hole concentration for 0.5V forward bias.

2. Constants

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<td>T</td>
<td>300[K]</td>
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</table>

file://C:\Documents and Settings\BCANNON\Desktop\PWell Starting 2-12-10\1 GHZ 4 Periods Good Transient.mph
**3. Geom1**

Space dimensions: 2D

Independent variables: x, y, z

### 3.1. Scalar Expressions

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<td>Doping concentration</td>
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<td>Charge neutrality electron concentration</td>
</tr>
<tr>
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<td>1/m³</td>
<td>Charge neutrality hole concentration</td>
</tr>
<tr>
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<tr>
<td>RSRH</td>
<td>(on-top-ni²)<em>(taup</em>(cn+n)+tau_p*(cp+ni))</td>
<td>V</td>
<td>Recombination term</td>
</tr>
</tbody>
</table>

### 3.2. Mesh

#### 3.2.1. Mesh Statistics

<table>
<thead>
<tr>
<th>Description</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Number of degrees of freedom</td>
<td>189018</td>
</tr>
<tr>
<td>Number of mesh points</td>
<td>21963</td>
</tr>
<tr>
<td>Number of elements</td>
<td>43688</td>
</tr>
<tr>
<td>Triangular</td>
<td></td>
</tr>
<tr>
<td>Quadrilateral</td>
<td>0</td>
</tr>
<tr>
<td>Number of boundary elements</td>
<td>1344</td>
</tr>
<tr>
<td>Number of vertex elements</td>
<td>33</td>
</tr>
<tr>
<td>Minimum element quality</td>
<td>0.62</td>
</tr>
<tr>
<td>Element area ratio</td>
<td>0</td>
</tr>
</tbody>
</table>

---

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3.3. Application Mode: Electrostatics (es)

Application mode type: Electrostatics
Application mode name: es

3.3.1. Scalar Variables

<table>
<thead>
<tr>
<th>Name</th>
<th>Variable</th>
<th>Value</th>
<th>Unit</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>epsilon0</td>
<td>8.854187817e-12</td>
<td>F/m</td>
<td>Permittivity of vacuum</td>
</tr>
</tbody>
</table>

3.3.2. Application Mode Properties

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Default element type</td>
<td>Lagrange - Quadratic</td>
</tr>
<tr>
<td>Input property</td>
<td>Forced voltage</td>
</tr>
<tr>
<td>Frame</td>
<td>Frame (ref)</td>
</tr>
<tr>
<td>Weak constraints</td>
<td>Off</td>
</tr>
<tr>
<td>Constraint type</td>
<td>Ideal</td>
</tr>
</tbody>
</table>

3.3.3. Variables
Dependent variables: psi
Shape functions: shlag(2,'psi')
Interior boundaries active

3.3.4. Boundary Settings

<table>
<thead>
<tr>
<th>Boundary</th>
<th>1, 3, 5, 32-33</th>
<th>2, 18</th>
<th>12, 19, 34-35</th>
</tr>
</thead>
<tbody>
<tr>
<td>Type</td>
<td>Zero charge/Symmetry</td>
<td>Electric potential</td>
<td>Continuity</td>
</tr>
<tr>
<td>Surface charge density (rhos)</td>
<td>C/m²</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Electric potential (V0)</td>
<td>V</td>
<td>0</td>
<td>psi_init</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Boundary</th>
<th>13, 20</th>
<th>4, 11, 24, 26</th>
<th>14-17, 21-23, 25</th>
</tr>
</thead>
<tbody>
<tr>
<td>Type</td>
<td>Surface charge</td>
<td>Surface charge</td>
<td>Electric potential</td>
</tr>
<tr>
<td>Surface charge density (rhos)</td>
<td>C/m²</td>
<td>rhos</td>
<td>rhos</td>
</tr>
<tr>
<td>Electric potential (V0)</td>
<td>V</td>
<td>psi_init</td>
<td>0</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Boundary</th>
<th>6-10, 27-31</th>
</tr>
</thead>
<tbody>
<tr>
<td>Type</td>
<td>Electric potential</td>
</tr>
<tr>
<td>Surface charge density (rhos)</td>
<td>C/m²</td>
</tr>
<tr>
<td>Electric potential (V0)</td>
<td>V</td>
</tr>
</tbody>
</table>

3.3.5. Subdomain Settings

<table>
<thead>
<tr>
<th>Subdomain</th>
<th>1, 4</th>
<th>2-3, 5-6</th>
</tr>
</thead>
<tbody>
<tr>
<td>Relative permittivity (epsilon)</td>
<td>1</td>
<td>[epsilon(0,0,0),epsilon(1,0,0)]</td>
</tr>
<tr>
<td>Space charge density (rho)</td>
<td>C/m²</td>
<td>q*(N-cn+cp)</td>
</tr>
</tbody>
</table>

Subdomain initial value: 1, 4

3.4. Application Mode: Convection and Diffusion (cd)

Application mode type: Convection and Diffusion
Application mode name: cd

3.4.1. Application Mode Properties

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Default element type</td>
<td>Lagrange - Quadratic</td>
</tr>
<tr>
<td>Analysis type</td>
<td>Transient</td>
</tr>
<tr>
<td>Equation form</td>
<td>Conservative</td>
</tr>
<tr>
<td>Frame</td>
<td>Frame (ref)</td>
</tr>
<tr>
<td>Weak constraints</td>
<td>On</td>
</tr>
<tr>
<td>Constraint type</td>
<td>Ideal</td>
</tr>
</tbody>
</table>

3.4.2. Variables

Dependent variables: cn
3.4.3. Boundary Settings

<table>
<thead>
<tr>
<th>Boundary</th>
<th>Type</th>
<th>Concentration ($c_0$) mol/m$^3$</th>
<th>$n_{init}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1, 32</td>
<td>Insulation/Symmetry</td>
<td>0</td>
<td>$n_{init}$</td>
</tr>
<tr>
<td>2, 18</td>
<td>Concentration Continuity</td>
<td></td>
<td>0</td>
</tr>
<tr>
<td>3, 5-10, 12, 14-17, 19, 21-23, 25, 27-31, 33-35</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Boundary</th>
<th>Type</th>
<th>Concentration ($c_0$) mol/m$^3$</th>
<th>$n_{init}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>4, 11, 24, 26</td>
<td>Convective flux</td>
<td>0</td>
<td>$n_{init}$</td>
</tr>
<tr>
<td>13, 20</td>
<td>Convective flux</td>
<td></td>
<td>0</td>
</tr>
</tbody>
</table>

