RAPIDLY SOLVING PHYSICS-BASED MODELS FOR UNCERTAINTY PROPAGATION IN NONDESTRUCTIVE EVALUATION

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By

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Abstract


Recent research in extending nondestructive evaluation (NDE) methods toward damage and materials characterization has led to an emphasis on the development of physics-based forward models in NDE. Furthermore, a desire to quantify levels of uncertainty in NDE inspections, particularly in Air Force applications, has driven the need for quick solving surrogate models for the traditional forward models, which have largely focused on accurately capturing many aspects of the problem with little emphasis on computational effort. In the past 5 years, many different techniques for creating lower-fidelity, quickly solving models to be used in place of the expensive high fidelity simulations have been explored in the context of NDE simulations, however there is still much to be done. This dissertation is focused on the development of physics-based models which rely on approximations to simplify the calculations while maintaining accuracy. Models were developed for prediction of the signal from random, heterogeneous materials during eddy current testing (ECT) inspections with absolute and reflection differential coils. A model was also developed for a specific scanning acoustic microscopy (SAM) experiment that has been used previously to characterize the elastic properties of a material. Furthermore, improvements were made to the post-processing of the data from these experiments that enabled high fidelity analysis of the wave behavior in single crystals of titanium alloys. The models developed as part of this work were shown to be relatively accurate, but much quicker to solve than the commercially available software for performing the same simulations. The models were tested against considerable amounts of experimental data from four samples with known microstructure, and they were found to be in good qualitative agreement with the experiments in most cases. The models were also verified against other numerical techniques for performing the same computations.
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Chapter 1

Introduction

The field of nondestructive evaluation (NDE) has traditionally been centered around detection of discrete flaws in materials as well as changes in the bulk properties of materials as a function of wear and processing. The methods used typically involve propagation of energy into a material and measuring the interaction of the energy with the material properties of both the host material as well as the flaw. While the signals generated by measuring this interaction carry a large amount of information about the flaw, the traditional focus on strictly detection has limited the useful information withdrawn from the signal to a binary flaw/no-flaw estimation. However, with increasing fidelity of numerical modeling and simulation methods related to NDE inspections as well as a strong focus on low/multi-fidelity modeling to increase the speed of model evaluations, nonlinear iterative inverse techniques have been implemented for estimation of the properties of flaws from the signals collected during an inspection. The properties of the flaw, such as those related to the geometry and location, can be used to manage the remaining life of the component. Furthermore, this technology has opened the door for a much wider application of traditional NDE techniques to materials characterization on a variety of length scales aside from bulk material properties. NDE for characterization of microstructure features such as mean grain size in a polycrystalline aggregate has seen a significant increase in interest in the last 15 years.
While many numerical techniques have been developed for solving physics-based forward models (e.g. finite element method (FEM), boundary element, and volume integral simulations), a large focus has been placed on the development of new and application of existing surrogate modeling techniques to reduce computation time. Modeling and simulation using traditional approaches such as FEM is too computationally expensive for use in an inversion algorithm or for uncertainty propagation and quantification. There has been significant progress on development of surrogate models to date, yet there are still many research opportunities in this area. For instance, there is very little emphasis on taking advantage of physics-based approximations such as reduced dimensionality and low material property change conditions to reduce the size/complexity of numerical simulations. This type of low-fidelity approximation-based model could drastically increase the speed of simulations while maintaining accuracy, provided the assumptions made during derivation hold. In the area of surrogate modeling for NDE applications, much emphasis has been placed on polynomial interpolation techniques such as probabilistic collocation method (PCM) and sparse grid techniques. These methods have provided drastic reduction in computational resources in the area of uncertainty quantification, but little emphasis has been placed on propagation of uncertainties from the microstructure of the material system through forward models to determine the distribution of the NDE response. This often dominates the noise in the signal when the material is heterogeneous and anisotropic, especially in the areas of eddy current testing of titanium components as well as ultrasonic testing of most engineering alloys and composite systems. A combination of expansion techniques with low-fidelity modeling in NDE could provide the computational benefit of the surrogate modeling approaches that have been explored in the past, but with uncertainty from the material system such as that from microstructure.

An uncertainty propagation framework in which the variability in the inspection is analyzed in terms of the physical interaction of the NDE signal with heterogeneous materials could provide significant payoff for computational design of materials. There has
been heavy emphasis in recent research on digital design of materials and how materials processing and property models fit in with the engineering design optimization process. Using digital tools for predicting the properties of a material given the chemistry and processing, aspects of the material system (e.g. fatigue strength, yield strength, cost, etc.) can be included as an objective function and/or a constraint in a design optimization routine. This is especially important when designing complex structures that can only be fabricated using additive manufacturing techniques. However, one key factor typically not considered in the design and analysis of structures is the inspectability of the underlying material. Anisotropic, heterogeneous materials act as a source of noise in NDE inspections, as is evidenced by the fact that the documented NDE capability in titanium is worse than that in nickel due to the anisotropic electrical conductivity. This noise and the subsequent effect it has on detectability of flaws has a direct correlation to inspection intervals, and thus sustainment costs, of a component. A set of digital tools in which the fundamental physical limit of detectability of flaws in a material system can be determined given the microstructure predicted from a set of processing and chemistry parameters would allow designers to consider sustainment costs in their designs as either separate objective functions or as constraints.

The focus of the work in this dissertation is uncertainty propagation when the primary source of variability in the NDE inspection stems from the microstructure of the material. This uncertainty propagation routine relies on an expansion technique known as the Karhunen-Loeve method where the microstructure can be randomly sampled given known statistics that could be acquired digitally from processing models. These samples are then fed through rapidly-solving forward models of NDE inspections (eddy current and ultrasound inspections) to determine the statistics of the NDE sensors, and thus the fundamental limit of detectability of flaws in a material designed in a purely digital framework. Thus, in this work, the focus is on predicting the noise in an inspection given known microstructure and not on predicting the signal from flaws.
This dissertation documents advances in approximation-based modeling techniques for microstructure characterization and uncertainty propagation. Specifically, the dissertation discusses:

- Development of a new approximate model for calculating the response of absolute eddy current coils over heterogeneous materials.
- Development of a new approximate model for calculating the response of reflection differential eddy current coils over heterogeneous materials.
- Development of an approximate model for defocused-probe Rayleigh surface wave (RSW) imaging techniques
- Development of a new method of calculating the RSW velocity as a function of anisotropic elastic constants and Euler angles for materials characterization with RSW imaging probes.
- Development of new methodologies for analyzing the experimental results to improve local quantitative measurement of the material properties in RSW imaging methods.

The main goal of this work was to provide a framework for uncertainty propagation from randomly heterogeneous materials in nondestructive evaluation. Development of these quick-solving, physics-based forward models as well as advancements to the experimental techniques for the purpose of validation were crucial steps toward achieving this goal, and have each provided advances in the state-of-the-art.

The dissertation is organized with this chapter providing a thorough background and literature review for the above listed contributions, the next chapter describing the material, its properties, and the statistical representations for the properties, and then a chapter dedicated to each contribution for further development and analysis (Chapters 3, 4, and 5).
The final chapter provides a short summary of the contributions made thus far as well as proposed future research.

1.1 Basics of Nondestructive Evaluation

This dissertation is focused on modeling and simulation in the context of material state characterization with NDE. Since NDE is not a well known field, the fundamentals are discussed in this chapter as well as some historical uses for NDE techniques. The chapter starts with a general discussion of concepts related to all techniques and then gives brief descriptions of several of the more common techniques used.

1.1.1 General Nondestructive Evaluation Methodologies

NDE is a set of methodologies that can be used to determine the state of a material system or a component made from the material. In this context, a material system is any material from which engineering components can be made, though usually NDE is used on structural materials such as metals, composites, or concrete in civil structures. The state of a material system or component is a collection of attributes that together define the components ability to meet the designed-to functional requirements. In this sense, there can be a great deal of diverse attributes that are important to a particular component. For instance, a beam may be designed to not deflect to within a certain tolerance when a load is applied. The attributes of this beam that define its ability to withstand this deflection would be the Young’s modulus, the shape parameters of the beam, and the means by which the beam is restrained. NDE could then be redefined as a set of methodologies that can be used to measure attributes of a component that define its ability to perform its function, with the intent of monitoring the component before ultimate failure occurs.

NDE can be applied in several different scenarios. If a change in attributes is expected to occur during normal use (e.g. material loss due to fluid flow and erosion across...
the beam), NDE could be applied to monitor the attribute and determine when the beam should be removed from service or repaired. Some attributes that have been traditionally monitored with NDE include:

- Geometry changes such as thinning of pipe walls [3].

- Bulk material parameters such as electrical conductivity [4–6], thermal conductivity [7–9], electrical permittivity [10], magnetic permeability [11], and elastic constants [12].

- Presence of macro-scale damage such as fatigue cracks [13, 14], corrosion[15, 16], stress corrosion cracking [17], and impact damage in composites [18].

- Presence of micro-scale damage such as micro-cracking [19], porosity [20], and creep damage [21].

- Presence of nano-scale damage such as increasing dislocation density [19]

While these examples all pertain to material and component degradation as a function of usage, NDE can also be used to monitor the manufacturing techniques used to produce components. Some process monitoring techniques in NDE include curing of resins in composites [22], progression of microstructure in heat treatment of metal components [23], and characterization of porosity in concrete [24].

The references given in the previous paragraph are all recent research papers in NDE. They are by no means inclusive, but they illustrate how diverse NDE methodologies can be. The types of methodologies and the equipment used are typically tailored to the material system, geometry of the component, and the attribute being measured. Examples of NDE methodologies include ultrasound, eddy current, magnetic particle, visual, radiography, thermography, and penetrant testing. Each of these can then be broken down further into techniques by the type of equipment used, the range of operation (typically frequency based), and various other factors that distinguish the different techniques. For instance,
eddy current methodology is a low frequency, near-field electromagnetic technique that uses coils as sensors to detect damage (the physics of eddy current will be discussed in Section 1.1.2). This basic sensor can be adapted to various testing scenarios by changing the geometry of the probe. For instance, detection of surface breaking damage on flat surfaces requires a different probe geometry than bolthole inspections with eddy current. These are two different techniques that both rely on the same methodology.

While there are a great variety of techniques for NDE, there are some generalities that apply to all methodologies that can help to clarify the use of each one. NDE techniques all rely on energy interacting with a material such that the material properties can be measured or characterized. Typically, some form of energy is emitted from a source, the energy interacts with the material, and whatever energy reflects off of or transmits through the material is measured by a sensor. Any change in the material properties will cause a change in the interaction, which will change the received signal at the sensor. This indicates that there is a physical aspect of the material that has changed in the inspection. Typically, the sensor reports the interaction of energy to the user as a signal. An example signal can be seen in Fig. 1.1. This figure shows a plot of the response of an eddy current coil as the coil is moved over a fatigue crack in a sample. The energy from the eddy current coil interacts with the material through its material properties (electrical conductivity and magnetic permeability), but these properties have changed in the area of a flaw. This change is represented by a change in the signal of the sensor. The sensor is generally located directly above a flaw, but multiple sensors can be used to improve the spatial resolution of the probe and enhance the contrast of the flaw with respect to the background noise.

Encoded in this signal is three different interactions between the energy and the components of the inspection. These interactions describe 1) how energy is generated at the source and delivered to the component, 2) how energy interacts with the component and material system, and 3) how energy is transmitted to the sensor and converted to a signal. Understanding the information contained within an NDE signal requires an analysis
of each interaction, but the fundamental descriptor of an NDE methodology is the way in which energy interacts with a material system. It defines what material systems an NDE methodology can be applied to and what damage modes or material characteristics that methodology may be sensitive to. The other two interactions merely mask the portion of the signal that is described by the material interaction by way of introducing uncertainty in the analysis. There is concerted effort to reduce the effects of sensor variation in experimental NDE, but no NDE signal is completely free of the variability introduced by sensor and source discrepancies. Furthermore, the interaction with the material also contains uncertainty due to component geometry changes and material noise. A very successful approach for removing or isolating these sources of variation (nuisance parameters) from the material effects has been in model-based methods such as inverse problems. As such, physics-based modeling and simulation of all of the interactions for nearly every NDE technique is an active field of research.

Energy interaction with a component and the material system is governed by the properties of the material, and implicitly by the geometry of the component. Every NDE technique is sensitive to a subset of material properties. Damage or abnormalities are simply

![Typical NDE Sensor Response Over Flaw](image_url)

**Figure 1.1:** A plot of a typical NDE signal. The sensor response is shown as a function of the position of the sensor relative to a fatigue crack. This is a clear indication that damage is present in the material.
a change to one or more of the properties, either locally (e.g. fatigue cracks have different material properties than their surroundings) or globally (e.g. measuring the elastic properties of a material prior to use for quality assurance). Furthermore, the contrast (i.e. signal-to-noise ratio or signal amplitude) that can be achieved in an NDE technique can be related to the contrast in the material properties from healthy to damaged states.

In the following sections, two different NDE methodologies are discussed. They are each be characterized by the type of energy that they use, the material properties that they interact with, their strengths and weaknesses, and several different techniques in which they are employed.

1.1.2 Eddy Current Testing

1.1.2.1 Basics of Eddy Current Testing

Eddy current testing (ECT) is an NDE methodology that uses low frequency electromagnetic energy to interrogate materials. The electromagnetic waves are often generated by coils, though not necessarily. Low frequency electromagnetic waves are generated and impinge (primary field) on the surface of a material. These waves propagate into the material and portions of the waves reflect back to the sensor. When the waves propagate in a conductive material, the electric field does work on the free charges and entices them to move (Lorentz forces). This motion of free charges is referred to as eddy currents. Energy is dissipated in the material and the electromagnetic waves die down as an exponential function of distance traveled into the material. The eddy currents oppose the electromagnetic field (Lenz’s law) and thus create their own electromagnetic field (the secondary field) that propagates back to the source. This field generates opposing forces within the coil that serves to increase the resistance and change the electrical impedance (complex resistance) of the coil. Thus, by monitoring the impedance of a coil being excited with an AC signal, conductive materials in the vicinity of the coil can be detected.
Any disruption to the flow of eddy currents in the conductive material will cause a change in the secondary field that the coil sees, but to understand the type of changes that could cause a disruption requires understanding which material properties govern the interaction of energy with the material. The total current density created in electromagnetic wave propagation is a contribution from many different sources. This can be seen in:

\[
\nabla \times (\bar{\mu}^{-1} \cdot \mathbf{B}) = \mathbf{J}_{\text{tot}} = \bar{\sigma} \cdot \mathbf{E} + \bar{\varepsilon} \cdot \frac{\partial \mathbf{E}}{\partial t} + \mathbf{J}_e
\]

(1.1)

where \( \mathbf{B} \) is the magnetic flux density, \( \bar{\mu} \) is the magnetic permeability tensor, \( \mathbf{J}_{\text{tot}} \) is the total current density, \( \bar{\sigma} \) is the electric conductivity tensor, \( \mathbf{E} \) is the electric field, \( \bar{\varepsilon} \) is the permittivity tensor, and \( \mathbf{J}_e \) is an externally applied current density such as that in a wire. This equation is a version of Ampere’s circuital law. In words, it states that a current density in space and/or a time changing electric field will create a magnetic field with nonzero curl, or conversely that a magnetic field with nonzero curl cannot exist without some form of current density. The total current density can come from multiple different sources, several of which are shown in the right hand side of the equation.

The first term represents induced currents that are generated by an electric field applying force to free charges. The notion that the electric field does work on the free charges implies that as it propagates into a material, it loses energy. This dissipation of energy is often stated as skin depth which in an isotropic, homogeneous and nondispersive material is:

\[
\delta = \sqrt{\frac{2}{\omega \sigma \mu}}
\]

(1.2)

In this equation, \( \delta \) is the skin depth of the material, \( \omega \) is the angular frequency of the electromagnetic wave, \( \sigma \) is the scalar conductivity, and \( \mu \) is the scalar permeability. The skin depth is the distance a plane wave would have to travel into a conductive material to decay to \( 1/e^1 \) of its original value. This figure is often used in eddy current as an approximation of how deep the flaw can be and still be detected with eddy current probes.
Table 1.1: Skin depths in some metals at different frequencies.

<table>
<thead>
<tr>
<th>Material</th>
<th>Skin Depth (µm) at 100kHz</th>
<th>Skin Depth (µm) at 2MHz</th>
</tr>
</thead>
<tbody>
<tr>
<td>Annealed Copper</td>
<td>208</td>
<td>52.8</td>
</tr>
<tr>
<td>Gold</td>
<td>236</td>
<td>46.4</td>
</tr>
<tr>
<td>Aluminum</td>
<td>262</td>
<td>58.5</td>
</tr>
<tr>
<td>Titanium</td>
<td>1180</td>
<td>265</td>
</tr>
<tr>
<td>Nickel</td>
<td>11.8</td>
<td>2.56</td>
</tr>
</tbody>
</table>

It is not accurate at lower frequencies due to the plane wave approximation breaking down, but it is valid in typical eddy current ranges [25]. An example of skin depths in some materials is shown in Table 1.1. As this table indicates, most of the fields that penetrate the sample are restricted to within 1mm of the sample, making eddy current difficult to use for anything but surface breaking flaws, thought many authors have used pulsed eddy current [26] and low frequency magnetic field-based techniques [27] as a means to interrogate further into the material.

The second term on the right hand side of (1.1) is called the displacement current term. Part of this term is the displacement currents in free space, which aren’t actually currents but the electric field which must arise when a magnetic field with nonzero curl exists in a vacuum. Another contribution to displacement currents is polarization in a medium when the material can react to an electric field. The vacuum permittivity is a constant, but polarization in a medium can be a tensorial quantity and can be heterogeneous and dispersive. In (1.1), it is non-dispersive, but no other assumptions are made about any of the material properties. In almost all applications of ECT methodologies, the frequencies used are sufficiently low and the conductivity of the material high enough that displacement currents can be neglected. Thus, the material properties that influence the fields most in ECT inspections are conductivity and permeability. As such, eddy current is mostly useful on metal materials where the anomaly and metal are drastically different in conductivity and/or permeability.
Eddy current is used extensively for inspections in damage tolerant design of aircraft. Coils are typically used as both transmitter and receiver, and bridge circuits are used to determine the impedance of the coil, making the inspection equipment for an ECT inspection relatively inexpensive (compared to other NDE methods aside from visual). Furthermore, because of the high contrast in material properties from a metal structure to a crack, the signals in ECT tend to be strong compared to the noise of the inspection.

1.1.2.2 Types of Eddy Current Probes

Eddy current probes can be used in multiple different configurations [28]. The more common configurations for inspection of aircraft structure and propulsion components are absolute, differential, and reflection differential. In an absolute configuration, one coil is excited with current and the impedance of that coil is measured as a function of the position over the surface of the sample. Absolute coils are highly sensitive to changes in the host conductivity of the material, but they are also sensitive to the material properties themselves. Thus, absolute coils can be used for detection of flaws as well as measurement of the absolute electrical properties of the sample. In certain inspections, this sensitivity can be a nuisance and is thus minimized by shielding the coil and/or placing a core in the center of the coil to focus the magnetic field lines more toward the center. Liftoff (distance between the coil and sample) is a significant source of variability in this configuration.

Differential probes have two coils that are both excited and wound in opposite directions. This has the effect of essentially taking the difference between the impedance of the two coils. This means that large-scale changes such as long-wavelength electromagnetic interference as well as large undulations in the surface geometry have less effect on the response than in absolute configuration. This type of probe is very sensitive to small discontinuities in the electrical conductivity of the sample such as small surface breaking cracks.

Reflection differential probes operate similar to the differential probe, but use a trans-
mitting coil to excite eddy currents in the sample. Two receive coils wound in opposite direction are used to sense the changes in the material properties. Often the receive coils are inside the transmit coil. This probe is even more sensitive to fatigue cracking in the sample and has the added advantage of providing conductive shielding to the inner receive coils to mitigate the effect of edges and other geometrical features. These probes are often used in bolt-hole inspections and inspections on edges of components.

1.1.2.3 Microstructure Characterization with Eddy Current Testing

Eddy current probes are sensitive to the electrical and magnetic properties of the host material, hence many authors have shown the applicability of ECT in microstructure characterization. ECT has been used extensively in characterization of steels and steel alloys because the various constituent phases in steels have very different magnetic and electrical properties [29–34]. In addition, work in characterization of microstructure in nickel-based superalloys has been performed where the various precipitates that form in the material during manufacturing and thermal aging contribute differently to the conductivity [35, 36]. These characterization techniques were all empirical by nature and used large coils (1-10mm) and low frequencies (10-1000Hz) to obtain a homogenized bulk conductivity aggregated from small microstructure features of interest (1-40\(\mu\)m). These empirical studies provided estimates of volume fractions of electrically and magnetically different phases that constitute an aggregate and did not provide spatially dependent information.

Investigation of microstructure characterization with ECT in titanium alloys has been very limited. Most of the research has focused on using ECT as a tool to measure the bulk conductivity of a material without considering local perturbations of the conductivity due to small coil geometries. Bulk electrical conductivity measured in titanium alloys with eddy current instruments has been used to detect oxygen contamination due to high temperature exposure and changes in wear resistance due to changes in chemistry of the material [37–39]. Recently, ECT bulk electrical conductivity measurements were used to estimate the
volume fraction of different phases and $\beta$ transus temperature in titanium alloys [40]. The $\beta$ transus temperature marks the temperature at which the alloy transitions from an $\alpha$-$\beta$ phase mixture to being entirely composed of $\beta$-phase. A physics-based rule of mixtures was used to relate the microstructure to the ECT response, which enabled quantification of $\beta$ transus and composition on more than an empirical basis.

Yin et al [41] used effective medium theory and finite element method (FEM) to estimate the electromagnetic properties and its relation to ferrite fraction and morphology in steel. Both of these studies used bulk measurement techniques, but they showed the value of relating the estimated material parameters to the microstructure through physical arguments. In this way, more properties could be quantified using the eddy current signal.

Eddy current methods have been used in the past to characterize spatial inhomogeneity of conductivity on an extremely fine scale (50-100nm) [42]. This work achieved excellent contrast with changing conductivity at different spatial locations below the sensor but required a very precise experimental setup. No previous work has addressed characterization of spatial features of microstructure with ECT coils in the resolution range between 1mm and 100nm. In titanium, it has been shown [43] that the spatial variations in microstructure can have dramatic effects on ECT probes due to the average sizes of the grains (10-20µm) and ensembles of similarly oriented grains (100µm to multiple mm’s) relative to the size of probes (0.05-1mm). While this work clearly showed contrast with changing orientation of the grains, the hypothesis was never tested by comparison of the ECT images with data from orientation imaging. Furthermore, no theoretical justification was made to establish the limits of orientation imaging with ECT based on percent change in conductivity.

1.1.2.4 Modeling in Eddy Current Testing

Traditional ECT models calculate the impedance change of an idealized coil in the presence of local conductivity changes in a host material so that the response of an eddy current coil due to damage can be predicted. This section introduces the basic formula for modeling
the response of an eddy current coil and the aspects of solving the equation that have been studied in the literature in relation to damage detection. Furthermore, modeling of ECT coils in relation to microstructure characterization is discussed as well as the limitations to current state-of-the-art modeling techniques.

In [44] a relationship was given for the impedance change due to a local discrepancy in the conductivity of a host material. The expression was derived using principles of conservation of energy of an electromagnetic field given by Poynting’s theorem to arrive at a surface integral equation:

$$\Delta Z = \frac{1}{I^2} \int_S (E_b \times H_a - E_a \times H_b) \cdot n \, dx \quad (1.3)$$

$\Delta Z$ is the change of impedance due to the presence of the damage, $I$ is the input current, $E$ is an electric field quantity, $H$ is a magnetic field quantity, the subscript $b$ represents the field due to an unflawed part, the subscript $a$ is a field due to the flawed part, $S$ is a surface encompassing the notch or flawed region, and $n$ is an inward pointing unit vector normal to the surface $S$. This equation can also be expressed as a volume integral. These equations give a solution for the change of impedance of a coil due to an arbitrarily shaped flaw for any coil provided the flawed and unflawed fields are known at all points on the surface of the flaw.

The unflawed field can be calculated for a number of different scenarios described by the geometry of the conductor and the coil. For instance, Dodd and Deeds [45] provided analytical solutions for flat pancake coils over multilayered samples and cylindrical coils surrounding tubes. These results were extended by many authors (e.g.[46–49]) to include several more complex situations such as varying probe and sample geometries, as well as deviations from simple media.

The second aspect of calculating the impedance change with equation (1.3) is the calculation of the flawed field quantities. This is an issue of great interest and constitutes
significant motivation for the development of eddy current forward models. One method
to accomplish this is to solve for a set of dipole point sources distributed in the region of
the crack that act as a barrier to current flow [50]. A popular method to accomplish this
is by the volume integral method (VIM) as described in [51]. Essentially, the field due to
the dipole source is calculated as a Greens function and the integral along the entire flaw
region is calculated with the method of moments. This results in a full matrix calculation,
but since the flaw region is the only region that needs to be meshed, the matrix sizes are
relatively small. The obvious attractive part of this method is that it is quick, but it is
restricted to the problems for which the analytical Greens functions can be calculated.
Boundary element methods have also been used [52], but again, this method relies on the
calculation of Greens functions that might not be available for complicated geometries. A
more general way of solving this problem is with a finite element method (FEM) scheme.
FEM is computationally expensive, but the breadth of problems that it can handle makes
it a useful method in its own right. FEM for eddy current problems has been studied
by various recent authors [53–55]. Examples of other modeling methods that have been
explored include distributed point source method (DPSM) [56] and Nyström discretization
[57].

The modeling methods discussed previously are all discretization based numerical al-
gorithms. Since they are intended to solve for the response of a coil over a discrete flaw
in the material, they rely on having fine meshes in the area of the flaw. In the case of
microstructure simulations, the flaw is the size of the material with which the coil inter-
acts. This implies that for any of the previously discussed methods to be successful, they
would have to allow for a relatively fine mesh over the entirety of the sample. This makes
microstructure simulations with these methods computationally intensive. For the sake of
microstructure characterization with inverse techniques, a lower-cost alternative is needed.
A quick model for prediction of ECT signals above anisotropic polycrystalline materials
does not currently exist. A new model for calculation of the eddy current response above
a spatially heterogeneous material is shown in Chapter 3. This model was applied to both absolute and reflection differential configurations and verified/validated using multiple different samples.

1.1.3 Ultrasonic Testing

Ultrasonic testing (UT) is an NDE methodology that employs the interaction of acoustic and elastic waves with a material. The energy emitter is a transducer that converts electrical impulses to mechanical displacements through a piezoelectric material such as lead zirconate titanate (PZT). The transducer is often coupled to the test article through some fluid media, and pressure waves are excited in the fluid by the mechanical displacement. The pressure waves impinge on the surface of the test article and a large portion of the energy contained within the pressure waves is reflected back to the transducer or in a different direction. The portion of energy that isn’t reflected is transmitted into the sample as mechanical displacements. These mechanical displacements then travel through the material as a wave. Any local change in the elastic properties of the material causes a reflection of energy which is detected by the transducer using the inverse piezoelectric effect.

1.1.3.1 Velocity of Bulk Waves

Mechanical waves in a solid material propagate as either longitudinal, fast shear, or slow shear modes. Pure longitudinal waves propagate with particle displacements parallel to the direction of wave propagation, and pure shear waves have particle displacements perpendicular to the direction of wave propagation. These waves propagate at a velocity that is a function of the material properties, and in an isotropic material, the propagation velocity
for each is given as:

\[
\begin{align*}
 v_l &= \sqrt{\frac{\lambda + 2\mu}{\rho}} \\
 v_t &= \sqrt{\frac{\mu}{\rho}}
\end{align*}
\]  

where \( v_l \) is the velocity of the longitudinal wave, \( v_t \) is the velocity of the transverse wave, \( \lambda \) is the first Lamé parameter, \( \mu \) is the second Lamé parameter, and \( \rho \) is the density of the material. In an isotropic material, both fast shear and slow shear propagate at the same velocity. Because of the connection between elastic parameters and velocity of waves in a material, time-of-flight ultrasound has been used extensively to characterize the elastic constants of solid materials [58].

In many different structural metals, the equations shown in (1.4) give similar results when using the homogenized isotropic properties of a material. For instance, Table 1.2 shows the isotropic properties, the density, and the longitudinal and shear wave velocity of Ti64, Al-7075-T6, and AISI 4130 steel. The values shown here are all very similar. In fact, it is impossible to identify a material by ultrasonic velocity alone, and the density must be estimated independently for true elastic constant characterization with ultrasound techniques.

Materials vary much more drastically when considering single crystal, anisotropic elastic behavior. In anisotropic materials, the velocity is a function of the propagation

<table>
<thead>
<tr>
<th>Material</th>
<th>Young’s Modulus</th>
<th>Poisson Ratio</th>
<th>Density</th>
<th>Longitudinal Wave Velocity</th>
<th>Shear Wave Velocity</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ti64</td>
<td>113.8 GPa</td>
<td>0.33</td>
<td>4430 kg/m³</td>
<td>6170 m/s</td>
<td>3107 m/s</td>
</tr>
<tr>
<td>Al-7075-T6</td>
<td>71.7 GPa</td>
<td>0.34</td>
<td>2810 kg/m³</td>
<td>6270 m/s</td>
<td>3086 m/s</td>
</tr>
<tr>
<td>AISI 4130 Steel</td>
<td>205 GPa</td>
<td>0.29</td>
<td>7850 kg/m³</td>
<td>5850 m/s</td>
<td>3182 m/s</td>
</tr>
</tbody>
</table>
direction of the wave and the connection between elastic properties and the velocity of the wave is not as straightforward as that shown in (1.4). The velocity must be determined from analysis of the general 3D equations of motion in elastic, non-dispersive materials free of body forces, given by:

\[ c_{ijkl} \frac{\partial^2 u_k}{\partial x_j \partial x_l} = \rho \frac{\partial^2 u_i}{\partial t^2} \] (1.5)

where repeated indices in a product indicate summation over those indices. In this equation, \( i, j, k, l = 1, 2, 3 \), \( c_{ijkl} \) are the elastic moduli, and \( u_i \) is the displacement component in the \( i \)th direction, \( x_i \). Assuming bulk waves propagating as plane waves, the solution to this equation has the form:

\[ u_i = A_0 a_i \exp \left[ -i(x_m k_m - \omega t) \right] \] (1.6)

where \( A_0 \) is the amplitude associated with the entire wave, \( a_i \) is the component of the wave in the \( i \)th direction, \( i = \sqrt{-1} \), \( k_m \) is the component of the wave vector \( k \) in the \( m \)th direction, and \( \omega \) is the frequency of the wave. This solution is differentiated and substituted into the governing differential equation (1.5) to yield the eigenvalue problem:

\[ (c_{ijkl} k_l k_j - \rho \omega^2 \delta_{ik}) a_k = 0 \] (1.7)

where \( \delta_{ik} \) is the Kronecker delta function. Equation (1.7) is the Christoffel equation for anisotropic solids. It is rearranged into a \( 3 \times 3 \) eigenvalue problem and used to find the values of \( \rho \omega^2 \) for which the plane wave exists. These three eigenvalue solutions are then the phase velocity, \( v_p \), of the three component waves in the direction \( k \). This equation has been solved numerically and also analytically for the three component wave velocities given in many different texts [59].
1.1.3.2 Reflection and Refraction at Surfaces

At the fluid-solid boundary, portions of the energy in the wave are reflected and portions are transmitted based on a change in the material properties across the boundary. The same phenomenon occurs at the boundary between two solids with dissimilar elastic properties. When the wave falls on this boundary at oblique incidence, the reflected portion of the wave and the transmitted portion propagate in different directions. Furthermore, the longitudinal and shear portions of the transmitted energy propagate in different directions. Therefore, discrete damage such as cracks scatter the ultrasound energy and reflections from the cracks can be detected. Similarly, material features such as crystallites in a polycrystalline aggregate cause a significant reflection of energy that is detected in an ultrasound inspection.

1.1.3.3 Surface Acoustic Waves

As mentioned in the previous section, waves incident on a solid surface are partitioned into 4 different components, a reflected portion back into the fluid and three elastic waves in the elastic media of differing displacement components. One is compressional (or dilational) and the other two are shear waves polarized in different directions. These waves propagate at a fixed velocity according to the elastic properties, density, and in anisotropic materials, the angle of propagation. Furthermore, in a general anisotropic material, the velocities each differ from one another. An image of the wave components at the boundary is shown in Fig. 1.2. The angle of refraction of each wave can be determined from the generalized Snell’s law given by:

\[
\frac{\sin \theta_i}{c_i} = \frac{\sin \theta_L}{c_L} = \frac{\sin \theta_{S1}}{c_{S1}} = \frac{\sin \theta_{S2}}{c_{S2}} \quad (1.8)
\]

In this equation, \( c_i \) and \( \theta_i \) are the incident wave speed and incident angle, \( c_L \) and \( \theta_L \) are the velocity and refracted angle of the longitudinal wave, \( c_{S1} \) and \( \theta_{S1} \) are the wave speed and refracted angle of the fast shear wave, and \( c_{S2} \) and \( \theta_{S2} \) are the wave speed and refracted
angle of the slow shear wave. When the incident angle satisfies the expression:

\[ \theta_i = \arcsin \frac{c_i}{c_R} \]  

\( c_R \) is just the velocity of a refracted wave component, that specific component of the wave becomes an inhomogeneous wave and the displacements are restricted to the surface of the material. When all critical angles in the component are exceeded, the entire wave field is restricted to a thin layer on the surface of the material, thus creating a surface wave. The thickness of this layer is determined by the wavelength of the wave which implies it is dependent on the wave velocity and frequency.

1.1.3.4 Rayleigh Surface Waves and Phase Velocity Calculation Review

Surface acoustic waves such as Rayleigh waves are important in a number of industries and applications such as nondestructive evaluation, materials characterization and acoustic

![Image](image.png)

Figure 1.2: An image depicting the wave components at a fluid-solid interface. Each wave component in the solid propagates at a certain refraction angle relative to the vertical axis and at a specific velocity.
microscopy. These waves propagate with distinct particle motions due to the mixing of both shear and compressional modes, and thus also have a different velocity. Furthermore, in an anisotropic material the wave velocity and particle displacements change as a function of propagation direction. This is often represented with a slowness curve which gives the reciprocal of velocity as a function of propagation direction. While the method for calculating these curves is well understood for bulk longitudinal, slow shear waves, and fast shear waves [60], Rayleigh surface wave (RSW) velocity curves in crystals of arbitrary symmetry are much less common.

One application area has been in material property characterization. Measurement of RSW velocity on a single crystal in multiple directions of propagation has been used to calculate the single crystal elastic constants of a material [61]. More recently, modern experimental techniques have been used to measure the velocity of the surface waves much quicker than previously possible by using laser excitation and detection of elastic strains. In [2], RSW velocity measurements were used to characterize the orientation map of a sample by calculating the velocity given known orientations and elastic constants and then inverting the response to get to orientation. In [62], the response over the entire surface of the sample was used to characterize the elastic properties of a material by generating a distribution of velocities in the many different orientations present in a polycrystalline aggregate. In all of these studies, a key step in generating a useful technique was accurately calculating the RSW velocity given known orientation, propagation direction, and elastic constants. These methods all employed the methods of Farnell [63] for numerical computation of the RSW velocity.

While numerical methods have been used extensively in the past for calculation of the RSW velocity, there are a number of authors who have derived various equations for analytically calculating RSW velocities [64, 65]. These derivations often used the Stroh formalism for elastodynamic equations, although not always [66]. This formalism reorganizes the stiffness matrix in an elastic wave problem and, after application of boundary
conditions, results in an eigenvalue problem to determine the wave propagation constant. This leads to a polynomial equation whose roots are directly related to the wave velocity. Any arbitrary orientation can be solved by applying a rotation matrix to the stiffness tensor. However, the eigenvalue problem that results from the decomposition of the stiffness matrix is not analytically tractable in an arbitrarily rotated crystal also having arbitrary crystal symmetry.

Authors have used other methods and linear algebra techniques to argue past the eigenvalue problem to derive at a new determinant equation for calculating the secular equation for RSW velocity explicitly [67]. This was done for an arbitrary elasticity tensor in [68]. In this work, a determinant equation was derived that was a function of only the elastic constants and wave velocity. This equation was used to derive analytical secular equations that had previously been derived. This approach resulted in a very general method of calculating the coefficients of the secular equation explicitly as a function of elastic constants and rotation angles, but the generalized version of the equations are very difficult to derive, even in symbolic math languages such as Mathematica. Furthermore, these analytical results can not be used to determine the pseudo-surface wave velocities which will be discussed in §5.2.3.1. As a results, the equations are either solved for specific orientations, propagation directions, and crystal symmetries or numerical techniques are used to solve the equations [69].

Typical numerical solutions for RSW have used the iterative search procedure described in [63]. In this approach, the velocity space is searched over with non-gradient based optimization methods to find the velocities at which both the governing differential equation as well as the stress-free boundary conditions are satisfied. The optimization is performed many times to determine which of the many minima corresponds to the RSW velocity. This results in a non-trivial forward solution for the RSW velocity in all directions on the surface of arbitrarily oriented crystals. This has led to database approaches where a surrogate model is pre-computed and used as the forward solution in the inverse [2, 62].
new numerical algorithm that calculates surface wave velocities more efficiently than previous methods is shown in Chapter 5. This algorithm is quick enough that it can be directly applied as the forward solution in an inverse procedure. Application of the algorithm in an inversion for single crystal elastic constants is demonstrated in Chapter 5 as well.