3.4.4. Subdomain Settings

<table>
<thead>
<tr>
<th>Subdomain</th>
<th>Shape functions (shape)</th>
<th>Integration order (gorder)</th>
<th>Diffusion coefficient (D) m$^2$/s</th>
<th>Reaction rate (R) moil/m$^3$/s</th>
<th>$u$-velocity (u) m/s</th>
<th>$v$-velocity (v) m/s</th>
</tr>
</thead>
<tbody>
<tr>
<td>1, 4</td>
<td>shlag(2,'Im2') shlag(2,'cn')</td>
<td>4</td>
<td>Dn</td>
<td>-RSRH</td>
<td>$mun*psix$</td>
<td>$mun*psiy$</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Subdomain initial value</th>
<th>Concentration, $cn$ (cn) mol/m$^3$</th>
<th>$n_{init}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1, 4</td>
<td>$n_{init}$</td>
<td></td>
</tr>
</tbody>
</table>

3.5. Application Mode: Convection and Diffusion (cd2)

Application mode type: Convection and Diffusion
Application mode name: cd2

3.5.1. Application Mode Properties

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Default element type</td>
<td>Lagrange - Quadratic</td>
</tr>
<tr>
<td>Analysis type</td>
<td>Transient</td>
</tr>
<tr>
<td>Equation form</td>
<td>Conservative</td>
</tr>
<tr>
<td>Frame</td>
<td>Frame (ref)</td>
</tr>
<tr>
<td>Weak constraints</td>
<td>On</td>
</tr>
<tr>
<td>Constraint type</td>
<td>Ideal</td>
</tr>
</tbody>
</table>

3.5.2. Variables

Dependent variables: $cp$
Shape functions: shlag(2,'Im3'), shlag(2,'cp')

Interior boundaries not active
3.5.3. Boundary Settings

<table>
<thead>
<tr>
<th>Boundary</th>
<th>1, 32</th>
<th>2, 18</th>
<th>4, 11, 24, 26</th>
</tr>
</thead>
<tbody>
<tr>
<td>Type</td>
<td>Insulation/Symmetry</td>
<td>Concentration</td>
<td>Convective flux</td>
</tr>
<tr>
<td>Concentration (c0)</td>
<td>mol/m³</td>
<td>p_init</td>
<td>0</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Boundary</th>
<th>13, 20</th>
</tr>
</thead>
<tbody>
<tr>
<td>Type</td>
<td>Convective flux</td>
</tr>
<tr>
<td>Concentration (c0)</td>
<td>mol/m³</td>
</tr>
</tbody>
</table>

### 3.5.4. Subdomain Settings

<table>
<thead>
<tr>
<th>Subdomain</th>
<th>1, 4</th>
</tr>
</thead>
<tbody>
<tr>
<td>Shape functions (shape)</td>
<td>shlag(2,'Im3') shlag(2,'cp')</td>
</tr>
<tr>
<td>Integration order (gporder)</td>
<td>4</td>
</tr>
<tr>
<td>Diffusion coefficient (D)</td>
<td>m²/s</td>
</tr>
<tr>
<td>Reaction rate (R)</td>
<td>mol/(m³s)</td>
</tr>
<tr>
<td>x-velocity (u)</td>
<td>m/s</td>
</tr>
<tr>
<td>y-velocity (v)</td>
<td>m/s</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Subdomain initial value</th>
<th>1, 4</th>
</tr>
</thead>
<tbody>
<tr>
<td>Concentration, cp (cp)</td>
<td>mol/m³</td>
</tr>
</tbody>
</table>

3.6. Application Mode: Weak Form, Boundary (wb)

Application mode type: Weak Form, Boundary

Application mode name: wb

3.6.1. Application Mode Properties

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Default element type</td>
<td>Lagrange - Quadratic</td>
</tr>
<tr>
<td>Wave extension</td>
<td>Off</td>
</tr>
<tr>
<td>Frame</td>
<td>Frame (ref)</td>
</tr>
<tr>
<td>Weak constraints</td>
<td>Off</td>
</tr>
</tbody>
</table>

3.6.2. Variables

Dependent variables: rhos, rhos_t

Shape functions: shlag(2,'rhos')

Interior boundaries not active

3.6.3. Boundary Settings

<table>
<thead>
<tr>
<th>Boundary</th>
<th>4, 11, 13, 20, 24, 26</th>
</tr>
</thead>
<tbody>
<tr>
<td>Weak term (weak)</td>
<td>rhos_test&quot;(q<em>ntflux_cn_cd+q</em>ntflux_cp_cd2)</td>
</tr>
<tr>
<td>Time-dependent weak term (dweak)</td>
<td>rhos_test*rhos_time</td>
</tr>
</tbody>
</table>
4. Integration Coupling Variables

4.1. geom1

4.1.1. Source Boundary: 2, 18

<table>
<thead>
<tr>
<th>Name</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Variable name</td>
<td>ic</td>
</tr>
<tr>
<td>Expression</td>
<td>1e-6<em>q</em>(m2-lm3)</td>
</tr>
<tr>
<td>Order</td>
<td>4</td>
</tr>
<tr>
<td>Global</td>
<td>Yes</td>
</tr>
</tbody>
</table>

5. Solver Settings

Solve using a script: off

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Auto select solver</td>
<td>On</td>
</tr>
<tr>
<td>Solver</td>
<td>Time dependent</td>
</tr>
<tr>
<td>Solution form</td>
<td>Automatic</td>
</tr>
<tr>
<td>Symmetric</td>
<td>auto</td>
</tr>
<tr>
<td>Adaptive mesh refinement</td>
<td>Off</td>
</tr>
<tr>
<td>Optimization/Sensitivity</td>
<td>Off</td>
</tr>
<tr>
<td>Plot while solving</td>
<td>On</td>
</tr>
</tbody>
</table>

5.1. Direct (UMFPACK)

Solver type: Linear system solver

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pivot threshold</td>
<td>0.1</td>
</tr>
<tr>
<td>Memory allocation factor</td>
<td>0.7</td>
</tr>
</tbody>
</table>

5.2. Time Stepping

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Times</td>
<td>range(0,1e-11,4e-9)</td>
</tr>
<tr>
<td>Relative tolerance</td>
<td>0.001</td>
</tr>
<tr>
<td>Absolute tolerance</td>
<td>0.00010</td>
</tr>
<tr>
<td>Times to store in output</td>
<td>Specified times</td>
</tr>
<tr>
<td>Time steps taken by solver</td>
<td>Free</td>
</tr>
<tr>
<td>Maximum BDF order</td>
<td>5</td>
</tr>
<tr>
<td>Singular mass matrix</td>
<td>Maybe</td>
</tr>
<tr>
<td>Consistent initialization of DAE systems</td>
<td>Backward Euler</td>
</tr>
<tr>
<td>Error estimation strategy</td>
<td>Include algebraic</td>
</tr>
<tr>
<td>Allow complex numbers</td>
<td>Off</td>
</tr>
</tbody>
</table>

5.3. Advanced

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Constraint handling method</td>
<td>Elimination</td>
</tr>
</tbody>
</table>
### 6. Variables

#### 6.1. Boundary

6.1.1. Boundary 1-2, 4, 11-13, 18-20, 24, 26, 32, 34-35

<table>
<thead>
<tr>
<th>Name</th>
<th>Description</th>
<th>Unit</th>
<th>Expression</th>
</tr>
</thead>
<tbody>
<tr>
<td>unTEx_es</td>
<td>Maxwell surface stress tensor (x)</td>
<td>Pa</td>
<td>(-0.5 * (up(Dx_es) * up(Ex_es) + up(Dy_es) * up(Ey_es)) * [dx] + ([dx] * up(Dx_es) + [dy] * up(Dy_es)) * up(Ex_es))</td>
</tr>
<tr>
<td>unTEy_es</td>
<td>Maxwell surface stress tensor (y)</td>
<td>Pa</td>
<td>(-0.5 * (up(Dx_es) * up(Ex_es) + up(Dy_es) * up(Ey_es)) * [dy] + ([dx] * up(Dx_es) + [dy] * up(Dy_es)) * up(Ex_es))</td>
</tr>
<tr>
<td>dnTEx_es</td>
<td>Maxwell surface stress tensor (x)</td>
<td>Pa</td>
<td>(-0.5 * ([down](Dx_es) * [down](Ex_es) + [down](Dy_es) * [down](Ey_es)) * [ux] + ([ux] * [down](Dx_es) + [uy] * [down](Dy_es)) * [down](Ex_es))</td>
</tr>
<tr>
<td>dnTExy_es</td>
<td>Maxwell surface stress tensor (x, y)</td>
<td>Pa</td>
<td>(-0.5 * ([down](Dx_es) * [down](Ex_es) + [down](Dy_es) * [down](Ey_es)) * [ux] + ([ux] * [down](Dx_es) + [uy] * [down](Dy_es)) * [down](Ex_es))</td>
</tr>
<tr>
<td>unTx_es</td>
<td>Exterior Maxwell stress tensor (u)</td>
<td>Pa</td>
<td>[unTEx_es] + [unTMx_es]</td>
</tr>
<tr>
<td>unTMx_es</td>
<td>Exterior magnetic Maxwell stress tensor (u)</td>
<td>Pa</td>
<td>0</td>
</tr>
<tr>
<td>unTy_es</td>
<td>Exterior Maxwell stress tensor (u, y)</td>
<td>Pa</td>
<td>[unTEy_es] + [unTMy_es]</td>
</tr>
<tr>
<td>unTMy_es</td>
<td>Exterior magnetic Maxwell stress tensor (u)</td>
<td>Pa</td>
<td>0</td>
</tr>
<tr>
<td>dnTx_es</td>
<td>Exterior Maxwell stress tensor (d)</td>
<td>Pa</td>
<td>[dnTEx_es] + [dnTMx_es]</td>
</tr>
<tr>
<td>dnTMx_es</td>
<td>Exterior magnetic Maxwell stress tensor (d)</td>
<td>Pa</td>
<td>0</td>
</tr>
<tr>
<td>dnTy_es</td>
<td>Exterior Maxwell stress tensor (d, y)</td>
<td>Pa</td>
<td>[dnTExy_es] + [dnTMy_es]</td>
</tr>
<tr>
<td>dnTMy_es</td>
<td>Exterior magnetic Maxwell stress tensor (d)</td>
<td>Pa</td>
<td>0</td>
</tr>
</tbody>
</table>

---

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6.1.2. Boundary 3, 5-10, 14-17, 21-23, 25, 27-31, 33