1.1.3.5 Defocused-Probe Rayleigh Surface Wave Velocity Imaging

Rayleigh surface waves have been used extensively for materials characterization using scanning acoustic microscopy (SAM) [70, 71]. In a SAM setup, a piezoelectric element with a spherical or line focusing lens is excited with an electrical signal. Pressure waves generated in a coupling media such as water interact with the elastic material properties of the sample. The various wave modes excited in the sample send energy back to the transducer by reflecting off either the surface or objects below the surface. The advantage of the line focusing lens is that it is directionally sensitive and can be used to characterize the entire slowness surface of a single crystal [72]. The disadvantage is that line focused transducers require a relatively large single crystal to fit the entire focal spot within the sample. As such, it has been applied extensively in characterization of thin-film properties [73]. A spherically focused lens is not directionally sensitive but it has a very tight focal spot allowing it to fit within a large grain in a polycrystalline aggregate.

In a typical experimental setup, the focusing lens has a wide enough opening angle that the Rayleigh critical angle is exceeded, thus exciting a RSW in the material. Authors have used the technique to excite RSW on the surface of the sample and have used the time-domain response to estimate RSW velocity [72]. These RSW propagate at a distinct velocity when compared to the bulk waves of the material due to the particle displacements being a combination of shear and longitudinal modes. The RSW velocity can be used to characterize the elastic properties of a material with high precision [74]. The RSW velocity has also been used in the past to fully characterize the single crystal elastic moduli of a sample [62, 73] as well as the orientation of crystallites that make up a polycrystalline ag-
aggregate [75]. Furthermore, SAM measurements have been made to characterize the average RSW velocity in complex materials [76].

Three main electrical signals, tone burst (TB), continuous wave (CW), and impulse excitation (IE), have been used to excite the acoustic transducer for SAM. The earliest developed SAM systems as well as most systems currently available are based on TB excitation [77]. Enhanced contrast in the acoustic images is observed when the lens is operated at a specific defocus level. The location where optimal contrast is achieved is found by analysis of the $V(z)$ curve, where the variation of the gated signal amplitude is plotted as a function of the distance of the lens from the sample. When the focusing lens is wide enough to generate a RSW on the sample, the direct reflected wave (DRW) and the RSW interfere, causing oscillations in the $V(z)$ curve. The periodicity is related to the RSW velocity in the material, thus it has been used for local quantitative measurement of the elastic properties [70]. Alternatively, when CW excitation is used, the $V(z)$ curve is a mixture of acoustic standing waves in water and the RSW on the surface [78]. Analysis of the complex standing wave pattern is used to determine the RSW velocity in the material and the longitudinal wave velocity in the coupling fluid simultaneously. In both the tone burst and continuous wave excitation methods, the DRW and the RSW are not separated in the time domain. On the other hand, SAM based on IE signals allows the separation of the DRW and the RSW in the time domain [76, 79]. The amplitude of the RSW is used for imaging while the time separation between the DRW and the RSW at different defocus levels is used for quantitative measurement of the RSW velocity. This method, known as the two-point defocus impulse excitation (TDIE) method, has been used to generate maps of the RSW velocity. The method has also been extended to measure the surface skimming longitudinal wave (SSLW) velocity to quantify the isotropic elastic properties over the sample [80].

The principle of the TDIE technique is shown in Fig. 1.3. A wide angle focused UT probe is brought near the sample so that the distance between the probe and sample is close to the focal point of the transducer. The opening angle of the transducer is large enough
that a portion of the incoming energy exceeds the Rayleigh critical angle and generates Rayleigh waves. At focus, any energy returned from the RSW is obfuscated by the direct reflection. When the probe is defocused toward the sample, the path length of the RSW becomes larger, delaying the time at which the reflected energy arrives at the transducer. Furthermore, the path length of the direct reflection becomes shorter. This separates the RSW from the direct reflection in the time domain. The separation of these two reflected signals is shown in the image.

Time-domain data is collected at multiple different defocus levels and the RSW peak signal is tracked in the time domain. Using simple geometric relationships, the wave velocity is then calculated using

$$v_{SW} = \frac{2(z_1 - z_2)}{\sqrt{[(\Delta t_1 - \Delta t_2)^2 - (\Delta t_{r,1} - \Delta t_{r,2})^2]}}$$  \hspace{1cm} (1.10)

In this equation, $v_{SW}$ is the surface wave velocity, $z_1$ and $z_2$ are the two defocus levels, $t_1$ and $t_2$ are the times of the direct reflection peak at both defocus levels, and $t_{r,1}$ and $t_{r,2}$ are the times of the two RSW signals in at each defocus. What can be noted with this equation is that no absolute registration of the probe distance relative to the sample is needed. Only the changes in arrival times and defocus levels are needed for this computation. Thus any two defocus levels can be used to compute the velocity. Another aspect to note is that this technique is not restricted to measurement of the Rayleigh wave velocity. The same authors used the technique to measure the velocity of the surface skimming longitudinal wave as well as the Rayleigh wave, and combined these measurements to get an estimate of the isotropic elastic modulus [80].

This technique is very useful as a microscopy method due to the small spot size of the focused transducer at higher frequencies. For instance, the spot size of a focused transducer at 100MHz is 30µm. This is a fine enough resolution that the spot could be contained
within one large grain in a polycrystalline aggregate. However, at lower frequencies the
spot size of the transducer will fall in multiple grains, such as in the data shown in [80]. In
that work, scans were taken over large grained materials to verify the techniques. It was
clearly seen that the resolution of the longitudinal wave velocity images was lower due
to the larger defocus required to separate the longitudinal wave from the direct reflection.
This created the distorted images of longitudinal wave velocity. Furthermore, the analysis
performed in their work assumed that the material was isotropic. The velocities were re-
lated back to the elastic properties through the isotropic wave velocity equations. This gave
lower fidelity estimates of the elastic properties of the material. If a more rigorous charac-
terization of the material is required, an accurate model of the data collection process that
takes into account the anisotropy of the material is needed. A new model to approximate
the scans taken with this technique in the presence of realistic microstructure is presented
in Chapter 5.
1.2 Surrogate Modeling and Uncertainty Propagation in Nondestructive Evaluation

Many authors have developed simulations for NDE inspections. These simulations are often discretization-based (e.g. finite element method (FEM), volume integral method (VIM), boundary element method (BEM), etc.) and have been designed to capture as much realism in the inspection as possible. An example of this development is VIM for eddy current testing (ECT) problems. The modeling method was developed in the late 1980’s through the early 1990’s [51] and was implemented in the simulation tool Vic-3D® [81]. There has been significant push in the last 5 years to incorporate more complexity in this model with extensive experimental validation of the results [82, 83]. This has lead to successful demonstration of the model for characterization of damage in engine components with uncertainty quantification [84]. In this study, significant modifications and improvements were made to the simulation tool and benchmark experiments were performed to validate the modifications. This work clearly showed the need for model complexity and accuracy in materials state awareness (MSA).

The trade-off for increased model complexity/realism is that it often results in longer computation times. This is not always the case (multi-threading was used to keep simulation times down in [84]), but in general, discretization-based methods require significant time (from seconds to hours) to find a solution even in the most optimum configuration. When these simulation tools are used in the context of inverse problems and uncertainty propagation, many simulations are required (for instance in Matlab®’s lsqnonlin routine, the default maximum number of function evaluations is set to $100 \times$ the number of parameters). Furthermore, the number of simulations increases as a function of the number of parameters included in the problem. This has led researchers to develop fast solving, highly accurate surrogate models to use in place of the full discretized problem. Furthermore,
many authors are currently researching methods to combine models of varying fidelity in a multi-fidelity modeling framework [85–87]. In this section, surrogate models that have been applied in NDE simulations are discussed as well as their application in uncertainty propagation problems.

1.2.1 Surrogate Models for Uncertainty Propagation

Many researchers have used surrogate models in NDE. For instance, in [84] a full tensor grid covering the parameter space and linear interpolation were used to represent an ECT problem where the flaw dimensions were varying. This was used in the context of an inverse problem. In their work, near real-time inversion was enabled by using quick-solving linear interpolation. However, linear interpolation performs poorly if the function deviates sufficiently from linearity between the points in the full Cartesian grid. The authors in [88] and subsequent authors (e.g. [89], [90]) used polynomial chaos methods to generate surrogate models for uncertainty propagation. Polynomial chaos is based on orthogonal polynomial projections of the random variable to generate a series expansion of interpolation functions and expansion coefficients that converge to the random variable. The method has convergence advantages in uncertainty propagation problems as is discussed in [91], but the “curse of dimensionality” becomes a problem for the typical application of non-intrusive polynomial chaos methods. Authors [92–95] have used sparse grids in electromagnetic NDE problems to reduce the burden of added dimensions in both uncertainty propagation problems as well as inverse problems. Sparse grids have the advantage of retaining the accuracy of a full Cartesian product grid while requiring less computations. Furthermore, they can be nested making them adaptive. This makes refinement of the grid less demanding [93]. Authors have also used non-deterministic Kriging-based [96] surrogate models in the past for NDE applications [97, 98]. Kriging-based surrogate models are a generalization of typical spline interpolation models that have the advantage of being able to use points at any arbitrary location inside the parameter space. This makes them highly
adaptive and easy to refine as more data is collected from the high fidelity model.

1.2.2 Microstructure Signal in Uncertainty Propagation

In uncertainty propagation problems, propagating randomly heterogeneous material noise through forward models is often challenging. This is due to the high dimensionality of the stochastic process that represents the microstructure features in the sample. One approach of dealing with this problem is to expand the random process in terms of the eigendecomposition of the correlation function. This is known as the Karhunen-Loeve (K-L) expansion [99]. This expansion converges to the actual random process in mean square and can be truncated after a finite amount of terms, resulting in a series of random variables to propagate through the forward model. Any of the techniques used in the previous section for uncertainty propagation can be applied to propagate the resulting uncertainty through the model of an NDE inspection. Previous work has been done on this subject in the context of eddy current testing of titanium alloys. The authors in [100] showed that this expansion could be used to represent the orientation of the anisotropic crystallites to propagate the uncertainty from microstructure through Vic3D. The authors used a uniform random process to represent the microstructure and applied the assumptions made in deriving the K-L expansion for Gaussian random variables. Furthermore, a very specific set of correlation functions were considered. If the K-L expansion is applied to microstructure uncertainty propagation through NDE forward models, a more quantitative method of evaluating the convergence of the expansion in terms of the convergence of the correlation function is needed. Typical approaches for evaluating the convergence have been based on scree plots [101]. This is essentially the approach used in [100] as well. The authors used analysis of variance (ANOVA) to evaluate the convergence of the random process by noting that the eigenvalues are directly related to the total variance of each term in the expansion. This approach was also suggested in [99]. While convergence of the total variance gives accurate estimates for many applications, it does not guarantee convergence of the correlation
function, which is required for use in NDE forward uncertainty propagation. This issue is addressed in §2.3.1.2. Another issue with previous applications of the K-L expansion in the context of microstructure propagation through eddy current models was the assumption of uniform distributions. A method to change the distribution of instances of random processes generated from the K-L expansion is discussed and implemented in §2.3.1.3.

1.3 Organization of Dissertation

While significant progress has been made in modeling and simulation of NDE scenarios as well as application of UQ techniques for model-based reliability assessment of NDE techniques, more work is needed. Random signals from the material often confound NDE capability more than any other source of variability in an inspection. Thus, accurate material models must be leveraged to propagate uncertainty from the microstructure through forward models of NDE. These forward models should be efficient enough that many simulations can be run for propagation of uncertainty techniques. The goal of the work in this dissertation was development of fast and accurate approximation-based models for use in uncertainty propagation. Two different NDE techniques were chosen that represent different methodologies as well as spatial resolutions. Forward models that efficiently map microstructure information to the NDE response were developed. These models used physics-based approximations to alleviate the need for full discretization of the spatial domains, which resulted in highly efficient simulations in both cases.

Chapter 2 of this dissertation discusses the material properties of titanium alloys that are relevant to the NDE models. Several different methods for statistical representation of the material are introduced and discussed in brief detail. The output of the statistical representation is a map of the crystallographic orientation at each spatial location in a sample. The orientations from the representation are related to the anisotropic material properties, which are mapped through the NDE models to determine the theoretical response of the
sensor. In Chapter 3, a novel model for mapping the orientations to the ECT response is shown. This model has been tested and qualitatively validated against experimental data. The validation has been accomplished with both an absolute probe as well as a reflection differential probe using samples with large single crystals as well as samples with a significant volume fraction of microtexture regions. Chapter 4 shows the experimental methods in TDIE inspections as well as modifications made to the post-processing algorithms to enhance the contrast of images obtained in these scans. Chapter 5 shows a novel physics-based model for defocused UT inspections. A novel numerical routine was developed for quick calculation of the surface wave velocity in any arbitrary direction and on any plane of a single crystal sample. This routine was verified and validated. Finally, Chapter 6 summarizes the progress made thus far and documents the contributions to the state-of-the-art. Avenues for further work are discussed as well.
Chapter 2

Nondestructive Evaluation Related Material Properties of Titanium Alloys

This chapter discusses the material properties of titanium alloys that have the greatest effect on NDE signals. The chapter shows the linkage between the material system and the NDE physics, effectively mapping the orientation of crystallites in a polycrystalline aggregate to the NDE signal. Characterization methods for the materials are discussed with examples that were used to verify/validate the models developed in this dissertation. Statistical representations of these materials are discussed and the output of those representations is shown. The details of the Karhunen-Loeve (K-L) method are given in this chapter as it has been previously applied to NDE models. Enhancements are shown that alleviate the assumptions about the statistics of the random processes in the K-L method. Furthermore, an in-depth discussion of the convergence of the technique is shown. The outputs of statistical representations feed directly into the physics-based modeling routines to map the statistical representation of the material to the NDE response. Once this map is made, the models that are discussed in later chapters can be used to calculate the statistics of the NDE response digitally. This chapter is intended to give an introduction only to the material properties that feed into the models developed in the dissertation and to show how the fundamental aspects of single crystals map to these material properties, giving a consistent notation to
use throughout the rest of the dissertation.

2.1 Hexagonal Crystal Symmetry

Titanium alloys used in industry are either $\alpha$ or $\alpha + \beta$ phase and contain a significant volume fraction of $\alpha$-phase [102], thus for this work, the properties of the hexagonal crystal symmetry are discussed and the body centered cubic $\beta$-phase is ignored. In Fig. 2.1, the hexagonal prism represents the crystal structure of $\alpha$-phase Ti64. According to the standard Miller-Bravis indices for hcp crystals, the X-axis lies along the $[2\overline{1}\overline{1}0]$ direction, the Y-axis lies along the $[01\overline{1}0]$ direction, and the Z-axis lies along the $[0001]$ direction. The plane spanned by X and Y (the (0001) plane) is called the Basal plane, and the axis collinear with the Z-axis is called the c-axis of the crystal. The material properties can be thought of as isotropic in any direction along the basal plane and anisotropic in directions not lying in the basal plane.

2.1.1 Crystallographic Orientation

Single crystals of hexagonal close packed (HCP) materials are anisotropic in both electrical as well as elastic properties. This implies that the orientation of the crystal relative to the sample axes must be characterized and incorporated in the forward model of an NDE methodology to accurately predict the response of an NDE sensor. The orientation of any

Figure 2.1: Figure shows the subsequent rotations of the crystal from the global frame of reference to the crystal frame of reference.[1]
crystal is completely defined by 3 unique rotations, called Euler angles. In this dissertation, Bunge’s active notation [103] is used as the convention for determining how the rotations are applied to the crystal. In this convention, also known as the $Z$-$X'$-$Z''$ convention, $Z$ is a rotation about the first $Z$-axis or the $c$-axis of the crystal, $X'$ is a rotation about the new $X'$-axis, and $Z''$ a rotation about the new $Z''$-axis or again the $c$-axis. A schematic of these subsequent rotations is shown in Fig. 2.1. The angles corresponding to these three rotations are labeled ($\psi_1$, $\theta$, $\psi_2$).

### 2.1.2 Mapping the Orientation

Most engineering metals are not single crystals but aggregates of multiple crystallites. Thus, every point inside a sample will lie in a crystallite whose orientation is completely defined by the set of Euler angles shown above. To determine the orientation of each crystallite in a sample, a method that maps the orientation at discrete spatial locations is needed.

A common method for mapping the orientation in a polycrystalline sample is called electron backscatter diffraction (EBSD) [104]. This technique is a scanning electron microscopy technique that acquires the diffraction pattern of electrons through the crystal lattice of a material and compares that diffraction pattern against a database of patterns. Each orientation along a surface has a unique diffraction pattern so that the orientation can be mapped at each spatial location by finding the pattern that best fits the experiment.

![Figure 2.2: IPF map legend. The out of plane sample axis [001] is the reference direction for these maps.](image)
technique only works if the geometry of the underlying crystal system is known, which in
the case of $\alpha$-phase titanium is hexagonal, $6/mmm$ point group. This method is strictly
surface-based and requires a highly polished and flat surface. However, if the surface is
flat enough, a large area of orientations can be obtained automatically from a sample in a
relatively short amount of time. The orientation data collected with EBSD is stored, along
with spatial locations, in large ASCII text files or binary files, and the orientations are read
into analysis code.

A common method for displaying this data is called inverse pole figure (IPF) mapping.
Each orientation is mapped into its equivalent symmetric orientation in the unit cell of the
stereographic projection. The unit cell is color-coded based on the scheme shown in Fig.
2.2, and each spatial location is colored in a spatial map. This false color scheme tends
to illustrate symmetries and illuminates phenomena such as twinning better than coloring
by the Euler angles themselves. For the purpose of this work, the tilt of the c-axis of
the hexagonal crystal has the most bearing on the NDE signal. In these images, c-axis
orientations that are close to vertical are colored closer to red, and blue and green show
orientations where the c-axis is lying in the plane of the sample surface.

Below are four examples of this data collected over the samples that were used for
validation in this work. The first data set is from a large grained Ti64 sample that was
used for verification/validation in previous work [43]. This sample, shown in Fig. 2.3,
had large features that are visually observable without microscopy once the surface is pol-
ished. This sample was used because it has distinct features that can be registered between
datasets from multiple different modalities for quantitative comparison. A sample with
smaller grains would not have distinct features to use for comparison and could only give
validation in terms of the statistics of the signal predicted. Furthermore, this exact sample
has been used in multiple different previous studies for verification and validation [1, 43],
thus it provides a benchmark dataset to compare experimental methods and models against
previous work. This sample will be called Ti64-plate1 throughout the dissertation.
The Ti64-plate1 sample has features that are small enough that NDE techniques obscure them. Furthermore, while the techniques discussed in this dissertation are surface based with minimal subsurface penetration of energy, there still is interaction with the subsurface features. For instance, typical skin-depths for eddy current are in the $100 - 500\mu m$ range. For this reason, a second Ti64 sample (called Ti64-plate2) was used for verification and validation. This plate was specifically heat treated such that the grain boundaries are largely normal to the cut surface. This ensures that the grains are essentially pillars into the surface, making validation much easier. The EBSD data for this sample is shown in Figure 2.4.

The third sample used in this dissertation came from the study in [105]. This sample, shown in Fig. 2.5, was extracted from a large ingot made from coarse-grained Ti64, but had a relatively constant $\beta$-grain size compared with the previous sample. While the measurements are not sensitive to $\beta$-phase, the resulting $\alpha$-phase colonies after heat treatment where still relatively uniform across the sample, which gave more areas for verification and validation of the measurement techniques. Furthermore, the sample was larger than the
previous sample, which provided more area to perform NDE measurements. Throughout this dissertation, this sample is referred to as 2B-B-1-2AR-RF-B, following the notation used in the previous study.