<table>
<thead>
<tr>
<th>Name</th>
<th>Description</th>
<th>Unit</th>
<th>Expression</th>
</tr>
</thead>
<tbody>
<tr>
<td>unTEx_es</td>
<td>Maxwell surface stress tensor (x)</td>
<td>Pa</td>
<td>-0.5 * (up(Dx_es) * up(Ex_es) + up(Dy_es) * up(Ey_es)) * up(Dx_es) + up(Dy_es) * up(Ey_es)</td>
</tr>
<tr>
<td>unTEx_es</td>
<td>Maxwell surface stress tensor (y)</td>
<td>Pa</td>
<td>-0.5 * (up(Dx_es) * up(Ex_es) + up(Dy_es) * up(Ey_es)) * up(Dx_es) + up(Dy_es) * up(Ey_es)</td>
</tr>
<tr>
<td>dnTEx_es</td>
<td>Maxwell surface stress tensor (x)</td>
<td>Pa</td>
<td>-0.5 * (down(Dx_es) * down(Ex_es) + down(Dy_es) * down(Ey_es)) * down(Dx_es) + down(Dy_es) * down(Ey_es)</td>
</tr>
<tr>
<td>dnTEx_es</td>
<td>Maxwell surface stress tensor (y)</td>
<td>Pa</td>
<td>-0.5 * (down(Dx_es) * down(Ex_es) + down(Dy_es) * down(Ey_es)) * down(Dx_es) + down(Dy_es) * down(Ey_es)</td>
</tr>
<tr>
<td>unTx_es</td>
<td>Exterior Maxwell stress tensor (u), x component</td>
<td>Pa</td>
<td>unTEx_es+unTMx_es</td>
</tr>
<tr>
<td>unTMy_es</td>
<td>Exterior Maxwell stress tensor (u), y component</td>
<td>Pa</td>
<td>0</td>
</tr>
<tr>
<td>unTy_es</td>
<td>Exterior Maxwell stress tensor (u), y component</td>
<td>Pa</td>
<td>unTEx_es+unTMy_es</td>
</tr>
<tr>
<td>unTy_es</td>
<td>Exterior Maxwell stress tensor (u), y component</td>
<td>Pa</td>
<td>0</td>
</tr>
<tr>
<td>dnTx_es</td>
<td>Exterior Maxwell stress tensor (d), x component</td>
<td>Pa</td>
<td>dnTEx_es+dnTMx_es</td>
</tr>
<tr>
<td>dnTMy_es</td>
<td>Exterior Maxwell stress tensor (d), y component</td>
<td>Pa</td>
<td>0</td>
</tr>
<tr>
<td>dnTy_es</td>
<td>Exterior Maxwell stress tensor (d), y component</td>
<td>Pa</td>
<td>dnTEx_es+dnTMy_es</td>
</tr>
<tr>
<td>dnTy_es</td>
<td>Exterior Maxwell stress tensor (d), y component</td>
<td>Pa</td>
<td>0</td>
</tr>
<tr>
<td>dVolbd_es</td>
<td>Volume integration contribution</td>
<td>m</td>
<td>d_es</td>
</tr>
<tr>
<td>nD_es</td>
<td>Surface charge density</td>
<td>C/m^2</td>
<td>-unx * (down(Dx_es) - up(Dx_es)) - uny * (down(Dy_es) - up(Dy_es))</td>
</tr>
</tbody>
</table>

6.1.2. Boundary 3, 5-10, 14-17, 21-23, 25, 27-31, 33

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### 6.2. Subdomain

#### 6.2.1. Subdomain 1, 4

<table>
<thead>
<tr>
<th>Name</th>
<th>Description</th>
<th>Unit</th>
<th>Expression</th>
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</thead>
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<td>dVol_es</td>
<td>Volume integration contribution</td>
<td>m</td>
<td>d_es</td>
</tr>
<tr>
<td>Dx_es</td>
<td>Electric displacement, x component</td>
<td>C/m^2</td>
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<tr>
<td>Dy_es</td>
<td>Electric displacement, y component</td>
<td>C/m^2</td>
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<tr>
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<tr>
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<td>Ey_es</td>
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<td>Diffusive flux, on, x component</td>
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<tr>
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<tr>
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file://C:\Documents and Settings\BCANNON\Desktop\PWell Starting 2-12-10\1GHz4Pe... 4/20/2010
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<td>Volume integration contribution</td>
<td>m</td>
<td>d es</td>
</tr>
<tr>
<td>Dx es</td>
<td>Electric displacement, x component</td>
<td>C/m²²</td>
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<tr>
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<td>( \varepsilon_{xy} \cdot E_x + \varepsilon_{yy} \cdot E_y )</td>
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<tr>
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<td>Permittivity</td>
<td>F/m</td>
<td>( \varepsilon_0 \cdot \varepsilon_{xx} )</td>
</tr>
<tr>
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<td>Permittivity, xx component</td>
<td>F/m</td>
<td>( \varepsilon_0 \cdot \varepsilon_{xx} )</td>
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<td>( \varepsilon_0 \cdot \varepsilon_{xy} )</td>
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<td>F/m</td>
<td>( \varepsilon_0 \cdot \varepsilon_{xy} )</td>
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<td>( \varepsilon_0 \cdot \varepsilon_{yy} )</td>
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<td>Ey es</td>
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file://C:\Documents and Settings\BCANNON\Desktop\PWell Starting 2-12-10\1GHz 4 P... 4/20/2010
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<td>Convective flux, cn, y component</td>
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<tr>
<td>grad_cn_y_cd</td>
<td>Concentration gradient, cn, y component</td>
<td>mol/m^4</td>
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<tr>
<td>grad_cn_x_cd</td>
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<td>grad_cn_y_cd</td>
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<td>grad_cn_y_cd</td>
<td>Total flux, cn, y component</td>
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<td>Equation residual for cn</td>
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<td>grad_cn_x_cd</td>
<td>Shock capturing residual for cn</td>
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<td>da_cn_cd</td>
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Appendix D: COMSOL Settings for Contaminated Photomask

The following is a COMSOL auto-generated report that corresponds to the FEM simulation results that were presented in Section 3.1. The report provides information about FEM model properties, meshing settings, boundary conditions, solver settings, solver variables, constants used, etc.
1. Model Properties

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<th>Value</th>
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<tr>
<td>Author</td>
<td>COMSOL</td>
</tr>
<tr>
<td>Company</td>
<td>COMSOL</td>
</tr>
<tr>
<td>Department</td>
<td></td>
</tr>
<tr>
<td>Reference</td>
<td>Copyright (c) 1998-2008 by COMSOL AB</td>
</tr>
<tr>
<td>URL</td>
<td><a href="http://www.comsol.com">www.comsol.com</a></td>
</tr>
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Application modes and modules used in this model:

- Geom1 (2D)
  - In-Plane Electric Currents (AC/DC Module)

2. Geom1

Space dimensions: 2D

Independent variables: x, y, z

2.1. Mesh

2.1.1. Mesh Statistics

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<th></th>
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<td>Number of elements</td>
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File name: C:\Documents and Settings\BCANNON\Desktop\ASML 70nm diameter particle True Absorber Conductivity Values\ASML_Oim.mph
### 2.2. Application Mode: In-Plane Electric Currents (emqvw)

Application mode type: In-Plane Electric Currents (AC/DC Module)

Application mode name: emqvw

#### 2.2.1. Scalar Variables

<table>
<thead>
<tr>
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<th>Variable</th>
<th>Value</th>
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<th>Description</th>
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#### 2.2.2. Application Mode Properties

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<th>Value</th>
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</thead>
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File: C:\Documents and Settings\BCANNON\Desktop\ASML 70nm diameter particle True... 4/20/2010
### 2.2.3. Variables

Dependent variables: V, Ax, Ay, redAx, redAy, psi

Shape functions: $\text{shlag}(2,'\text{Im1}')$, $\text{shlag}(2,'V')$

Interior boundaries active

### 2.2.4. Boundary Settings

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<table>
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<td>magtype</td>
<td>Magnetic insulation</td>
<td>Magnetic insulation</td>
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<table>
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<tr>
<th>Boundary</th>
<th>26, 30</th>
<th>31-33, 40</th>
<th>34-36, 47-49, 51</th>
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<tbody>
<tr>
<td>Electric potential (V</td>
<td>0</td>
<td>-1</td>
<td>-1</td>
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<td>Port number (portnr)</td>
<td>10</td>
<td>2</td>
<td>8</td>
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<tr>
<td>Inport</td>
<td>0</td>
<td>0</td>
<td>0</td>
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<tr>
<td>eltype</td>
<td>Floating potential</td>
<td>Port</td>
<td>Port</td>
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<td>magtype</td>
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2.2.5. Subdomain Settings

<table>
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<tr>
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<th>2, 9</th>
<th>3</th>
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</thead>
<tbody>
<tr>
<td>Shape functions (shape)</td>
<td>shlag(2, 'lm1') shlag (2, 'V')</td>
<td>shlag(2, 'lm1') shlag (2, 'V')</td>
<td>shlag(2, 'lm1') shlag (2, 'V')</td>
</tr>
<tr>
<td>Integration order (gorder)</td>
<td>4</td>
<td>4</td>
<td>4</td>
</tr>
<tr>
<td>name</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Electric conductivity (sigma)</td>
<td>S/m</td>
<td>(0, 0; 0, 0)</td>
<td>(10e6, 0; 0, 10e6)</td>
</tr>
<tr>
<td>Relative permittivity (epsilon)</td>
<td>1</td>
<td>(1, 0, 0.1)</td>
<td>(2, 0, 0.2)</td>
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<tr>
<td>Source point (nTsrcpnt)</td>
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<td>(0, 0)</td>
<td>(0, 0)</td>
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<table>
<thead>
<tr>
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<th>11</th>
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<tbody>
<tr>
<td>Shape functions (shape)</td>
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<tr>
<td>Integration order (gorder)</td>
<td>4</td>
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<tr>
<td>name</td>
<td>particle</td>
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<tr>
<td>Electric conductivity (sigma)</td>
<td>S/m</td>
</tr>
<tr>
<td>Relative permittivity (epsilon)</td>
<td>1</td>
</tr>
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<td>Source point (nTsrcpnt)</td>
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3. Solver Settings

Solve using a script: off

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<tr>
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<th>Time-harmonic electric currents</th>
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<tbody>
<tr>
<td>Auto select solver</td>
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<tr>
<td>Solver</td>
<td>Stationary</td>
</tr>
<tr>
<td>Solution form</td>
<td>Automatic</td>
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<tr>
<td>Symmetric</td>
<td>auto</td>
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<tr>
<td>Adaptive mesh refinement</td>
<td>Off</td>
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<tr>
<td>Optimization/Sensitivity</td>
<td>Off</td>
</tr>
<tr>
<td>Plot while solving</td>
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3.1. Direct (UMFPACK)

Solver type: Linear system solver

<table>
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<tr>
<th>Parameter</th>
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</thead>
<tbody>
<tr>
<td>Pivot threshold</td>
<td>0.1</td>
</tr>
<tr>
<td>Memory allocation factor</td>
<td>0.7</td>
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3.2. Stationary
### 3.3. Advanced

<table>
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<tr>
<th>Parameter</th>
<th>Value</th>
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<tbody>
<tr>
<td>Constraint handling method</td>
<td>Elimination</td>
</tr>
<tr>
<td>Null-space function</td>
<td>Automatic</td>
</tr>
<tr>
<td>Automatic assembly block size</td>
<td>On</td>
</tr>
<tr>
<td>Assembly block size</td>
<td>5000</td>
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<tr>
<td>Use Hermitian transpose of constraint matrix and in symmetry detection</td>
<td>Off</td>
</tr>
<tr>
<td>Use complex functions with real input</td>
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</tr>
<tr>
<td>Step if error due to undefined operation</td>
<td>On</td>
</tr>
<tr>
<td>Store solution on file</td>
<td>Off</td>
</tr>
<tr>
<td>Type of scaling</td>
<td>Automatic</td>
</tr>
<tr>
<td>Manual scaling</td>
<td>On</td>
</tr>
<tr>
<td>Row equilibration</td>
<td>On</td>
</tr>
<tr>
<td>Manual control of reassembly</td>
<td>Off</td>
</tr>
<tr>
<td>Load constant</td>
<td>On</td>
</tr>
<tr>
<td>Constraint constant</td>
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<tr>
<td>Mass constant</td>
<td>On</td>
</tr>
<tr>
<td>Damping (mass) constant</td>
<td>Off</td>
</tr>
<tr>
<td>Jacobian constant</td>
<td>On</td>
</tr>
<tr>
<td>Constraint Jacobian constant</td>
<td>On</td>
</tr>
<tr>
<td>Assembly block size</td>
<td>5000</td>
</tr>
<tr>
<td>Use complex functions with real input</td>
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</tr>
<tr>
<td>Step if error due to undefined operation</td>
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<tr>
<td>Store solution on file</td>
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<tr>
<td>Type of scaling</td>
<td>Automatic</td>
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<tr>
<td>Manual scaling</td>
<td>On</td>
</tr>
<tr>
<td>Row equilibration</td>
<td>On</td>
</tr>
<tr>
<td>Manual control of reassembly</td>
<td>Off</td>
</tr>
<tr>
<td>Load constant</td>
<td>On</td>
</tr>
<tr>
<td>Constraint constant</td>
<td>On</td>
</tr>
<tr>
<td>Mass constant</td>
<td>On</td>
</tr>
<tr>
<td>Damping (mass) constant</td>
<td>Off</td>
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<tr>
<td>Jacobian constant</td>
<td>On</td>
</tr>
<tr>
<td>Constraint Jacobian constant</td>
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### 4. Variables