The last set of samples were created in the study by Pilchak et al. [102]. These samples were Ti-8Al-1Mo-1V (Ti811) with nearly 65% $\alpha$ phase and the rest primarily $\alpha + \beta$ colonies. Multiple slices of this material were cut from different locations in a billet, and the statistics were estimated from these slices. These samples contained much smaller average grain sizes ($10 - 20 \mu m$) compared with the previous samples, but they also contained a significant volume fraction of microtexture regions (MTR). MTRs are large regions where the c-axis of the hexagonal crystals will align in very similar orientations. This has been known to cause significant noise in eddy current scans of titanium [106], and is thus of interest in uncertainty quantification for eddy current models in this work. Due to the subsurface interaction discussed previously, it was not expected that the models would predict the experiment exactly. Rather, the large scale microtexture makes these samples ideal for verification and validation of the statistics that the ECT model predicts in the experiment, namely the correlation functions in the eddy current response. This necessitates an in-depth analysis of the convergence of the expansion techniques in terms of the correlation function, as will be shown in §2.3.1.2. An example IPF map for this material is shown in Fig. 2.6.

![Figure 2.5: Inverse pole figure map of 2B-B-1-2AR-RF-B.](image)
2.2 Overview of Relevant Material Properties

The orientation of each crystallite relative to the sample surface discussed in the previous section is a fundamental property of the crystal system. However, the orientations do not directly map into the physics-based simulations. The input to the physics-based models are material properties, generally coming from some constitutive law such as Ohm’s law or Hooke’s law. Since the material properties in a hexagonal system are anisotropic, the properties must be expressed as tensors with multiple values describing the behavior in different directions. In the following sections, these properties are discussed as well as the rotations to the tensor quantities using Euler angles.

2.2.1 Electromagnetic Properties

Titanium alloys are relatively poor conductors for metals, with an average conductivity in the $0.9 - 3\, \%\text{IACS}$ range ($\%\text{IACS}$ being the percent of the conductivity of annealed copper). They have a relative permeability near 1, making them essentially non-magnetic. Furthermore, at the frequency ranges of eddy current, the electromagnetic fields have very little interaction with the electrical permittivity. Thus the electrical conductivity is the only

Figure 2.6: Inverse pole figure map of a slice of the Ti811 material. Fiducial marks can be seen in the lower portion of this data set.
relevant material property in (1.1) for ECT in titanium. The constitutive relationship that governs this interaction is called Ohm’s law, and it relates induced currents to the electric field through the conductivity tensor. The single crystal conductivity tensor is expressed as:

\[
\bar{\sigma} = \begin{bmatrix}
\sigma_{xx} & 0 & 0 \\
0 & \sigma_{xx} & 0 \\
0 & 0 & \sigma_{zz}
\end{bmatrix}
\]  

(2.1)

The electrical conductivity is isotropic in the Basal plane and anisotropic in any direction not lying this Basal plane. The conductivity in any direction is described by an ellipsoid with semi-axes equal to the diagonal terms shown in this tensor.

The tensor in (2.5) is given for a crystal with axes collinear with the sample axes, \(xyz\). To rotate this tensor to the correct orientation, a rotation matrix is applied. The rotation matrix used here is given by:

\[
R = \begin{bmatrix}
c_1c_3 & s_1c_2s_3 & -c_1s_3 - s_1c_2c_3 & s_1s_2 \\
s_1c_3 & c_1c_2s_3 & c_1c_2c_3 - s_1s_3 & -c_1s_2 \\
s_2s_3 & s_2c_3 & c_2
\end{bmatrix}
\]  

(2.2)

Here, \(c_i\) is the cosine of the \(i^{th}\) angle, \(i \in \{1, 2, 3\}\) corresponding to the index of the respective Euler angles \((\psi_1, \theta, \psi_2)\) and \(s_i\) is the sine of the \(i^{th}\) angle. The rotated conductivity tensor is then given as

\[
\bar{\sigma}_R = R\bar{\sigma}R^T = \begin{bmatrix}
\sigma_{11} & \sigma_{12} & \sigma_{13} \\
\sigma_{12} & \sigma_{22} & \sigma_{23} \\
\sigma_{13} & \sigma_{23} & \sigma_{33}
\end{bmatrix}
\]  

(2.3)
where

\begin{align}
\sigma_{11} &= \sigma_{xx}(1 - s_1^2 s_2^2) + \sigma_{zz} s_1^2 s_2^2 \\
\sigma_{12} &= 2s_1 c_1 s_2^2 (\sigma_{xx} - \sigma_{zz}) / 4 \\
\sigma_{13} &= -s_1 c_2 s_2 (\sigma_{xx} - \sigma_{zz}) \\
\sigma_{22} &= \sigma_{xx}(1 - s_2^2 + s_1^2 s_2^2) + \sigma_{zz} s_2^2 (1 - s_1^2) \\
\sigma_{23} &= c_1 c_2 s_2 (\sigma_{xx} - \sigma_{zz}) \\
\sigma_{33} &= \sigma_{zz}(1 - s_2^2) + \sigma_{xx} s_2^2
\end{align}

An important part of these equations is that there is no \(c_3\) or \(s_3\) in any of them. This agrees with intuition in that the conductivity is isotropic in the basal plane of the hcp unit cell. This implies that the electromagnetic response that relies on the conductivity is invariant under rotations about the \(c\)-axis of the unit cell, which is well documented in literature \[43\]. The third angle, \(\psi_2\) is simply one final rotation about the crystal \(c\)-axis, thus the eddy current response is not sensitive to it.

For the purpose of this work, the average conductivity was estimated using the 4-point calibration technique on each sample. This number was then decomposed into the single crystal components by assuming that the average estimated conductivity is close to the average of the primary axes of the conductivity ellipse. This gave an estimate of the conductivity to use for the models. The average conductivity measured for Ti64 was 1.1\%IACS and the average value for the Ti811 samples was 1.0\%IACS. Assuming that
σ_{zz} is 94% of σ_{xx}, the single crystal conductivities used for each of the material systems is:

\[
\sigma_{Ti64} = \begin{bmatrix}
5.98e5 & 0 & 0 \\
0 & 5.98e5 & 0 \\
0 & 0 & 5.62e5 \\
\end{bmatrix} \text{ S/m}
\]

\[
\sigma_{Ti811} = \begin{bmatrix}
6.58e5 & 0 & 0 \\
0 & 6.58e5 & 0 \\
0 & 0 & 6.18e5 \\
\end{bmatrix} \text{ S/m}
\] (2.5)

### 2.2.2 Elastic Properties

The constitutive relationship for the elastic behavior of a material system is Hooke’s law, which can be written as:

\[
s_{ij} = C_{ijkl} \varepsilon_{kl}
\] (2.6)

In this equation, \(s_{ij}\) is the stress component corresponding to stress on the \(i^{th}\) face in the \(j^{th}\) direction of an infinitesimal cube with faces normal to the \(x_i\) axes \((i, j, k, l \in [1, 2, 3])\). The \(\varepsilon_{kl}\) are strain components defined similarly to stresses, and \(C_{ijkl}\) are the material linear elastic constants which relate the strains to the stresses. The linear elastic behavior of a material for ultrasound is completely defined by these \(C_{ijkl}\) plus the density, \(\rho\) of the material. In the equation, summation notation is used to simplify the expressions, where repeated indices such as those on the right hand side are summed over.

An alternative representation of the equation is known as Voigt notation and it is writ-
ten as:

\[
\begin{bmatrix}
  s_{11} & s_{12} & s_{13} \\
  s_{22} & s_{23} & s_{21} \\
  s_{33} & s_{32} & s_{31}
\end{bmatrix}
\begin{bmatrix}
  C_{11} & C_{12} & C_{13} & C_{14} & C_{15} & C_{16} \\
  C_{21} & C_{22} & C_{23} & C_{24} & C_{25} & C_{26} \\
  C_{31} & C_{32} & C_{33} & C_{34} & C_{35} & C_{36} \\
  C_{41} & C_{42} & C_{43} & C_{44} & C_{45} & C_{46} \\
  C_{51} & C_{52} & C_{53} & C_{54} & C_{55} & C_{56} \\
  C_{61} & C_{62} & C_{63} & C_{64} & C_{65} & C_{66}
\end{bmatrix}
\begin{bmatrix}
  \varepsilon_{11} \\
  \varepsilon_{22} \\
  \varepsilon_{33} \\
  2\varepsilon_{23} \\
  2\varepsilon_{13} \\
  2\varepsilon_{12}
\end{bmatrix}
\]

(2.7)

where \(C_{IJ}\) are related to \(C_{ijkl}\) as shown in [107]. In hexagonal crystals, the symmetry of the crystal system reduces this equation to:

\[
\begin{bmatrix}
  s_{11} & s_{12} & s_{13} \\
  s_{22} & s_{23} & s_{21} \\
  s_{33} & s_{32} & s_{31}
\end{bmatrix}
\begin{bmatrix}
  C_{11} & C_{12} & 0 & 0 & 0 \\
  C_{21} & C_{22} & 0 & 0 & 0 \\
  C_{31} & C_{32} & 0 & 0 & 0 \\
  0 & 0 & C_{44} & 0 & 0 \\
  0 & 0 & 0 & C_{44} & 0 \\
  0 & 0 & 0 & 0 & C_{11} - C_{12}/2
\end{bmatrix}
\begin{bmatrix}
  \varepsilon_{11} \\
  \varepsilon_{22} \\
  \varepsilon_{33} \\
  2\varepsilon_{23} \\
  2\varepsilon_{13} \\
  2\varepsilon_{12}
\end{bmatrix}
\]

(2.8)

Thus, 5 independent constants need to be known to define the elastic behavior in these crystals.

There are a wide range of numbers reported in literature for Ti64 elastic constants, e.g. [108, 109]. In general, these measurements are based either on resonance techniques [110] or on measuring the bulk ultrasound velocity in specific crystallographic directions. Ideally, the sample would be used to determine the constants, but these techniques require significant work to be placed on sample prep and great care must be taken in making the measurements. For this reason, it is enough for model verification and validation to use the values reported in literature. In this dissertation, the constants that were used were from
The density of Ti64 was assumed to be 4430 kg/m$^3$. Ti811 was not used for validation of the ultrasound code in this dissertation, so the constants are not reported here.

In elasticity, the rotation matrix (2.2) can be applied to the 4th rank tensor, $C_{ijkl}$, by using:

$$C'_{ijkl} = R_{im}R_{jn}R_{kp}R_{lq}C_{mnpq}$$  \hspace{1cm} (2.10)

In fact, being able to apply a physical rotation in this way defines the $C_{ijkl}$ as a 4th rank tensor. Alternatively, the method of building the tensors in Voigt’s notation can be used to generate a rotation matrix in Voigt notation that can be applied to the $C_{I,J}$ matrix.

### 2.2.3 Properties in a Physical Model and Microtexture

In the previous two sections, the single crystal properties are shown for both electrical conductivity as well as elastic wave motion. Rotations are applied to the matrices to connect the fundamental microstructure property of orientation to the material properties. The material properties as a function of the sample spatial coordinates are the inputs to the physics-based models. Thus, the map from microstructure to the physics-based models has been made. The spatial map of orientation over a sample surface can be mapped to the material properties, which then is input into the physics-based models that will be shown in later chapters. The response of the NDE probes is dictated by these rotation matrices,
and thus the orientations at every point on the surface. Any set of orientations where the rotation matrices has the same effect on the material property tensor is called a symmetry direction (e.g. rotations about the c-axis in hexagonal systems).

This leads to an effect that is very common in titanium alloy mill products called microtexture region (MTR) formation [111]. MTR’s are regions where multiple crystallites within a sample align to have similar orientations. This leads to negative impacts on the performance of the material both from a fatigue standpoint as well as from a creep standpoint. From an NDE perspective, these MTR’s are large regions (> 100µm) where the material properties are very close to one another. If the surrounding area has orientations that are sufficiently different from the MTR, the NDE signal changes. In fact, a sample with microtexture typically has a significant amount of “material noise” that acts as a confounding factor in NDE inspections [106]. For the purpose of uncertainty propagation, a method must be found that can generate samples of a titanium alloy digitally that can incorporate this microtexture signal. This will be discussed in the next section.

2.3 Statistical Representations of Microstructure

In the previous sections, the link between the orientation map and the NDE physics-based model is shown. The IPF maps shown in the figures thus far were collected using EBSD on real samples. While this provides an excellent data set with which to validate forward models, the orientation maps can also be generated using numerical algorithms, effectively creating digital instantiations of the material. These numerical algorithms use statistics estimated from the data collected in EBSD maps that describe the material, and then randomly sample those statistics to generate instantiations of that material. In this section, methods that have been used previously to represent materials in NDE are discussed. This statistical representation of the material is crucial for uncertainty propagation through NDE forward models.
Characterization of the distribution of heterogeneous materials using ECT has been a subject of interest for some time. In 2004, a substantial amount of work was done on looking at rough surfaces with eddy current testing [112]. In this work, a simplified model was created based on Rayleigh scattering on the surface of the material assuming a sinusoidal distribution of the scatterers. The spectral decomposition of the random process was then used to generate random samples of the rough surface, and multiple correlation functions were analyzed for their applicability to the surface roughness in ECT. In 2006, the authors in [113] used this spectral decomposition to look at a multi-Gaussian random process to represent the surface roughness. More recently and more appropriate to the problem at hand, the authors in [114] used the Karhunen-Loeve (eigendecomposition) expansion to represent the microstructure of a titanium sample. In this work, significant progress was made in representation of randomly oriented conductivity changes in a host material for the purposes of eddy current testing. The advantage that the authors noted in using the K-L expansion was that it resulted in the optimal expansion in a mean-square sense to propagate through the forward models. The authors used the computational code Vic3D to compute the ECT response over many different realizations of the material system and then calculated statistics on the responses.

In their work, the authors in [100] and later [114] made the assumption that the process was uniformly distributed. This assumption is rather limiting in that no realistic material behaves in a purely untextured way. However, the authors clearly showed that there can be significant reduction in dimensionality of the random process as well as in the terms needed from the rotation matrix applied to the conductivity tensor. This lends significant interest in developing the K-L expansion methods further for use in ECT. In the following sections, the details of the K-L expansion will be discussed as well as methods for applying the expansion technique to arbitrarily distributed random processes.
2.3.1 Karhunen-Loeve Expansion Techniques

The Karhunen-Loeve expansion is a widely used approach to handle spatially heterogeneous noise in uncertainty propagation problems [91, 115, 116]. In problems where the noise in an experiment is Gaussian with high spatial correlation, this method is a very effective tool used to reduce the infinite dimensional random process to a finite dimensional series of deterministic functions and random coefficients.

Microstructure has two separate attributes that are randomly generated, the shape/geometry/location of the grains and the orientation of each grain. In reality, the signals that interact with the microstructure in an NDE experiment are of a spatial resolution where the grain size is not as significant as the spatial correlation and distribution of the orientations. In UT experiments, there has been evidence that this is not true and that the morphology as well as the orientation needs to be considered to accurately model the scattering/attenuation/homogenized velocity [117]. However, in the context of larger spatial resolution defocused UT techniques as well as in ECT experiments, the coils are significantly larger than the average grain size. If there are enough grains within the “spot size” of the transducer or eddy current coil, it effectively averages them and the shapes of the grains are not significant. Therefore, the signals are more likely affected by long range correlations of the orientations of the grains rather than the shape and morphology of the grains themselves. These long range correlations are characteristic of MTRs. In this work, the coils were large enough that long range correlations such as those from microtexture regions were the dominant features.

The goal of the Karhunen-Loeve method is to find an expansion that represents the random process so that samples can be drawn from the random process. Drawing a sample from random variables with well-defined probability density functions results in a number that lies somewhere in the domain of the random variable. The K-L expansion decomposes the random process to a series of deterministic functions and random variables. Sampling
from the process then becomes a matter of sampling from random variables and applying the samples in the series expansion.

Given a random process, $\Phi(x)$, where the random variable, $\Phi$, is a function of the spatial variable $x$, the orthogonal decomposition of the form:

$$\Phi(x) = \sum_{i=1}^{\infty} C_i \psi_i(x)$$  \hspace{1cm} (2.11)

can be used to represent the random process. The random variable $\Phi$ is a random quantity of interest, for instance an Euler angle or another quantity representing the orientation. In this expansion, each $C_i$ is also a random variable:

$$C_i = \int_{x_1}^{x_2} \int_{x_1'}^{x_2'} \psi_i(x) \Phi(x) dx$$  \hspace{1cm} (2.12)

and each $\psi_i(x)$ is a deterministic basis function, the form of which is discussed later. If the distribution of $C_i$ is known, it can be sampled numerically and the summation in (2.11) can be carried out. If this series is shown to converge to the actual random process, then it can be truncated and used to effectively sample from the random process, reducing the dimensionality of the random process to the number of terms retained after truncation.

The functions, $\psi_i(x)$, are the eigenfunctions of the correlation function kernel operator:

$$\int_{x_1'}^{x_2'} \int_{x_1}^{x_2} K(x, x') \psi_i(x') dx' = \lambda_i \psi_i(x)$$  \hspace{1cm} (2.13)

where $K(x, x')$ is the correlation function of the random process (e.g. the kernel of the operator), $\psi_i(x)$ is the $i^{th}$ eigenfunction of this operator, and $\lambda_i$ is the $i^{th}$ eigenvalue associated with this eigenfunction. Using the eigenfunctions to build the expansion in (2.11) ensures that the expansion converges to the random process in mean-square convergence. These eigenfunctions are rarely known analytically for arbitrary covariance functions and have to be determined numerically in most cases, which is an $O(n^3)$ operation, where $n$ is
the number of spatial locations for which the orientation must be known. However, once
the eigenvalue decomposition is obtained, the truncated expansion is simply a combina-
tion of random coefficients and deterministic functions of space, effectively reducing the
dimensionality of the random process.

This expansion is called the K-L expansion. It is very useful for Gaussian random
processes, as the expansion coefficients have an analytically determined form for their PDF
given by:

$$f_{c_i}(c_i) = N[m_i, \lambda_i]$$  \hspace{1cm} (2.14)

where

$$m_i = \int_{x_1}^{x_2} m(x) \psi_i(x) dx$$  \hspace{1cm} (2.15)

In this expression, $m(x)$ is the mean function of the random process. It was assumed to
be zero for the microstructure signals in this work, thus the mean of each of the expansion
coefficients was also zero. This analytical expression for the distributions of the expansion
coefficients makes the K-L expansion for Gaussian random processes extremely useful as
none of the parameters of the distributions need to be estimated. Even in conservative
problems where 20 expansion terms are required, each having unknown 1st and 2nd order
moments, the parameter estimation problem would be extremely data intensive and require
a significant amount of characterization results. Thus, unless the distributions of the coef-
ficients can be determined analytically, the expansion is not useful for this problem.