#### 4.1. Boundary

##### 4.1.1. Boundary 1, 3-4, 6-9, 16, 21, 26, 28, 37, 39, 41, 46, 50, 62-54, 66-60

<table>
<thead>
<tr>
<th>Name</th>
<th>Description</th>
<th>Unit</th>
<th>Expression</th>
</tr>
</thead>
<tbody>
<tr>
<td>dVolbd_ emqvw</td>
<td>Area integration contribution</td>
<td>m</td>
<td>d_emqvw</td>
</tr>
<tr>
<td>rJ_ emqvw</td>
<td>Normal current density</td>
<td>A/m²</td>
<td>r_emqvw * 3x_emqvw + ny_emqvw * 3y_emqvw</td>
</tr>
<tr>
<td>uTExav_ emqvw</td>
<td>Electric Maxwell surface stress tensor, time average, x component</td>
<td>Pa</td>
<td>real(-0.25 * (Ex_emqvw_up * conj(Dx_emqvw_up)) + Ey_emqvw_up * conj(Dy_emqvw_up)) * dnx + 0.5 * (dx_x * Ex_emqvw_up + dny * Ey_emqvw_up) * conj(Dx_emqvw_up))</td>
</tr>
<tr>
<td>dTExav_ emqvw</td>
<td>Electric Maxwell surface stress tensor, time average, x component</td>
<td>Pa</td>
<td>real(-0.25 * (Ex_emqvw_down * conj(Dx_emqvw_down)) + Ey_emqvw_down * conj(Dy_emqvw_down)) * unx + 0.5 * (ux_x * Ex_emqvw_down + uny * Ey_emqvw_down) * conj(Dx_emqvw_down))</td>
</tr>
<tr>
<td>uTEyav_ emqvw</td>
<td>Electric Maxwell</td>
<td>Pa</td>
<td>real(-0.25 * (Ex_emqvw_up * conj(Dx_emqvw_up))</td>
</tr>
<tr>
<td>Term</td>
<td>Description</td>
<td>Unit</td>
<td>Equation</td>
</tr>
<tr>
<td>------</td>
<td>-------------</td>
<td>------</td>
<td>----------</td>
</tr>
<tr>
<td>surface stress tensor, time average, y component</td>
<td></td>
<td></td>
<td>$+E_y \cdot q_{vw} \cdot \text{up} \cdot \text{conj}(D_y \cdot q_{vw} \cdot \text{up}) \cdot \text{conjdny} + 0.5 \cdot (\text{dnx} \cdot E_x \cdot q_{vw} \cdot \text{up} + \text{dnx} \cdot E_x \cdot q_{vw} \cdot \text{up}) \cdot \text{conj}(D_x \cdot q_{vw} \cdot \text{up})$</td>
</tr>
<tr>
<td>$dnT_{Ey\cdot q_{vw}}$</td>
<td>Electric Maxwell surface stress tensor, time average, y component</td>
<td>Pa</td>
<td>$\text{real}(0.25 \cdot (E_x \cdot q_{vw} \cdot \text{down} \cdot \text{conj}(D_x \cdot q_{vw} \cdot \text{down}) + E_y \cdot q_{vw} \cdot \text{down} \cdot \text{conj}(D_y \cdot q_{vw} \cdot \text{down})) \cdot \text{uny} + 0.5 \cdot (\text{unx} \cdot E_x \cdot q_{vw} \cdot \text{down} + \text{uny} \cdot E_y \cdot q_{vw} \cdot \text{down}) \cdot \text{conj}(D_y \cdot q_{vw} \cdot \text{down})$</td>
</tr>
<tr>
<td>$nJ_s \cdot q_{vw}$</td>
<td>Source current density A/m$^2$</td>
<td></td>
<td>$\text{unx} \cdot (\text{down}(J_x \cdot q_{vw}) - \text{up}(J_x \cdot q_{vw})) + \text{uny} \cdot (\text{down}(J_y \cdot q_{vw}) - \text{up}(J_y \cdot q_{vw}))$</td>
</tr>
<tr>
<td>$tE_{x\cdot q_{vw}}$</td>
<td>Tangential electric field, x component</td>
<td>V/m</td>
<td>$-V_Tx$</td>
</tr>
<tr>
<td>$tE_{y\cdot q_{vw}}$</td>
<td>Tangential electric field, y component</td>
<td>V/m</td>
<td>$-V_Ty$</td>
</tr>
<tr>
<td>$tD_{x\cdot q_{vw}}$</td>
<td>Tangential electric displacement, x component</td>
<td>C/m$^2$</td>
<td>$\epsilon_0 \cdot \epsilon_{\text{rbnd}} \cdot E_x \cdot q_{vw} \cdot \text{conjdEx}$</td>
</tr>
<tr>
<td>$tD_{y\cdot q_{vw}}$</td>
<td>Tangential electric displacement, y component</td>
<td>C/m$^2$</td>
<td>$\epsilon_0 \cdot \epsilon_{\text{rbnd}} \cdot E_y \cdot q_{vw} \cdot \text{conjdEy}$</td>
</tr>
<tr>
<td>$\text{normtE}<em>{x\cdot q</em>{vw}}$</td>
<td>Tangential electric field, norm</td>
<td>V/m</td>
<td>$\sqrt{\text{abs}(E_x \cdot q_{vw})^2 + \text{abs}(E_y \cdot q_{vw})^2}$</td>
</tr>
<tr>
<td>$\text{normtD}<em>{x\cdot q</em>{vw}}$</td>
<td>Tangential electric displacement, norm</td>
<td>C/m$^2$</td>
<td>$\sqrt{\text{abs}(D_x \cdot q_{vw})^2 + \text{abs}(D_y \cdot q_{vw})^2}$</td>
</tr>
<tr>
<td>$uT_{x\cdot q_{vw}}$</td>
<td>Exterior Maxwell stress tensor (u), x component</td>
<td>Pa</td>
<td>$uT_{Ex\cdot q_{vw}} + uT_{Mx\cdot q_{vw}}$</td>
</tr>
<tr>
<td>$uT_{Ex\cdot q_{vw}}$</td>
<td>Exterior electric Maxwell stress tensor (u), x component</td>
<td>Pa</td>
<td>$0$</td>
</tr>
<tr>
<td>$uT_{Mx\cdot q_{vw}}$</td>
<td>Exterior magnetic Maxwell stress tensor (u), x component</td>
<td>Pa</td>
<td>$0$</td>
</tr>
<tr>
<td>$uT_{y\cdot q_{vw}}$</td>
<td>Exterior Maxwell stress tensor (u), y component</td>
<td>Pa</td>
<td>$uT_{Ey\cdot q_{vw}} + uT_{My\cdot q_{vw}}$</td>
</tr>
<tr>
<td>$uT_{Ey\cdot q_{vw}}$</td>
<td>Exterior electric Maxwell stress tensor (u), y component</td>
<td>Pa</td>
<td>$0$</td>
</tr>
<tr>
<td>$uT_{My\cdot q_{vw}}$</td>
<td>Exterior magnetic Maxwell stress tensor (u), y component</td>
<td>Pa</td>
<td>$0$</td>
</tr>
<tr>
<td>$dT_{x\cdot q_{vw}}$</td>
<td>Exterior Maxwell stress tensor (d), x component</td>
<td>Pa</td>
<td>$dT_{Ex\cdot q_{vw}} + dT_{Mx\cdot q_{vw}}$</td>
</tr>
<tr>
<td>$dT_{Ex\cdot q_{vw}}$</td>
<td>Exterior electric Maxwell stress tensor (d), x component</td>
<td>Pa</td>
<td>$0$</td>
</tr>
<tr>
<td>$dT_{Mx\cdot q_{vw}}$</td>
<td>Exterior magnetic Maxwell stress tensor (d), x component</td>
<td>Pa</td>
<td>$0$</td>
</tr>
<tr>
<td>$dT_{y\cdot q_{vw}}$</td>
<td>Exterior Maxwell stress tensor (d), y component</td>
<td>Pa</td>
<td>$dT_{Ey\cdot q_{vw}} + dT_{My\cdot q_{vw}}$</td>
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<tr>
<td>$dT_{Ey\cdot q_{vw}}$</td>
<td>Exterior electric Maxwell stress tensor (d), y component</td>
<td>Pa</td>
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### 4.1.2. Boundary 2, 5, 10-14, 16-20, 22-24, 26-27, 29-36, 38, 40, 42-45, 47-49, 51, 55

<table>
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<th>Name</th>
<th>Description</th>
<th>Unit</th>
<th>Expression</th>
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<tbody>
<tr>
<td>dVolbnd_emqvw</td>
<td>Area integration contribution</td>
<td>m</td>
<td>dEmqvw</td>
</tr>
<tr>
<td>dTMy_emqvw</td>
<td>Exterior magnetic Maxwell stress tensor ((\mathbf{d})) y component</td>
<td>Pa</td>
<td>0</td>
</tr>
<tr>
<td>nJ_emqvw</td>
<td>Normal current density (\mathbf{nJ}) emqvw</td>
<td>A/m²²</td>
<td>(\mathbf{r}_x) Emqvw * (\mathbf{n}_x) Emqvw + (\mathbf{n}_y) Emqvw</td>
</tr>
<tr>
<td>uTExav_emqvw</td>
<td>Electric Maxwell surface stress tensor, time average, x component</td>
<td>Pa</td>
<td>real(-0.25 * ((\mathbf{E}_x) Emqvw_up * conj(Dx_emqvw_up)) + (\mathbf{E}_y) Emqvw_up * conj(Dy_emqvw_up)) * dnx + 0.5 * (dnx * (\mathbf{E}_x) Emqvw_up + dny * (\mathbf{E}_y) Emqvw_up) * conj(Dx_emqvw_up))</td>
</tr>
<tr>
<td>dTExav_emqvw</td>
<td>Electric Maxwell surface stress tensor, time average, x component</td>
<td>Pa</td>
<td>real(-0.25 * ((\mathbf{E}_x) Emqvw_down * conj(Dx_emqvw_down)) + (\mathbf{E}_y) Emqvw_down * conj(Dy_emqvw_down)) * dnx + 0.5 * (dnx * (\mathbf{E}_x) Emqvw_down + dny * (\mathbf{E}_y) Emqvw_down) * conj(Dx_emqvw_down))</td>
</tr>
<tr>
<td>uTEyav_emqvw</td>
<td>Electric Maxwell surface stress tensor, time average, y component</td>
<td>Pa</td>
<td>real(-0.25 * ((\mathbf{E}_x) Emqvw_up * conj(Dx_emqvw_up)) + (\mathbf{E}_y) Emqvw_up * conj(Dy_emqvw_up)) * dny + 0.5 * (dny * (\mathbf{E}_x) Emqvw_up + dnx * (\mathbf{E}_y) Emqvw_up) * conj(Dy_emqvw_up))</td>
</tr>
<tr>
<td>dTEyav_emqvw</td>
<td>Electric Maxwell surface stress tensor, time average, y component</td>
<td>Pa</td>
<td>real(-0.25 * ((\mathbf{E}_x) Emqvw_down * conj(Dx_emqvw_down)) + (\mathbf{E}_y) Emqvw_down * conj(Dy_emqvw_down)) * dny + 0.5 * (dny * (\mathbf{E}_x) Emqvw_down + dnx * (\mathbf{E}_y) Emqvw_down) * conj(Dy_emqvw_down))</td>
</tr>
<tr>
<td>nJx_emqvw</td>
<td>Source current density (\mathbf{nJ}_x) emqvw</td>
<td>A/m²²</td>
<td>Iml/d Emqvw</td>
</tr>
<tr>
<td>tEx_emqvw</td>
<td>Tangential electric field, x component</td>
<td>V/m</td>
<td>(-\mathbf{V}_T\mathbf{x})</td>
</tr>
<tr>
<td>tEy_emqvw</td>
<td>Tangential electric field, y component</td>
<td>V/m</td>
<td>(-\mathbf{V}_T\mathbf{y})</td>
</tr>
<tr>
<td>tDx_emqvw</td>
<td>Tangential electric displacement, x component</td>
<td>C/m²²</td>
<td>(\epsilon_0) Emqvw * (\epsilon_{rbnd}) Emqvw * tEx_emqvw</td>
</tr>
<tr>
<td>tDy_emqvw</td>
<td>Tangential electric displacement, y component</td>
<td>C/m²²</td>
<td>(\epsilon_0) Emqvw * (\epsilon_{rbnd}) Emqvw * tEy_emqvw</td>
</tr>
<tr>
<td>normE_emqvw</td>
<td>Tangential electric field, norm</td>
<td>V/m</td>
<td>sqrt(abs(tEx_emqvw)² + abs(tEy_emqvw)²)</td>
</tr>
<tr>
<td>normD_emqvw</td>
<td>Tangential electric displacement, norm</td>
<td>C/m²²</td>
<td>sqrt(abs(tDx_emqvw)² + abs(tDy_emqvw)²)</td>
</tr>
<tr>
<td>uTx_emqvw</td>
<td>Exterior Maxwell stress tensor ((\mathbf{u})), x component</td>
<td>Pa</td>
<td>uTEx_emqvw + uTMx_emqvw</td>
</tr>
<tr>
<td>uTEx_emqvw</td>
<td>Exterior electric Maxwell stress tensor ((\mathbf{u})), x component</td>
<td>Pa</td>
<td>0</td>
</tr>
<tr>
<td>uTMx_emqvw</td>
<td>Exterior magnetic Maxwell stress tensor ((\mathbf{u})), x component</td>
<td>Pa</td>
<td>0</td>
</tr>
<tr>
<td>uTy_emqvw</td>
<td>Exterior Maxwell stress tensor ((\mathbf{u})), y component</td>
<td>Pa</td>
<td>uTY_emqvw + uTMy_emqvw</td>
</tr>
<tr>
<td>uTEy_emqvw</td>
<td>Exterior electric Maxwell stress tensor ((\mathbf{u})), y component</td>
<td>Pa</td>
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### Photomask Geometry