2.3.1.1 Eigendecomposition of Correlation Function

One difficult aspect of applying the K-L expansion is computing the eigendecomposition
from (2.13). This is a Fredholm integral of the first kind and ample literature exists that
describes the solution to this equation. One kernel for which this Eigenvalue problem has
been solved analytically is for processes that follow Poisson statistics, which are modeled
with the exponential correlation function. In general, it is reasonable to assume that the
long range correlations from microtextured regions as well as the single crystal $\alpha$-particles can be modeled effectively with Poisson statistics. The correlation function is written as:

$$ K(x, x') = P \exp \left[ -\frac{|x - x'|}{\gamma} \right] $$

In this expression, $\gamma$ is the correlation length and $P$ is the mean square error of the random process. The integral in (2.13) is carried out for one dimension on the interval $[-T, T]$. In application, $T$ is half the length of a sample for which the material properties are a random function of space. The eigenfunctions and eigenvalues of this kernel function have been determined analytically using the solution method outlined in [99] in their Example 6.2 from §6.4.1, or in [115] in their §6.2.3. In this method, (2.13) is differentiated and the eigenvalues and eigenfunctions are found as the solutions to the resulting ordinary differential equation. The eigenvalues are given as:

$$ \lambda_i = \frac{2P}{\gamma (\gamma^2 + b_i^2)} $$

where $b_i$ are given as the solutions to the transcendental equation:

$$ (\tan bT + b\gamma) \left( \tan bT - (b\gamma)^{-1} \right) = 0 $$

The eigenfunctions for this correlation function are written as:

$$ \psi_i(x) = \begin{cases} 
T \left( 1 + \frac{\sin 2b_i T}{2b_i T} \right)^{-\frac{1}{2}} \cos b_i x, & i \text{ is odd} \\
T \left( 1 - \frac{\sin 2b_i T}{2b_i T} \right)^{-\frac{1}{2}} \sin b_i x, & i \text{ is even}
\end{cases} $$
Assuming that the correlation function for both dimensions can be written as the product of the two separate dimensions, or as:

\[
K(x_1, x_1', x_2, x_2') = P \exp \left[ -\frac{|x_1 - x_1'|}{\gamma_1} - \frac{|x_2 - x_2'|}{\gamma_2} \right]
\]  

(2.20)

then the integrations in (2.13) can be carried out separately and the eigenfunctions of this expression are just the product of the constituent eigenfunctions.

In [102], an alternate form of the correlation function is given that is relevant in Ti811. It is reasonable to assume that the long range correlations from microtextured regions as well as the single crystal \( \alpha \)-particles can be modeled effectively with Poisson statistics. However, the off-diagonal directions are better modeled by relating the autocorrelation to the distance from the origin. This can be accomplished by using:

\[
K ((x_1, x_1'), (x_2, x_2')) = P \exp \sqrt{\frac{(x_1 - x_1')^2}{\gamma_1^2} + \frac{(x_2 - x_2')^2}{\gamma_2^2}}
\]  

(2.21)

In this equation, \( \gamma = [\gamma_1, \gamma_2] \) are the correlation lengths in the \( x_1 \)- and \( x_2 \)-directions, respectively. The difference between (2.20) and (2.21) is that the equation in (2.21) is not separable in \( x_1 \) and \( x_2 \), which implies that the eigenvalue decomposition cannot be performed for each spatial dimension separately. The combined correlation function for both the fine \( \alpha \)-particles as well as the microtextured regions can be expressed as:

\[
K(x, x') = C_\gamma \exp \sqrt{\frac{(x_i - x_i')^2}{\gamma_i^2}} + C_\kappa \exp \sqrt{\frac{(x_i - x_i')^2}{\kappa_i^2}}
\]  

(2.22)

where \( \gamma \) is the correlation length of the \( \alpha \)-particles, \( \kappa \) is the correlation length of the microtextured regions, and the coefficients \( C_\kappa \) and \( C_\gamma \) are the mixing coefficients for the two functions. The difficulty is that this kernel does not have an analytical eigenvalue decomposition and numerical techniques must be used to solve it. Once again, this is an \( O(n^3) \)
operation and thus a heavy computational burden when a wide field of view is needed.

### 2.3.1.2 Numerical Results

Numerical examples were used to show the output of the K-L expansion and to test the convergence for distributions with correlation functions similar to that from the Ti811 samples. Samples were drawn from a random process that has a Gaussian distribution with a separable exponential correlation function, as discussed in §2.3.1.1. The correlation function is shown in Equation (2.20). This is the simplest correlation function to use for testing due to the fact that the eigendecomposition for each dimension can be done analytically and then combined later. No numerical eigenvalue problem need be solved for this function, which implies that a relatively wide range of view can be generated. A $10 \times 10 mm$ area was simulated with correlation lengths of $\gamma_1 = 0.2 \text{mm}$ and $\gamma_2 = 0.9 \text{mm}$. A plot of the actual correlation function is shown in Fig. 2.7. The skewed nature in the y-axis can clearly be seen in this figure. Furthermore, the “diamond” shape comes from the separable assumption. For the sake of testing convergence of the K-L method with increasing eigen-

![Figure 2.7: The 2-D correlation function from $-5$ to $5$ with correlation lengths of $\gamma_1 = 0.2$ and $\gamma_2 = 0.9 \text{mm}$.](image)


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values, samples and the estimated correlation functions were plotted for multiple different numbers of eigenvalues retained. The results are shown in Fig. 2.8, where the left side is one sample of the truncated distribution, the right side is the estimated correlation function, and each row is an increased number of retained eigenvalues in the expansion.
One approach at viewing the convergence of the K-L expansion is by viewing the decay in the eigenvalues using a scree plot. This was shown in [101] and the expansions in that work were shown to converge after no more than 6 eigenfunctions were included in the expansion. The scree plot for the eigenvalues from the 2D random process described here can be seen in Fig. 2.9. From (2.14), it can be seen that the eigenvalue essentially gives the standard deviation of the magnitude of each term in expansion (2.11) and is also related to the spatial frequency of each eigenfunction defined in (2.19). So, as the eigenvalue increases in magnitude, the spatial frequency of the particular term in the expansion is decreased and the variance or “randomness” of that term is increased. This implies that for random fields where the correlation lengths are small compared with the sample size, or $T$, more terms will have to be retained to capture enough spatial “randomness”. This can be seen in the plot shown in Fig. 2.10. This plot shows the number of eigenvalues needed before their value fell below $1/10^{th}$ the maximum eigenvalue, which is plotted against the ratio of correlation length, $\gamma$ vs half the total length of the field of view, $T$. It can be seen in the plot shown in Fig. 2.10. This plot shows the number of eigenvalues needed before their value fell below $1/10^{th}$ the maximum eigenvalue, which is plotted against the ratio of correlation length, $\gamma$ vs half the total length of the field of view, $T$. It can be

---

Figure 2.9: Scree plot for the Karhunen-Loeve expansion eigenvalues for the 2D random process described in §2.3.1.4.
Figure 2.10: This plot shows the number of eigenvalues needed before the eigenvalue drops below 0.1 times the maximum eigenvalue on the y-axis and the ratio of the correlation length to the total field of view for the sample on the x-axis. Clearly, as correlation length is increased, less eigenvalues need to be retained in the K-L expansion.

clearly seen from this plot that the total number of eigenvalues needed to be retained in the expansion increases exponentially with decreasing correlation length. In the work of [101], this ratio was roughly 0.68, whereas in the numerical example analyzed here, the ratio is 0.04. Furthermore, the expansions in this work represent a 2D process, which inherently requires more eigenvalues. Thus, in using the K-L expansion to represent a random field, the range of view relative to the correlation length should be considered as well as the dimensionality required.

While eigenvalue decay is a good way to estimate the convergence of the expansion, the true quantity of interest is the correlation length. Once the expansion is built using a set total number of eigenvalues, it can be sampled multiple times and the autocorrelation of each sample can be calculated. However, the autocorrelation calculated in this way is determined using samples from multiple random variables (i.e. the expansion coefficients...
in (2.12)) and is thus a random variable itself. An example of convergence plots for the correlation length are shown for the correlation in the x-direction in Fig. 2.11 as well as the correlation in the y-direction in Fig. 2.12. To create this plot, K-L expansions were built based on 50, 100, 200, 500, 1000, 1500, and 2000 eigenvalues, and each expansion was sampled 50 times. The autocorrelation length was calculated for each sample in both spatial dimensions, and the results were plotted. The estimates of correlation length were based on fitting an exponential correlation function to the data in each direction. The horizontal line in each plot shows the actual correlation length in that spatial dimension, or 0.2 in the x-direction and 0.9 in the y-direction. The estimates of correlation length should converge to this horizontal line, which is clearly the case in these plots. What can be noted from this plot is that the correlation length has converged after 500 eigenvalues and that there are diminishing returns after this. The 500\textsuperscript{th} eigenvalue has 5\% the magnitude of the largest eigenvalue, indicating that this is a good cutoff criterion when analyzing the scree plot (Fig. 2.9) for application of this expansion technique. It should also be noted that the correlation length will always have the scatter shown in these plots regardless of how many eigenvalues are in the expansion. This is due to the fact that the sample extents themselves, or \( T \), are not infinite. Thus, one sample is not enough to determine the correlation length in the output from the NDE physics models, and multiple samples should be propagated through the NDE models.

In applying the K-L expansion, 500 terms were required for convergence, which is a significant computational burden. For instance, simply sampling the expansion 50 times required 3.5 minutes on a laptop with a Core\textsuperscript{TM}i7-3630QM, 2.4GHz processor and 16GB of RAM. If analytical results for the correlation function were not available, as is usually the case, building the expansion would require calculating the first 500 eigenvalues and eigenvectors of a \( 1.5e6 \times 1.5e6 \) correlation matrix, which is a full matrix. One method that has been proposed for improved computational performance is Stochastic Kriging (Gaussian
process fitting) [96], where the Gaussian random process parameters are fit to the random field using parameter estimation, essentially building a statistical model using regression that can be sampled. A challenge with this method is that the inverse of the correlation matrix must be found, which can be computationally expensive. However, if fewer spatial locations are required than by using eigendecomposition, the problem could be tractable. This method has not been analyzed in the context of propagation of uncertainty through NDE forward models, but should be investigated in further research. Alternatives to the full eigenvalue problem that have been pursued will be discussed in §2.3.1.4.

2.3.1.3 Alternate Distributions

The results that have been obtained in literature for the Karhunen Loeve expansion are almost entirely based on the assumption that the random process is Gaussian in distribution. However, the distributions of the Euler angles are clearly non-Gaussian. This limitation

Figure 2.11: Plots showing the convergence of the estimated correlation length in the x-direction as a function of increasing expansion length.
Figure 2.12: Plots showing the convergence of the estimated correlation length in the y-direction as a function of increasing expansion length.

could potentially be overcome by one of the two following arguments. The first is that, as will be seen in Chapter 3, the eddy current response above the randomly heterogeneous material is essentially a summation. If the ECT coil is big enough that it is averaging over a significant amount of grains, the distribution of the signal will likely be Gaussian no matter the distribution of the microstructure. It is enough to ensure that the signal merely acquires the proper moments from the distribution. To show this, the raw data from an experiment was whitened using ZCA whitening [118] and the distribution of the resulting transformed data was analyzed. The signal from an experiment using one of the Ti811 samples is shown in Fig. 2.13. The raw data is plotted on the top of this figure and the whitened signal is plotted in the bottom. It can be seen that there is still some spatial correlation left in the whitened image, but it is clearly less significant than in the raw data. Essentially, the data is closer to independently and identically distributed noise, and the statistics of the data can be analyzed as such. To show that the distribution of the raw data is effectively normal, the
Figure 2.13: Image of the (top) raw data as well as an image of the (bottom) whitened data.

estimated probability density function from the histogram of the data is plotted on the left side of Fig. 2.14 in red circles and the normal distribution using the estimated mean and variance is plotted on the same plot. These distributions are clearly very close. This can also be seen in the normal quantile-quantile (Q-Q) plot shown in the right side of Fig. 2.14. This plot indicates that there is only significant deviation from normal behavior (i.e. deviation from the 45° line) in the tails of the distribution. Thus, the distribution of the signal from an eddy current coil above the Ti811 material is very close to normal, indicating that there is not significant sensitivity to the first order properties of the input random process.

The second method to overcome this limitation is to take a standard normal distribution and perform a monotone transform using the inverse cumulative distribution function (CDF) to produce an arbitrary distribution [119]. This was shown in the work by [120], and later by [121] in the context of generating instantiations of microstructures for use within an NDE model. This technique assumes that the fractile correlation, rather than the usual
product moment correlation, is known. The reason for this is that, under monotone transforms such as a CDF transform, the fractile correlation function is conserved. In a Gaussian random process, the fractile and product moment correlation functions are related to one another through the transform [122]:

$$\rho = 2 \sin \left( \frac{\pi r}{6} \right)$$ \hspace{1cm} (2.23)

So, if the CDF of the actual data (in this case, the CDF of the Euler angles) can be found or approximated, a standard normal distribution can be used to generate a sample and the CDF transform can be used to change the distribution of that sample. This will ensure that the sample has the proper first order distribution as well as the correct fractile correlation function. To test this, a new expansion was built on 2000 eigenvalues based on the correlation lengths of 250µm in the x-direction and 200µm in the y-direction to better match the numbers found in [102] for the Ti811. 50 samples were drawn in the same manner as before, and each sample was run through the inverse CDF transform using the estimated CDF from the second Euler angle in the data. This CDF is shown in Fig. 2.15, with the solid line showing the estimated CDF of θ and the dashed line showing the CDF of one
sample after the monotone transform. These results show similar behavior in distribution, although there are still slight deviations after the transform. This deviation is due to using the standard normal distribution to transform the sample. Although the K-L expansion theoretically produces standard normal samples, these samples were built on incomplete eigenvalue decompositions, thus their distributions deviated from standard normal. The distribution is still much closer to the actual distribution of the Euler angle than previous results. The estimated CDF’s indicate that there will be less low-angle grains than in the actual sample and more high-angle grains, but not by a significant amount. A better estimate of the CDF of the K-L sample should be obtained to improve this fit.

The correlation lengths were estimated as in the previous example and are compiled in Table 2.1. These numbers clearly indicate that even the product-moment correlation functions match well after the CDF transform is performed in the case of exponential correlation functions. Thus, in this framework the limitations in poor recovery of the first order distribution noted in the previous work on K-L transforms applied to eddy current [100, 123] have been overcome by changing the distribution of the expansion using the inverse CDF transform.

### 2.3.1.4 Limitations and Alternate Methods

There are further assumptions made in the previously applied expansion method that must also be mentioned. For instance, the theory has been discussed in terms of a stationary random process, but in reality a microstructure with significant microtexture is non-stationary.

<table>
<thead>
<tr>
<th></th>
<th>$\gamma_x$</th>
<th>$\gamma_y$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Before Transform</td>
<td>0.278mm</td>
<td>0.225mm</td>
</tr>
<tr>
<td>After Transform</td>
<td>0.273mm</td>
<td>0.221mm</td>
</tr>
</tbody>
</table>
Figure 2.15: Image of the CDF estimated from the second Euler angle, $\theta$ (solid line), and the estimated CDF of one sample after the inverse CDF transform (dashed line).

in first order statistics. This assumption may be valid for materials with little texture, but titanium with significant amount of microtexture has multiple component orientation distribution functions (ODF’s) [124] that change based on the location on the surface of the sample. Another weakness in the model is that the random process generated is treated as a continuous function whereas microstructure is a discrete random process where grain boundaries act as discontinuities. Again, the assumption of continuous function realizations may not affect the NDE model significantly, but this has not been rigorously addressed. Lastly, each angle was treated independently of one another, which is an assumption that may not be true for any microstructures. Often, the symmetry of the crystal structure breaks this assumption.

One approach to overcome the limitations and confounding assumptions in kernel-based methods was discussed in [125]. In this method, the orientation across the entire sample surface is treated as a mixture of component ODF’s, and the EBSD data is segmented according to which ODF each group of spatial locations belongs to. The K-L
expansion is used to generate Gaussian random fields which are thresholded to give an integer response for assigning each spatial regions to an individual component ODF by using a plurigaussian model. This gives assignments for each spatial location to a component ODF, which can then be sampled. The advantage to this method is that first order statistics of the material can vary as a function of space, which is crucial for simulation of random fields with microtexture such as that in titanium. The computations required using this method are less severe as the eigendecomposition was performed using incomplete Cholesky factorization. Furthermore, Gaussian process fitting (Kriging) was used to improve the resolution of the data set so that the K-L expansion did not need to be sampled heavily. Thus, it can be applied for fairly large fields of view relative to the simple application of the K-L transform. At the time of publication, this method is still actively in development.

There has also been a significant amount of effort in the materials science community in generating synthetic materials having quantified the statistics of a representative sample, e.g. [126, 127]. The method is implemented in an open-source software tool known as DREAM.3D. It starts by initializing a grid of voxels in a computational volume where the sample is to be generated. The volume is randomly packed with primary features whose shapes are predetermined (often ellipsoidal is used) and whose sizes are determined by sampling from a distribution defined either manually or calculated from data. Then, the orientations are assigned to each feature, again from a set of statistics (e.g. the orientation distribution function, the misorientation distribution function, etc.) that are either manually entered to computed from EBSD data. The final result from this process is a grid of voxels representing the microstructure that is statistically very similar to the microstructure of the sample from which the statistics were estimated. The DREAM.3D suite has the tools for both generation of statistically equivalent instantiations as well as the analysis of orientation data for extraction of the relevant statistics from real data. This tool is likely to be ideal if large fields of view are needed, as the memory requirements are much less
restrictive than the previously discussed Kernel-based methods. The primary limitation of this method is that currently there is no guarantee that the correlation lengths are conserved in the instantiations. Again, this is currently in development at the time of writing this dissertation.

2.4 Conclusion

In this chapter, the material properties of titanium alloys that are relevant to NDE models were discussed. The properties were shown by first defining the notation and terminology used to describe the orientation of each crystallite that makes the polycrystalline aggregate. This orientation was linked to the fundamental material properties that define the behavior of the NDE physics in the material of interest. Methods of generating spatial maps of the orientation were discussed, and the link between the physics of the NDE method and the crystallographic orientation of the crystallites was thus made. A simplified method of sampling from the statistics of a microstructure based on the Karhunen-Loeve method to generate many instantiations of the material was then discussed. Advancements were made beyond the previous applications of this method so that arbitrary distributions could be represented using this expansion. A detailed analysis of the convergence of the expansion was given to show the amount of terms needed for proper reconstruction of the 2-point statistics of the random fields analyzed in this work. The applications and limitations of the method were discussed, and more sophisticated methods of generating microstructure instantiations were shown that could potentially alleviate these limitations. Any of these methods could be used to sample the microstructure provided a careful analysis of the assumptions is performed and they are not found to greatly degrade the accuracy of the results. Each of these methods generate samples of microstructure in the form of spatial maps of the Euler angles that map to the NDE response through the material properties discussed in §2.2, and then through the models that will be discussed in the following chapters. This is
crucial for uncertainty propagation when the variability from heterogeneous materials is to be quantified.
Chapter 3

Physics-Based Model for Microstructure Signal in Eddy Current

This chapter shows the development of two low-fidelity, fast-solving forward models to predict the change in impedance of an eddy current probe in the presence of heterogeneous materials that have features slightly smaller than the size of the eddy current testing (ECT) probe. The two models are based on the Born approximation, which is considered valid within a certain percent change in the material properties of the scatterer, as well as discontinuity of the fields at the grain boundaries. The validity of the approximations was shown based on analytical calculation of the impedance change on both isotropic and anisotropic homogeneous materials. The orientation maps discussed in Ch. 2 were used in the model to predict the eddy current signal. These predictions were compared with experimental eddy current data collected with a commercial ECT probe to validate the predictions in the case of heterogeneous, anisotropic materials.

3.1 Eddy Current Approximations

Two different methods were developed to approximate the eddy current signal above a heterogeneous, anisotropic material. The first was based on the assumption that the aggregate
effect of the grains below the coil is simply a weighted average of each grain, with weights
based on the shape of the electric field below the coil. The second was based on the inte-
gral equation that arises from deriving Poynting’s theorem for electromagnetic fields and
resulted in an integral solution for the response of the sensor. These two methods predict
similar solutions, though they are not equivalent. The first was found to be computationally
more efficient than the second, but was not as accurate. In this section, both methods are
discussed as well as the limitations and the verification and validation results.

3.1.1 Reduced Conductivity Approximation

In the reduced conductivity approximation (RCA) (discussed in [1]), the spatial grid of
EBSD data points is filtered to those just below a fictitious coil in a particular scan position.
A directional conductivity is defined for each point based on the position relative to the
center of the coil. In Fig. 3.1, a coil is shown above a random patch of grains from which
EBSD data has been collected in a regular grid. The entire grid of data has been filtered
down to this subset that corresponds to this particular coil position. At a point in the grid
\((p_i)\), a line is drawn from the center of the coil to the point \((d_i)\), and then a tangential unit
vector to that line is drawn \((r_i)\). This unit vector is the direction in which the directional
conductivity for this point is calculated. These directional conductivities are calculated for

\[
\mathbf{r}_i \cdot \mathbf{d}_i \quad \mathbf{r}_i \quad \mathbf{p}_i
\]

Figure 3.1: Image of a fictitious coil above a random patch of grains. A vector from
the center of the coil \((d_i)\) is drawn to each point in the orientation imaging microscopy
data set \((p_i)\) and the unit normal to that vector \((r_i)\) is used as \(\mathbf{r}_e\) in computing directional
conductivity. [1]
each point below the coil and then averaged to get a total reduced conductivity for the coil at that scan position.

The directional conductivity is calculated with an application of the constitutive relation for induced current density given by

\[ \mathbf{J} = \bar{\sigma}_R \cdot \mathbf{E} \]  
(3.1)

In this equation, \( \mathbf{J} \) is the electric current density, \( \mathbf{E} \) is the electric field, and the rotated conductivity tensor was introduced in Section 2.2.1. This is typically substituted into Maxwell’s equations, for instance to derive the wave equation in a conductive media. However, if it is assumed that the electric field is known, the induced current density can then be derived from a simple application of (3.1). The unit vector, \( \mathbf{r}_E \), pointed in the direction of the known electric field is determined. In the case of the eddy current coil, the electric field is assumed to be directed along the tangential direction to the coil everywhere below the coil. This implies that \( \mathbf{r}_E \) coincides with \( \mathbf{r}_i \), and the constitutive relation at a point below the coil can be written as

\[ \mathbf{J} = J \mathbf{r}_i = E \bar{\sigma}_R \mathbf{r}_i \]  
(3.2)

where \( J \) is the magnitude of the induced current density, \( E \) is the magnitude of the electric field, and \( \mathbf{r}_i \) is the direction of the induced currents given the known electric field. Taking the magnitude of this expression gives

\[ J = E \sqrt{\mathbf{r}_i^T \bar{\sigma}_R^T \bar{\sigma}_R \mathbf{r}_i} \]  
(3.3)

From this equation, the directional conductivity at the \( i^{th} \) point is defined as

\[ \sigma_i = \sqrt{\mathbf{r}_i^T \bar{\sigma}_R^T \bar{\sigma}_R \mathbf{r}_i} \]  
(3.4)
Averaging each of the N conductivities below the coil gives the reduced scalar conductivity as

\[ \sigma_r = \frac{1}{N} \sum_{i=1}^{N} \sigma_i \]  

(3.5)

At this point, any numerical algorithm that solves the one layer Dodd and Deeds problem in [45] gives an estimate of the impedance of the coil above this particular patch of grains. These computations are performed with \( \sigma_r \) at each coil position to give the approximate ECT response.

One of the key assumptions made in the process of deriving this expression for reduced conductivity was that the electric field was known. If Maxwell’s equations are solved with a coil above an isotropic half space, the field within the half space has a semi-analytical expression given by Dodd and Deeds. A change in the conductivity is introduced as a subspace of the half space, but in the case of heterogeneous microstructure features the change is small relative to the typical case in which a void is introduced in the sample. Though this is a low frequency solution to Maxwell’s equations in the near field, the disturbances to the secondary field can be considered a scattered field. As the change in the material properties of the scatterer is low, the transmitted field inside the scatterer can be approximated as the impending field, in a similar manner as an application of the Born approximation in typical scattering theory [128]. This provides a potential limit to the applicability of this algorithm based on the percent change in the conductivity. If the change is too high, this algorithm should break down at some point producing inaccurate results. This is explored in Section 3.2.2.

### 3.1.2 Approximate Impedance Integrals

The second approximation is called the approximate impedance integral (AII). It gives similar results to the RCA method, but has a much stronger basis in fundamentals of electromagnetic wave propagation. The approximation starts with an analysis of Maxwells
equations from a conservation of power perspective. In the absence of applied external fields and with induced and displacement currents being the only currents considered, Amperes law and Faradays law are written in differential form as

\[ \nabla \times \mathbf{H} = j\omega \varepsilon \mathbf{E} + \bar{\sigma}_R \cdot \mathbf{E} \]
\[ \nabla \times \mathbf{E} = -j\omega \mu \mathbf{H} \] (3.6)

In these expressions, \( \mathbf{H} \) is the magnetic field intensity, \( \omega \) is the angular frequency, \( \mu \) is the permeability and \( \varepsilon \) is the permittivity. The assumptions about the media in which these fields exist are that it is linear, homogeneous, and anisotropic in conductivity, isotropic in all other properties. These equations are combined in a similar manner as in [128] to give

\[ \oint_S (\mathbf{E} \times \mathbf{H}) \cdot \mathbf{n} \, dS = \int_V [j\omega \mu \mathbf{H} \cdot \mathbf{H} + j\omega \varepsilon \mathbf{E} \cdot \mathbf{E} + \mathbf{E} \cdot (\bar{\sigma}_R \cdot \mathbf{E})] \, dV \] (3.7)

In [44], an expression relating this surface integral around the flawed region to the change in impedance of the coil was derived. Denoting the fields that result from the coil excitation above an isotropic half-space with \( a \) in the subscript and the fields that result from an excitation above an anisotropic half-space with \( b \), this equation gives the change of impedance, \( \Delta Z \), as:

\[ \Delta Z = \frac{1}{I^2} \oint_S (\mathbf{E}_b \times \mathbf{H}_a - \mathbf{E}_a \times \mathbf{H}_b) \cdot \mathbf{n} \, dS \]
\[ = \frac{1}{I^2} \int_V [j\omega \mu (\mathbf{H}_a \cdot \mathbf{H}_a - \mathbf{H}_b \cdot \mathbf{H}_b) + j\omega \varepsilon (\mathbf{E}_a \cdot \mathbf{E}_a - \mathbf{E}_b \cdot \mathbf{E}_b) + \mathbf{E}_a \cdot (\sigma_a I_{3\times3} \cdot \mathbf{E}_a) - \mathbf{E}_b \cdot (\bar{\sigma}_b \cdot \mathbf{E}_b)] \, dV \] (3.8)

In this expression, \( S \) is the closed surface containing the patch where the conductivity changed, \( V \) is the volume enclosed by this surface, \( I^2 \) is the current in the coil, \( \sigma_a \) is the isotropic conductivity of the half space (referred to as the reference conductivity from here...
on), $\bar{\sigma}_b$ is the anisotropic conductivity tensor that has been rotated by the Euler angles in $V$. $I_{3 \times 3}$ is a $3 \times 3$ identity tensor, and permeability and permittivity remain constant from flawed to unflawed configuration. This expression gives the change of the impedance of the coil in relation to the change of the energy of the magnetic and electric fields, as well as the change in the work done by the electric fields on electric charges.

In the case where the conductivity change is low, the Born approximation can be used in the region of the scatterer. In this work, the scatterer is the region enclosed by $S$ which means that the $b$ subscripts attached to the fields in (3.8) become $a$, leading to the simplified form of the equation

$$\Delta \mathbf{Z} = \frac{1}{I^2} \int_V \left[ \mathbf{E}_a \cdot (\sigma_a I_{3 \times 3} - \bar{\sigma}_b) \cdot \mathbf{E}_a \right] dV \quad (3.9)$$

This equation is used to approximate the eddy current response over a heterogeneous half space. Essentially, the conductivity tensor at each point below a coil is known as in the effective conductivity approximation. Since the field dies out at a distance away from the central axis of the probe, this integral only needs to be calculated in a small region that extends slightly beyond the probe. This distance is related to the skin depth in the material. The integrations in this work were performed using the 2D trapezoidal method.

The reference electric field, $\mathbf{E}_a$, can be calculated using either the semi-analytical solution or by using a numerical algorithm. In this work, a linear FEM simulation was constructed for calculation of the reference electric field values at the surface of the sample when the reference material is an isotropic, homogeneous half-space. This simulation was set up and computed in COMSOL® Multiphysics with a geometry shown in Fig. 3.2. The geometry depicts the cross section of a coil above a half-space with isotropic conductivity, resulting in radial symmetry about the line of symmetry shown. This indicates that the only non-zero component of the electric field is the $\phi$-component. Second order triangular elements with Lagrange interpolation functions were used, which prevents the need for the
Figure 3.2: A general depiction of the geometry used in the FEM simulations to calculate the reference electric field.

typical "rule of thumb" 2 elements per skin depth. The solution was calculated for several different levels of discretization and convergence was reached after a max element size of $\delta/1.5$ on the surface of the sample, where $\delta$ was the minimum skin depth between the two principal axes of the anisotropic material. An element size of $\delta/3$ was used simply to ensure accuracy. The 2D axisymmetric model need only be run once before the AII approximation routine is run, and it solves in $4s$ on a workstation computer with a quad-core hyperthreaded processor and 48GB of RAM.

3.1.3 Model for the Reflection Differential Coil

The previous model applies to absolute coils only. While the absolute coil is used in many inspections, the reflection differential configuration is heavily relied upon in bolt-hole inspections as well as inspections on edges. A model that spatially maps the response of an eddy current reflection differential coil over a heterogeneous material in two dimensions has not been shown previously in literature. The AII model will be discussed in this section for a reflection differential coil design. Application of the RCA model will not be discussed
as it is fairly straightforward to apply to differential coil configurations.

The impedance of a reflection differential probe such as that shown in Fig. 3.3 can be calculated by finding the mutual impedance between the external excite coil and both of the internal D-shaped coils. The mutual impedance, $\Delta Z_{ij}$, of each of these two-port networks is expressed as [44]:

$$
\Delta Z_{12} = \frac{i\omega I^2}{2} \int_{V_f} \left[ H_a \cdot \{(\mu' - \mu) \cdot H_b\} - E_a \cdot \{(\varepsilon' - \varepsilon) \cdot E_b\} \right] dV \\
\Delta Z_{13} = \frac{i\omega I^2}{2} \int_{V_f} \left[ H_a \cdot \{(\mu' - \mu) \cdot H_c\} - E_a \cdot \{(\varepsilon' - \varepsilon) \cdot E_c\} \right] dV
$$

where $\omega$ is the angular frequency of excitation, $\mu$ is the total magnetic permeability, $H$ is the magnetic field intensity, $E$ is the Electric field intensity, $\varepsilon$ is the electric permittivity, and $V_f$ is the volume of the "scatterer" or microstructure features which affect the impedance of the coil. This volume extends slightly beyond the diameter of the coil due to the skin effect and decaying current density beyond the coil [106]. The primes next to the permeability and permittivity refer to the properties of the sample with anomalous material properties from the microstructure, and the lack of primes refer to the test article in the reference state. The reference state is chosen based on convenience of the computations, and in this work it is again assumed to be isotropic with properties somewhat close to the properties of the actual anisotropic material. The subscript $a$ refers to the fields when the external transmit coil is active and the test article is in the reference state, $b$ refers to the fields when the first receive D-shaped coil is active and the microstructure is present, and $c$ refers to the fields when the second receive D-shaped coil is active and the microstructure is present. The permittivity is expressed as:

$$
\varepsilon = \varepsilon_0 \varepsilon_r + \frac{\sigma}{i\omega}
$$

In this equation, $\varepsilon_0$ is the permittivity of free space, $\varepsilon_r$ is the relative permittivity of the material, and $\sigma$ is the electrical conductivity of the material. In this work, it was assumed
that the material was non-magnetic (i.e. \( \mu' = \mu \)) and that the first term in the integrand could be ignored. It was also assumed that the frequency and characteristic length were such that the real part of the electric permittivity, i.e. the displacement field, could be ignored. Under these assumptions, (3.10) reduces to:

\[
\Delta Z_{12} = \frac{1}{I^2} \int_{V_f} E_a \cdot (\sigma - \sigma') \cdot E_b dV
\]

\[
\Delta Z_{13} = \frac{1}{I^2} \int_{V_f} E_a \cdot (\sigma - \sigma') \cdot E_c dV
\]

(3.12)

The signal, \( \Delta Z \), from the reflection differential probe is just the difference \( \Delta Z_{12} - \Delta Z_{13} \).

These equations are analytically intractable for realistic microstructure and must be solved numerically. In this work, a simplifying assumption was made that the fields inside the part with the anomalous conductivity were the same as the fields that would be in the part if the material was in the reference state. This is called the Born approximation and it is valid under the assumption that the anomalous conductivity is near the reference
conductivity. In this work, the reference conductivity was chosen as:

$$\sigma = \frac{\sigma_{XX} + \sigma_{ZZ}}{2}$$  \hspace{1cm} (3.13)

As shown previously, in titanium, the conductivity of the primary axes only differs by 94%, which implies that the average between the two primary axes is closer than 94% to the conductivity of each axis. The assumptions of the Born approximation hold under this condition, as will be shown in §3.2.

This simplification implies that the fields with all subscripts are equal to the fields calculated in the reference state without any anomalous conductivities. Furthermore, the reference fields only need to be calculated once at the beginning of the scan. The fields can be calculated with any numerical technique, such as finite element method, or may be calculated using an analytical solution if one exists. For the D-shaped inner coils and the racetrack external coil, no analytical solution exists and the finite element method was used to find the reference fields. One computation was run for the excite coil, and one for the inner D-shaped coils (the fields are the same for both coils).

For the purpose of this work, it was also assumed that the field magnitudes are negligible at a distance of $3\delta$ away from the extents of the coil, where $\delta$ is the skin depth in the reference material. The integral is a 3D volume integral over the entire flawed region. However, the “flaw” in this case is the conductivity from the randomly oriented crystallites in the anisotropic material. Thus, the integral would need to be performed over the entire sample. Since the fields decay exponentially toward zero after a certain spatial distance away from center. This distance is a function of both the geometry of the coils as well as the skin depth [106]. In this work, the volume integral computation was restricted to a distance of 3 skin depths beyond the external diameter of the excite coil.

Another important simplification was in the behavior of the fields as a function of depth into the sample. At high enough frequencies, the fields essentially behave as plane
waves and the skin depth approximation holds [25]. This work was focused on probes with operating frequencies of $2 - 6 MHz$, which was high enough to assume that the waves essentially propagate as plane waves into the sample. Thus, the wave could be expressed as:

$$E = E(x, y)e^{\beta z}e^{j\alpha z}$$  \hspace{1cm} (3.14)

where $\alpha$ and $\beta$ come from the wave vector $k = \alpha + j\beta$ and are both given as

$$\alpha \approx \beta \approx \sqrt{\frac{\sigma \omega \mu}{2}} = \frac{1}{\delta}$$  \hspace{1cm} (3.15)

Substituting this expression into (3.12) and performing the integration in $z$ from $(-\infty, 0]$ gives

$$\Delta Z_{12} = \frac{\hat{\delta}(1 - i)}{4I^2} \int_{S_f} E_a(x, y) \cdot (\sigma - \sigma'(x, y)) \cdot E_b(x, y) dS$$

$$\Delta Z_{13} = \frac{\hat{\delta}(1 - i)}{4I^2} \int_{S_f} E_a(x, y) \cdot (\sigma - \sigma'(x, y)) \cdot E_c(x, y) dS$$  \hspace{1cm} (3.16)

where $\hat{\delta}$ is the mean skin depth calculated using the conductivity in the $z$-direction at every point below the coil. Note that this integration is now a surface integral over the surface of the anomalous region, which further reduces the computational burden. This is now two 2-dimensional numerical integrals that can be evaluated using any numerical integration technique. In this work, the trapezoidal method was used for ease of implementation.

### 3.1.4 Frequency Dependence of the Approximations

The models previously discussed are only accurate above a certain low-frequency limit. The accuracy degrades relative to the non approximation-based models as the frequency is decreased due to lowering fidelity in the approximations made during the derivation. In
the current work, the frequency of 2MHz was seen to be accurate enough for application to microstructure characterization with eddy current coils. However, difficulty could arise at even modest frequency ranges in the 100kHz range. This effect was considered carefully when using the approximations in this dissertation.

3.2 Convergence, Verification and Validation

3.2.1 Convergence of the Integration Techniques

The convergence of the numerical integration was tested by generating an artificial microstructure file that represented a single crystal sample. The microstructure file contained extremely fine resolution data and was subsequently down-sampled to simulate coarsening of the data set (i.e. reducing the discretization level). The AII routine was run at each discretization level to calculate the impedance change of the coil to determine the discretization level needed for the integration technique to converge. The results of this convergence study are shown in Fig. 3.4. These results show that the algorithm reaches convergence after 180 elements per coil diameter. This is not hard to achieve for microstructure data because coil diameters are typically on the order of 1mm whereas the microstructure data is often taken at spatial resolutions of 1-10$\mu$m. This convergence rate is consistent with the convergence in reflection differential probes.