#### 4.2. Subdomain

#### 4.2.1. Subdomain 1, 3, 11

<table>
<thead>
<tr>
<th>Name</th>
<th>Description</th>
<th>Unit</th>
<th>Expression</th>
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<td>Width in radial direction default guess</td>
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</tr>
<tr>
<td>R0_guess_emqvw</td>
<td>Inner radius default guess</td>
<td>m</td>
<td>0</td>
</tr>
<tr>
<td>Sx_emqvw</td>
<td>Infinite element x coordinate</td>
<td>m</td>
<td>x</td>
</tr>
<tr>
<td>Sox_guess_emqvw</td>
<td>Inner x coordinate default guess</td>
<td>m</td>
<td>0</td>
</tr>
<tr>
<td>Sdx_guess_emqvw</td>
<td>Width in x direction default guess</td>
<td>m</td>
<td>0</td>
</tr>
<tr>
<td>Sy_emqvw</td>
<td>Infinite element y coordinate</td>
<td>m</td>
<td>y</td>
</tr>
<tr>
<td>Soy_guess_emqvw</td>
<td>Inner y coordinate default guess</td>
<td>m</td>
<td>0</td>
</tr>
<tr>
<td>Sdy_guess_emqvw</td>
<td>Width in y direction default guess</td>
<td>m</td>
<td>0</td>
</tr>
<tr>
<td>delta_emqvw</td>
<td>Skin depth</td>
<td>m</td>
<td>1/real(sqrt((j \cdot \omega_{emqvw} \cdot \mu_0_{emqvw} \cdot \mu_r_{emqvw} \cdot \sigma_{emqvw} + \omega_{emqvw} \cdot \epsilon_{0_{emqvw}} \cdot \epsilon_{r_{emqvw}})))</td>
</tr>
<tr>
<td>dVol_emqvw</td>
<td>Volume integration contribution</td>
<td>m</td>
<td>det_l_emqvw * d_emqvw</td>
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### 4.2.2. Subdomain 2, 9

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<td>$-\nu_{yy} \omega_{yy}$</td>
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photomask Geometry Jy_emqvw Total current density, y component A/m^2 Jy_emqvw * Jy_emqvw

normP_emqvw Electric polarization, norm C/m^2 \sqrt{\text{abs}(P_x)^2 + \text{abs}(P_y)^2}

normDx_emqvw Remanent displacement, norm C/m^2 \sqrt{\text{abs}(D_{rx})^2 + \text{abs}(D_{ry})^2}

normDy_emqvw Electric displacement, norm C/m^2 \sqrt{\text{abs}(D_{ry})^2 + \text{abs}(D_{rx})^2}

normE_emqvw Electric field, norm V/m \sqrt{\text{abs}(E_x)^2 + \text{abs}(E_y)^2}

normJp_emqvw Potential current density, norm A/m^2 \sqrt{\text{abs}(J_{px})^2 + \text{abs}(J_{py})^2}

normJd_emqvw Displacement current density, norm A/m^2 \sqrt{\text{abs}(J_{dx})^2 + \text{abs}(J_{dy})^2}

normJe_emqvw External current density, norm A/m^2 \sqrt{\text{abs}(J_{ex})^2 + \text{abs}(J_{ey})^2}

normJ_emqvw Total current density, norm A/m^2 \sqrt{\text{abs}(J_x)^2 + \text{abs}(J_y)^2}

Weav_emqvw Electric energy density, time average J/m^3 0.25 * \text{real}(E_x * \text{conj}(D_x) + E_y * \text{conj}(D_y))

Wav_emqvw Total energy density, time average J/m^3 Weav_emqvw

Qav_emqvw Resistive heating, time average W/m^3 0.5 * \text{real}(J_x * \text{conj}(E_x) + J_y * \text{conj}(E_y))

Ex_emqvw Electric field, x component V/m -\text{invJxx} * V_x

Ey_emqvw Electric field, y component V/m -\text{invJyy} * V_y

4.2.3. Subdomain 4-8, 10

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