3.2.2 Verification with Isotropic Semi-analytical Model

A simplified sample where an isotropic, homogeneous half-space changes bulk scalar conductivity from one reference value to a new value was analyzed for verification purposes. This problem has an analytical solution given by [45]. This not only allows for direct comparison with a generally accepted solution to a problem but also allows for further analysis
into the range in which the approximation methods are accurate. For an isotropic change in conductivity in a homogeneous material, the change in impedance can be expressed as

$$\Delta Z = \frac{1}{I^2} \int_V (\sigma_b - \sigma_a) \mathbf{E}_a \cdot \mathbf{E}_a dV$$  \hfill (3.17)

The following assumptions can simplify this expression such that it becomes analytical in conductivity change

1. The field does not change in the azimuthal direction (radially symmetric)
2. The only non-zero component of the field is the $\phi$ directed portion
3. The field is known at $z = 0$ via an FEM solution
4. The field varies in $z$ according to

$$E_\phi(r, z) = E_\phi(r, 0)e^{\beta z}e^{j\alpha z}$$  \hfill (3.18)

Figure 3.4: Convergence plots of (a) resistance and (b) reactance for the integration technique used in the AII.
where $\alpha$ and $\beta$ come from the wave vector $k = \alpha + j\beta$ and are both given as

$$\alpha \approx \beta \approx \sqrt{\frac{\sigma \omega \mu}{2}} = \frac{1}{\delta} \quad (3.19)$$

The first two assumptions are facts in this case because of isotropy and heterogeneity, plus the geometry of the coil. The known field at $z = 0$ is due to the Born approximation assumption made in deriving (3.17), and (3.18) comes from an assumption that the field is a plane wave travelling purely in the $z$-direction ($k$-vector is $z$-directed). Substituting this expression into (3.17) gives

$$\Delta Z = \frac{(\sigma_b - \sigma_a)\delta(\sigma_b)\pi}{P^2(1+j)} \int_0^\infty E_{\phi}^2(r,0) r dr \quad (3.20)$$

This is an approximate expression for the impedance change due to isotropic conductivity changes in a homogeneous half-space from $\sigma_a$ to $\sigma_b$. The validity of the expression can be judged based on solutions to Dodd and Deeds analytical expression, solved with the methods in [129]. An assumption at the beginning of the derivation was that the final results would only be valid in a small range of conductivity change. To test this assumption, the Dodd and Deeds model was solved along with the integral expression for a range of conductivities. The results are shown in Fig. 3.5. These plots indicate that within 50% of the reference conductivity, the results compare reasonably well with theory. In the material of interest, there is a maximum conductivity change from the basal plane to the c-axis of 6%, which is well within the linear limit of the approximation. This gives some confidence that not only will the results correspond to an impedance change, but that they can be considered reliable.
Figure 3.5: (a) Resistance and (b) reactance change of a coil above a conducting isotropic half-space with changing conductivity calculated using two different methods.

Figure 3.6: Plots of the real and imaginary components of the electric field at the surface $z = 0$.

### 3.2.3 Verification with Anisotropic Semi-analytical Model

The model from the study in [49] was used to determine accuracy of the approximations over multiple frequency ranges for calculating the impedance of a coil over an anisotropic sample. The coil in this verification study had dimensions shown in Table 3.1. To show the accuracy of the approximations, the models were used to calculate the total impedance change from that of an isotropic half-space. The impedance in an isotropic reference state
was calculated using the analytical expressions of Dodd and Deeds. The AII approximation was used to calculate the changes from this reference isotropic state to the anisotropic state for varying degrees of anisotropy. Lastly, the actual impedance in the anisotropic configuration was calculated using the analytical expressions of Burke.

According to the coordinates used in [49], the conductivity in the x-direction was varied from 10% of the value used in the paper to 100%, or from $1.47066 - 1.47067 \text{Sm}^{-1}$. The conductivity in the y-direction was set to $1.47067 \text{Sm}^{-1}$. This implied that when the conductivity in the x-direction was at 100% ($1.47067 \text{Sm}^{-1}$), the sample was an isotropic half-space. The reference electric field over the isotropic half space was calculated at a conductivity of $1.47067 \text{Sm}^{-1}$ using the 2D FEM model discussed previously.

The real and imaginary components of impedance were calculated using both the Burke model and the AII, and the change in resistance and reactance from the isotropic half-space to the anisotropic half-space is shown in Fig. 3.7. These plots show the change from the isotropic impedance calculated analytically to the anisotropic impedance calculated with both models as the conductivity in the x-direction is decreased (i.e. the anisotropy of the sample is increased). At 100%, both models give zero change as expected since this state is isotropic. As the conductivity in the x-direction is decreased, the AII approximation maintains reasonable accuracy relative to the analytical model in both resistance and reactance until about 70%.

This analysis was also performed at 7 kHz to judge the accuracy of the model as frequency decreases. The results for resistance and reactance change with respect to level of anisotropy are shown in Figures 3.8a and 3.8b, respectively. These results clearly demonstrate that the accuracy of the model is dependent on frequency. Even though the reactance seems to have improved in accuracy, the expression for resistance is nearly unusable for any range of anisotropy.
Table 3.1: Dimensions of the coil used for finding the accuracy of the anisotropic calculations.

<table>
<thead>
<tr>
<th>Probe Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Inner Radius</td>
<td>9.34mm</td>
</tr>
<tr>
<td>Outer Radius</td>
<td>18.4mm</td>
</tr>
<tr>
<td>Height</td>
<td>8.8mm</td>
</tr>
<tr>
<td>Number of Turns</td>
<td>408</td>
</tr>
<tr>
<td>Internal Liftoff</td>
<td>2.1mm</td>
</tr>
<tr>
<td>Frequency</td>
<td>70kHz</td>
</tr>
</tbody>
</table>

Figure 3.7: (a) Resistance change and (b) reactance change as a function of changing conductivity in one principal axis of an anisotropic half space. In these results, the conductivity of the x-axis is changing from 10% of the paper value up to 100% of the paper value.

### 3.2.4 Verification with Other Numerical Models

Several computational methods such as FEM and VIM were discussed in Section 1.1.2.4 for solving ECT problems numerically for small flaws. It was stated that these methods would require meshes of significant size to solve microstructure problems. This is true for realistic microstructures, but in a simplified case, such as that shown in Fig. 3.9, FEM and VIM can calculate solutions with reasonable mesh discretization levels. This problem was solved with the parameters shown in Table 3.2 with FEM, VIM, the AII approximation,
Figure 3.8: (a) Resistance change and (b) reactance change as a function of changing conductivity in one principal axis of an anisotropic half space at a lower frequency. The resistance plot clearly shows the degradation of the fidelity of the approximations as the frequency is lowered.

Figure 3.9: Problem setup for verification with numerical codes. The red patch is a square of anisotropic material and the gray area is isotropic. The coil beginning and end positions are shown.

and the RCA approximation. Brief introductions to the FEM and VIM models are given in the following sections, and the results from each model are shown.
Table 3.2: Parameters of model for verification against numerical codes.

<table>
<thead>
<tr>
<th>Probe Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Inner Radius</td>
<td>9.34mm</td>
</tr>
<tr>
<td>Outer Radius</td>
<td>18.4mm</td>
</tr>
<tr>
<td>Height</td>
<td>9mm</td>
</tr>
<tr>
<td>Number of Turns</td>
<td>408</td>
</tr>
<tr>
<td>Liftoff</td>
<td>2.03mm</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
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<th>Value</th>
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</thead>
<tbody>
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</tr>
<tr>
<td>Sample Height</td>
<td>12.7mm</td>
</tr>
<tr>
<td>Patch Width</td>
<td>41mm</td>
</tr>
<tr>
<td>Patch Height</td>
<td>9mm</td>
</tr>
<tr>
<td>$\sigma_{XX}$</td>
<td>5.9e6 S/m</td>
</tr>
<tr>
<td>$\sigma_{ZZ}$</td>
<td>$0.94 \times \sigma_{XX}$</td>
</tr>
</tbody>
</table>

3.2.4.1 Finite Element Model Setup

The full 3D FEM model was set up according to the procedure in [130]. The theory of FEM simulation of eddy current problems has been extensively reviewed in [131]. A full 3D model was used in this work due to the lack of axial symmetry induced by the anisotropic patch. The mesh consisted of irregular tetrahedral elements with second order Lagrange interpolation functions, and is displayed in Fig. 3.10. The mesh on the top surface of the anisotropic patch consisted of triangles whose individual dimensions were no more than half the skin depth of the material calculated with conductivity $\sigma_{XX}$. This ensured adequate refinement in depth such that 2 elements per skin depth was achieved. The mesh was relatively coarse around the coil, air, and isotropic material domains. The FEM model solves for the magnetic vector potential, $\mathbf{A}$, and the electric scalar potential, $\psi$, at every point in space. These quantities can be used to calculate the physical field values $\mathbf{E}$ and $\mathbf{B}$.
using the relations:

\[ E = -\frac{\partial A}{\partial t} - \nabla v \]
\[ B = \nabla \times A \]  

(3.21)

The induced current density is calculated by substituting the resulting \( A \) and \( v \) from the FEM model into (3.21) and (3.1). These various results can be used to give the impedance change given in (1.3) where the unflawed part is an FEM simulation with the patch domain set to the reference conductivity and the flawed part is a simulation with the patch domain set to the anisotropic conductivity tensor. Two simulations are performed at each coil position and the results are used to calculate the change in conductivity. Both simulations are run at each position to reduce mesh noise from re-meshing at each coil position. This results in a simulation that takes well over 1 hour to solve on a workstation with dual hex-core processors, each clocked at a nominal 2.7GHz, and 48GB of RAM.

3.2.4.2 Volume Integral Method Model Setup

The theory of the VIM is discussed in several references including [50] and [51]. In this work, a software program called VIC-3D® was used to solve the model shown in Fig. 3.9. The first layer was set to the properties of air, and the second layer was set to the isotropic reference conductivity. The anisotropic patch was meshed with a regular grid that was discretized with \( 16 \times 16 \times 4 \) elements. Solving for air core coils with the volume integral method requires only the flaw domain to be meshed. Furthermore, since the computer on which the simulations were run had sufficient memory to solve the system of equations with direct LU decomposition, the simulation ran in 4s. This is efficient for the simplified problem, but in reality the grid would likely have to be much finer if true microstructure detail were included in the simulation, such as that shown in Fig. 2.3. Still, VIC-3D® was very efficient for the large-scale microstructure problem, especially when compared with
3.2.4.3 Approximation-Based Model Setup

A microstructure file was prepared for input to the RCA and AII methods for this problem. The Euler angles were set to zero in the isotropic domain, and the second Euler angle, $\theta$, was set to 90 in the anisotropic domain. The reference conductivity used for the AII method was given by (3.13). An element size of $200\mu m$ was used which resulted in a total simulation time of 8s. This was substantially higher than the volume integral method, but the refinement of the grid used in this study is sufficient for any microstructure detail needed in ECT scans. Furthermore, this method runs in Matlab and optimizations of the computations, such as parallelization and pre-compilation, have not been performed.

3.2.4.4 Discussion of Results

The results of this scan for all of the simulations are shown in Fig. 3.11. The data clearly shows that the results for all methods are somewhat close. The FEM results are slightly shifted from the VIM results over the patch, which is likely due to poor mesh refinement in the FEM model. The AII method performs the poorest of the low-fidelity models when attempting to predict the impedance directly over the patch. However, it seems to perform better as the conductivity change is lowered, moving closer to the edge of the sample. The
data is only for one test problem and the accuracy of both methods and the differences between them should be more thoroughly analyzed in future work. The plot indicates both methods predict the response relatively well when compared with the widely accepted numerical solutions to the problem. This builds confidence in their use. Furthermore, the simulation times for the methods are significantly lower than the FEM method, and are comparable to the VIM solution.

### 3.2.5 Validation with Experimental Data

The sample shown in Fig. 2.3 was scanned with an eddy current probe and this data was compared with the predictions from the computational routines to validate the simulations. An absolute, 2MHz center frequency Uniwest pencil probe (model# P-.187 2MHz) was used. The data was collected with a Nortec 19eII eddy current scope [132]. The advantage of collecting data with an eddy current scope is that the noise levels are generally lower than in an impedance analyzer, allowing the grain structure to be seen in the data. In fact, in this experiment, the noise in the large single crystal sections had standard deviation on the order of $1/100^{th}$ of the max signal change from one grain to another. The drawback
to using the eddy current scope is that the measurements only produce a voltage which coincides with a change in impedance from one area to another. There was no calibration block with known parameters to directly compare the signals taken from the experiments with the model results due to the calibration blocks saturating the instrument. Because of this, the experiments could not be used for direct quantitative comparison of impedance values from the numerical methods. Still, the experimental data gives a representation of the changes relative to changing orientation from one grain to another, and the contrast in the normalized images can be used to compare to the model results. The frequency of operation of the probe was shown to be in an accurate range for the models in the study in [132]. The experimental data is shown in Fig. 3.12. The approximate dimensions of the coil used in the fem simulation for each of the approximation techniques are shown in Table 3.3.

Both approximations were run using this information and the OIM data, and the results are shown in Figs. 3.13 and 3.14. The scales of both approximation techniques as well as the experimental data have been normalized for direct comparison. Several things can be noted from these results. First, both model approximations seem to be able to predict the experimental results fairly accurately, qualitatively. The AII approximation appears to have predicted the experiments slightly better, as the contrast in Fig. 3.14 is closer to the experimental data (this is very apparent in region 4 of the images).

Table 3.3: Dimensions of the coil used in the validation studies with perpendicular grain boundaries.

<table>
<thead>
<tr>
<th>Probe Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Inner Radius</td>
<td>1mm</td>
</tr>
<tr>
<td>Outer Radius</td>
<td>1.5mm</td>
</tr>
<tr>
<td>Height</td>
<td>3mm</td>
</tr>
<tr>
<td>Number of Turns</td>
<td>100</td>
</tr>
<tr>
<td>Internal Liftoff</td>
<td>0.25mm</td>
</tr>
</tbody>
</table>
The models are somewhat noisy due to the coarseness of the OIM data. The integrations and averages have not quite converged, resulting in numerical noise. This is especially true around the grain boundaries themselves. Still, there are aspects of the solutions that agree with intuition around the boundaries. For instance, Fig. 3.15 shows the tilt of the $c$-axis of each crystal relative to the $z$-axis (i.e. the second Euler angle, $\theta$). This is the primary source of sensitivity in ECT measurements due to isotropy of the conductivity in the basal plane. In moving from region 1 to region 2 in this image, there is no discernable difference in the tilt of the $c$-axis between the two regions. However, the IPF map in Fig. 2.3 shows that these are two distinct grains. Since their $c$-axis tilt is very similar, the regions appear very close in color scale in the experimental data as well as the model results. The slight perturbation along the boundary is due to the fact that the first Euler angle is not identical in the two grains. This essentially tilts the in-plane conductivity ellipses relative to one another, causing a change in the conductivity in the direction normal to the boundary. However, since the coil is circular, the scale of the response in each grain is identical. An oblique coil would be able to see the two grains distinctly due essentially to polarization of the incident field. The other area of note is region 3. The OIM data is slightly noisy in this region, which results in noise in the simulations that is not present in the experiments. Otherwise, the simulations are in satisfactory agreement with the experimental data.
3.2.6 Validation of the Reflection Differential Probe Model

The reflection differential probe model was run on the EBSD data from Ti64-plate1 and also scanned experimentally with a D20 reflection differential coil. A commercially available eddy current scope (Uniwest US-454A) was used to measure the impedance of the probe with the real and imaginary values of impedance represented by voltages in the output. These voltages were collected in a laptop computer through an external analog-to-digital converter. 5 values were sampled at each spatial location in the scan and averaged to reduce the noise in the signal. Furthermore, the low-pass filter on the instrument was
set to $120Hz$ to reduce the high frequency noise during the scan. This led to a noise level of $1/100^{th}$ the signal strength. The data for this experiment is shown in Fig. 3.16. Overall, these images show very good agreement considering the potential for subsurface microstructure features corrupting the scan relative to the model. Furthermore, the sample and probe mounting for these experiments was not highly controlled, leading to the potential for uncertainty in the orientation of the coils relative to the sample. Further quantitative analysis should be done to determine the areas in which poor agreement was achieved, which would give an indication of tilts in the coils relative to the sample surface. For the purpose of uncertainty propagation, this qualitative agreement is enough to proceed.

### 3.2.7 Validation with Ti811

The slices of Ti811 material were also scanned experimentally, and the EBSD data was run through the models to determine agreement in cases where the grain sizes are small and there is significant microtexture in the sample. The coil used for this experiment was a shielded, absolute coil with a $2MHz$ operating frequency. In the model, the reference fields

![Figure 3.16: Experimental data (top) compared with the model results (bottom) for this split-d coil. Many of the areas in the images agree well qualitatively, with subtle differences attributed to in-depth variation.](image)
were calculated using the 2-D axi-symmetric FEM model with a block for a ferromagnetic shield on the outside of the coil. The shielding was assumed to be non-conductive with a relative permeability of 2000. The coil dimensions were estimated by examining the coil behind the clear epoxy that surrounded it, but the height of the coil, core, and shielding were unknown. For this reason and for reasons stated previously in §3.2.5, no 1 to 1 comparison could be made between the experiment and model. Furthermore, it is not expected that the signals agree perfectly anyway due to the fact that subsurface information could potentially have a significant effect on the response at this size scale. The important aspect of this data that should be in agreement is the estimated autocorrelation function from both the model and the experiment.

An example of the experimental data from Slice 3 of the Ti811 is shown in Fig. 3.17. The data has been rotated in post-precessing such that the maximum amplitude response is in the horizontal axis so that non-conductivity change variations will be captured in the vertical axis. Thus, the only data considered for the current analysis was the horizontal channel. One thing that can be noted from the data is the trend from the bottom of each data set to the top. This long range trend was due to temperature fluctuations in the lab for the long running scans in the experiments, but the model results show a trend as well. This could be due to the fact that the microstructure is actually changing slightly from the top to the bottom of the EBSD data set due to different locations on the ingot having different material properties. This has not been validated using analysis of the EBSD data, but it could explain the variation seen here. Essentially, this means that the random field is non-stationary. This effect is more pronounced when viewing the estimated 2-D autocorrelation functions (Fig. 3.18). The light bands in the middle of the data show these long range correlations that are not related to the small scale variation in local microtexture.

To compensate for this effect, a 2nd order polynomial was fit to each column of the
Figure 3.17: Experimental data (top) compared with the model results (bottom) for a shielded absolute coil over the Ti811 material. The data shows a trend from north to south in both the model results as well as the experimental results.

Figure 3.18: Autocorrelation functions estimated from the data sets shown previously.
Figure 3.19: Experimental data (top) compared with the model results (bottom) for a shielded absolute coil over the Ti811 material. The data has been transformed to remove the long range correlations from either temperature or material variation.

Figure 3.20: Autocorrelation functions estimated from the transformed data.
data and removed from the data set by subtraction. This transform has the effect of removing the non-stationarity of the random process. The new data can be seen in Fig. 3.19. The new estimated correlation functions can be seen in Fig. 3.20. These images clearly show that the longer range correlations have been removed. A comparison between the model and experimental autocorrelation functions is shown in Fig. 3.21. In these images, the correlation functions are plotted in the x- and y-directions through the middle of the 2-D correlation function. The model and experiment clearly agree well under the transformations made in the data. These transformations should be analyzed further to assess their validity. Furthermore, they may be able to explain variation in the microstructure from different parts of the sample, which could provide useful information.

![x-Axis Correlation Function Comparison](image_url)

![y-Axis Correlation Function Comparison](image_url)

**Figure 3.21:** Plot of the correlation function in the (Top) x-axis and the (Bottom) y-axis. The solid line shows the experimental autocorrelation functions and the circles show the estimated function from the modeling results.
3.3 Conclusion

In this chapter, two different numerical approximations were developed to predict the results of an eddy current scan above a heterogeneous material with small spatial variations in conductivity. The methods were tested against other models of changing homogeneous material properties, both isotropic and anisotropic, and then against experimental data taken from an eddy current scan of a polycrystalline titanium alloy. The results from verification indicate that assumptions made during the derivation of the approximation methods are mostly valid within a conductivity change range of 50%. The relative changes of impedance in experimental data vs. that of the approximation methods is in relatively good agreement as well, especially in comparison with previous studies. Furthermore, the models were shown to require far less time for computation than the alternative discretization-based techniques. This model provides the forward simulation through which the microstructure instantiations from the sampling methods discussed in Ch. 2 can be propagated and mapped to the NDE response. This completes the framework for uncertainty propagation when material heterogeneity is the primary source of variability in the eddy current signal. The following chapters demonstrate verification and validation for similar forward models, but for an ultrasound inspection.
Chapter 4

Impulse Excitation Defocused Acoustic Microscopy Experiments

In this chapter, the experimental methods in continuous defocus impulse excitation (CDIE) scanning acoustic microscopy are presented. As discussed in 1.1.3.5, scanning acoustic microscopy is a useful technique for quantifying the material properties at very small length scales. TDIE excitation has been used to improve the local quantification of materials properties, but the technique still has limitations. CDIE mode has alleviated these limitations and provided highly accurate, rapid estimation of the elastic properties on a very localized scale. The chapter begins with a brief introduction to scanning acoustic microscopy, and continues with the in depth analysis of the experimental data in CDIE mode. It leads directly into the next chapter, which is a model-based analysis of the signals from the experiment. This chapter lays the foundation for building these models by introducing the experiments and providing the data necessary for verification and validation of the models.

4.1 Introduction

As discussed in §1.1.3.5, scanning acoustic microscopy (SAM) has been used to non-destructively quantify the local material properties in heterogeneous materials for many
decades [70, 71]. The TDIE experiments shown in that section have improved the localized quantitative capability of spherically focused lenses dramatically. However, the previous work has been limited to scans on relatively small samples due to the amount of time required for the scan. Furthermore, the quantitative results were obtained on samples that are isotropic, and anisotropic samples have been analyzed by assuming that the properties average to become isotropic.

This chapter discusses modifications made to the typical TDIE measurements that have improved the contrast in the images and fidelity of the quantitative data analysis. Novel instrumentation and analysis algorithms have been developed that extend the impulse excitation techniques. The new experimental method is called continuous defocus impulse excitation (CDIE) mode SAM. In CDIE mode, measurements are made at many different levels of defocus and the b-scans are analyzed for calculation of the wave velocities. This leads to improvements in the resolution as well as the repeatability of the measurements over the TDIE mode. Advanced analysis algorithms are used to determine the RSW velocity real-time during scan. These algorithms are based on analysis of the b-scans formed by plotting the transducer response as a function of the defocus depth, $z$, and the time, $t$, essentially forming a $V(z, t)$ curve [133]. In this work, further post-processing was performed that enhanced the contrast in the images and improved the quality of velocity estimation. The algorithms were tested on an optically flat E6 glass sample, and the standard deviation estimated over hundreds of spatial locations on the sample was found to be $\pm 2m/s$, which was an improvement over the previous methods. They were also tested on large grained Ti-6Al-4V (Ti64) samples to show the feasibility of using this method for spatial quantification of surface wave velocities in more complex material systems.
4.2 Continuous Defocus Impulse Excitation Method

In CDIE mode operation, the technique discussed in §1.3.5 is extended to collect data at multiple defocus levels. A 50MHz SAM transducer with a spherical focused lens with a 2 in focal spot was used to collect data. The transducer and sample was immersed in water and the transducer was excited with an impulse electrical source. The impulse was generated with a 50MHz center frequency JSR pulser/receiver with 20dB gain, and data was digitized at 1GSPS. A challenge for this setup is that the gain was restricted so that the direct reflected wave signal was not saturated. This necessarily made the RSW signal low, which led to challenges in the analysis of the signals in certain crystallographic orientations. This will be discussed in §4.4.

4.2.1 Continuous Defocus Impulse Excitation Experimental Method

Setup

A diagram of the CDIE setup is shown in Fig. 4.1. The DRW ray is shown down the middle of the transducer and the RSW ray is shown on either side of the DRW ray. In the previous experimental setup, two defocus points were used to calculate the velocity of the RSW in the sample using (1.10). Similar equations can be used to calculate the longitudinal wave velocity by defocusing the probe even further to decouple the SSLW from the DRW [80].

In the CDIE setup, multiple a-scans along the z-axis are collected, as shown on the right of Fig. 4.1. Each a-scan is then stacked on top of one another and a false color associated with the amplitude is applied to an image to build a b-scan. An example of this is shown in Fig. 4.2. The x-axis shows the time delay after the transducer was pulsed, and the y-axis shows the z-location of the probe with 0 simply being the original location close to focus. The probe is moved toward the sample in the negative z-direction to defocus it and move the RSW signal from the DRW signal in the time domain. The DRW and the
RSW can clearly be seen to separate further as the probe is defocused more. If a line is fit to each of the signals, the slope of each line can be used to determine the RSW velocity by using the equation

$$v_R = \frac{2}{\sqrt{m_{DRW}^2 - m_{RSW}^2}} \quad (4.1)$$

In this equation, $m_{DRW}$ and $m_{RSW}$ are the slope of the DRW line and the RSW line respectively. These lines are formed by considering the position along the $z$-axis as the independent variable and the time delay as the dependent variable. In that way, the dimensions of the slopes end up in $s/m$, which agrees with (4.1). Furthermore, if the RSW always separates more as the probe is defocused, then the quantity in the radical is guaranteed to be positive. This is only violated in extremely low amplitude cases when determining the RSW peak is so difficult that the repeatability of the measurement is not acceptable anyway.

During the experiment, fast algorithms are used to compute the RSW velocity as quickly as possible. This process is optimized to provide rapid feedback to the experimenter so that adjustments can be made real time during the experiment. This algorithm
finds the location of the DRW and RSW in the initial defocus level, when both peaks are the strongest. It then uses approximations of the RSW velocity to predict where the peak will move after the probe is defocused by a small increment, and performs another peak fitting routine on the a-scan in this new defocus level. This leads to highly efficient peak finding for the RSW peak, but it can get caught tracking the wrong peak if there are multiple peaks that are similar in magnitude within the wave packets. While this method is prone to error in difficult areas such as between grains, the algorithm runs in less than the time it takes the stages to move to the next location of the X-Y plane. The new experimental setup as a whole takes 0.5s per scan point as opposed to the 5s that the previous experiments required to calculate the RSW velocity at one spatial location [76].
4.2.2 Experimental Results on Benchmark Samples

The new experimental setup and algorithms were used to collect data from the Ti64-plate sample as well as the E6 glass. Both of these samples have been used in the past to assess the quantitative capability of the TDIE experiment, so they provide a good benchmark against which to judge the improvements in CDIE mode. The E6 glass was raster scanned over an $8 \times 9\text{mm}$ portion of the sample. The sample was leveled using time of flight of the direct reflected wave, as in the previous experiments. A c-scan depicting the RSW velocity calculated using the methods discussed above is shown in Fig. 4.3. The histogram of this data showed that this was roughly normal in distribution, and the mean and standard deviation of the calculated velocity in this material is $3042 \pm 2\text{m/s}$, which is very close to the previously obtained value, but has a higher precision. Furthermore, this standard deviation was estimated from multiple different computations by changing the spatial location, rather than simply performing the measurement in the same spatial location multiple times. Thus,
the CDIE method gives a significant improvement in the precision over the previous TDIE experiment as well as a reduction in the amount of time required per scan point.

Data from the Ti64-plate1 sample is shown in Fig. 4.4. This same sample has been scanned using in TDIE mode in [134]. Due to the improved time for scanning, more spatial locations could be measured over the sample, offering considerable improvements in the details in each image. Furthermore, due to the improvements in the repeatability of the measurements, the scans are less noisy than previously obtained data using the TDIE mode. These benchmark experiments clearly show the improvements of the CDIE mode over the TDIE mode of operation.

4.3 Post-Processing for Improved Rayleigh Surface Wave Velocity Calculations

While this method of velocity calculation improved significantly upon the TDIE mode, it is intended to calculate the velocity as quickly as possible so analysis can be done real time by the experimenter. However, there are difficulties with the technique that lead to incorrect calculation of the RSW velocity in certain samples, as can be seen in Fig. 4.5.
Figure 4.5: Calculated velocity map over sample 2B-B-1-2AR-RF-B. This map clearly shows corrupted data on many of the large grains as well as streaking on the top and bottom of the sample.

In this figure, the 2B-B-1-2AR-RF-B sample from Fig. 2.5 was scanned using the CDIE experiment. The image clearly shows corrupted scan data in the lower and upper portion of the image. One of the primary concerns with the on-the-fly calculation is that the algorithm tries to detect peaks based on the peaks found in the previous a-scans. This is extremely efficient and robust for quick computation, but the algorithm can get stuck following the wrong trajectory in the b-scan and thus miss tracking the RSW line entirely. Furthermore, when two separate peaks in the wave packet are close in amplitude, the algorithm tends to switch between the peaks, which was the issue in this image. In post-processing, it is possible to perform a more robust peak detection to enhance the image of RSW velocity.

4.3.1 Post-Processing Algorithm Theory

Digitization error in the signal is a difficulty that must be addressed with post-processing, as is shown in Fig. 4.6. The RSW signal is considerably lower than the DRW signal in the experiments in titanium. For instance, the maximum RSW amplitude found in the raw data from scans in 2B-B-1-2AR-RF-B was 7% the amplitude of the DRW in the same a-scan. However, the gain in the experiment had to be controlled to prevent saturation of the DRW signal. Thus, the signal-to-noise ratio (SNR) for the RSW signal was no higher than 3 in
all scans in titanium. For these experiments, an 8-bit digitizer was used to collect data. This implies that the amplitudes in the RSW signals were captured with no more than 12 discrete values.

A common approach for smoothing signals that have digitization errors is through low pass filtering. Essentially, the square waves in a digitized signal induce high frequency components of the signal in the frequency domain. One approach to handle this type of error is through filtering in the frequency domain using a low-pass sinc filter. In this work, a sinc filter was applied with successively increasing window size until the errors between the filtered signal and the raw signal were below the precision limit of the digitizer. This resulted in much smoother signals to perform peak-fitting with. However, this process is computationally expensive and performing this for all 12.8 million a-scans in the raw data from 2B-B-1-2AR-RF-B would take over 24 hours. Thus, the window size for a large sample of a-scans was determined, and the highest frequency window size was used for
analysis of the entire data set.

To limit the errors in peak finding due to switching between peaks in the low amplitude RSW signal, the wave packet envelope was calculated using the Hilbert transform. This has been successfully applied to ultrasound signals previously [135]. The effect of the transform can be seen in Fig. 4.7. In a sense, this converts the time-domain signal to the amplitude envelope which is plotted on the same time scale as the raw signal. The envelope has less major peaks than the raw signals, and if the RSW and the DRW are separated enough, should result in large single peaks corresponding to each wave packet. This effect can be clearly seen in the figure, where the envelope of the DRW is shown with the first peak marked with an x, and the envelope of the RSW is shown as the second peak marked. This combined with the smoothing algorithm makes it possible to use a nearest neighbor peak fitting routine to find the peaks corresponding to the center of the DRW signal and the RSW signal for each a-scan.
4.3.2 Results with the Post-Processing Algorithm

The post-processing algorithms were first tested on the E6 glass sample to verify that they gave similar results as the experimental methods. The algorithm found the average velocity of the E6 glass to be $3019 \text{m/s}$, which is slightly lower than both the values found by the experiment as well as the values found in literature using the two-point defocus method, but still within an acceptable range. The standard deviation using the post-processing algorithm was $\pm 6.2 \text{m/s}$, which is slightly higher than the experimental method. It is also higher than the values reported in literature for the two-point defocus method, but the average and standard deviation were found using values from over 7000 spatial locations on the E6 glass sample rather than performing the measurement 5 times at the same spatial location. This indicates that the precision is still significantly better than the two-point defocus method and similar to the smart-gate experimental algorithm.

While the post-processing algorithm produces a less precise estimation of the velocity, the value in using the algorithm is that it can find RSW peaks with more robustness.
and consistency than with traditional peak finding algorithms. The algorithm was used to perform peak fitting on the b-scan at each location of sample 2B-B-1-2AR-RF-B. An example of the lines fit to the peaks found in the b-scan can be seen in Fig. 4.8. In this image, the peaks that the algorithm found corresponding to the DRW signal and the RSW signal are given by green x’s. For each a-scan (a horizontal line in this image), the peaks corresponding to each reflection were estimated. The red lines in the image were then fit to these peaks to estimate the slope and intercept of the lines corresponding to the DRW and the RSW. These were used to perform the calculations in (4.1). This was done at every point on sample 2B-B-1-2AR-RF-B and a new map of the RSW velocity was generated. This is shown in Fig. 4.9. The color-scale on this image is the same as that of Fig. 4.5, but what can be seen from this image is that much of the corrupt data from Fig. 4.5 has been removed. The algorithm was able to find the peaks with much higher fidelity by fitting peaks in the Hilbert transform space. Eliminating the multiple peaks that can be associated with the wave packet by analyzing the wave envelope reduced the chances of the algorithm switching between peaks in each RSW signal in the a-scan.

![Calculated Velocity Map](image)

Figure 4.9: Improved map of the microstructure from RSW velocity measurements over the surface of 2B-B-1-2AR-RF-B.
4.4 Analysis of Results

While the spatial map of velocities shown in Fig. 4.9 is clearly improved over that shown in Fig. 4.5, further analysis reveals several key issues with this data which are discussed in this section. These issues were found to be related to the orientation of each grain within the sample. Thus, the velocity map of a portion of the sample from which EBSD data was available is shown next to the associated EBSD data in Fig. 4.10. The EBSD data shown here is color-coded according to the angle of the c-axis tilt, or the second Euler angle, as was done in §3.2.5. Specific grains relevant to the post-analysis of the data are labeled for convenience.

The grains with the most well defined velocities were ones such as Grain #2. This grain had a c-axis tilt of 25°. This finding was consistent across the entire sample, where any grain that had a relatively low c-axis tilt had very little scatter in the velocity calculation from the experiments. Furthermore, the velocity calculations in these grains were all between $3000\, m/s$ and $3200\, m/s$, which was well within the expected range for this material system. This was contrasted with grains such as Grain #3, where the tilt of this grain was 60°. It can be seen from the velocity map that the experimental velocity measurements had significantly more noise in this grain. For a quantitative comparison, the estimated standard deviation of surface wave velocity in Grain #2 was $10.6\, m/s$ whereas the estimated standard deviation in Grain #3 was $107.2\, m/s$. When a grain, e.g. Grain #1, had a c-axis tilt close to 90, the velocity became more predictable, with a standard deviation of $70.4\, m/s$. These findings were repeatable for multiple different grains in this sample. The poorest estimation was found in any grain that had orientation close to 64°, and the RSW calculations were predicted to be higher than the longitudinal wave velocity, which is physically impossible for this material. This indicates that the velocity calculation in this grain was very unreliable. Any of the grains that are white in this image had poor reproducibility in
Figure 4.10: (Top) Image of the second Euler angle mapped over the surface of a portion of sample 2B-B-1-2AR-RF-B, (Middle) new velocity map of the same portion, and (Bottom) image of the maximum fit amplitude over the b-scan. Specific grains are labeled with numbers for discussion.
the velocity calculation, and all of them were oriented between 60°-70°.

The physical reason for this artifact can be seen by looking at the b-scan in the grains. Figure 4.11 shows the b-scan from Grain #2 on top and the b-scan for Grain #4 on bottom. As can be seen in this image, the RSW signal in Grain #2 was very strong and the algorithm had no problem finding the peaks. The b-scan for the grain oriented at 64° had a very low RSW amplitude and thus the algorithm could not consistently find a RSW signal in these b-scans. This led to considerable noise and non-physical values of the RSW velocity. This implies that the RSW amplitude as well as the velocity are related to the tilt of the c-axis, though not in a linear relationship. In fact, the RSW signal disappeared almost entirely in this 60°-70° range only to gain amplitude again above 70°. This behavior is unexplained at this point and requires further investigation with multiple hexagonal material systems to verify. The high fidelity calculation of RSW velocity in regions where the RSW signal was strong enough to find peaks consistently, especially with the improved contrast over that which has been previously accomplished with the impulse excitation method, is promising.

The bottom image in Fig. 4.10 shows the maximum amplitude from the RSW fits on each a-scan in the b-scans. The amplitude is equivalent to that shown in Fig. 4.7 in the plot of the Hilbert transform of the a-scan. The image is saturated with any amplitude above 20 being the same color black to improve the contrast ratio of the lower amplitude grains. The grains with the lowest RSW amplitude clearly correspond to the grains in which RSW velocity was the least reliable. In fact, as can be seen in Fig. 4.7, the noise in the plot of the Hilbert transform was roughly on the order of 0 – 5, which was the same level as the amplitude of Grain #4. Lastly, the amplitude was clearly not unique with respect to the second Euler angle, as can be seen by looking at Grains #1 and #3. Given this fact, a combination of the velocity measurement as well as the amplitude in the grain would be required to uniquely identify the second Euler angle from data collected in this material. More work is required to determine this for other Hexagonal materials.
4.5 Summary and Conclusion

In this chapter, the continuous defocus impulse excitation (CDIE) mode of scanning acoustic microscopy (SAM) was shown. This mode has clear advantages over previous iterations of impulse excitation acoustic microscopy as was demonstrated by analyzing the E6 glass and Ti64-plate benchmark samples. Post-processing algorithms were developed
that improved the measurements further by making peak detection for low-level signals more robust using the Hilbert transform. These algorithms were applied to data from the 2B-B-1-2AR-RF-B sample and improvements in the robustness of peak detection over the raw experimental data were shown. This chapter introduced the experiments and discussed analysis techniques that were used to analyze the data, however estimation of the material constants from the velocity has not been addressed yet. Previous authors have attempted to relate the velocities back to the material properties, as was discussed in §1.1.3.5. Their work was primarily focused on assuming isotropic material properties below each transducer location on the surface of the sample. This assumption was limiting and led to inaccurate estimates of the material properties. Thus, in the following chapter, a model is shown that relates the anisotropic material properties to the estimated surface wave velocity in CDIE SAM experiments. The work shown in this chapter was crucial in demonstrating the data collected during a CDIE SAM experiment. Furthermore, the data from this chapter will be used for verification and validation of the models that are discussed in Ch. 5. The advancements made to the post-processing of the data have led to improved confidence and repeatability in the velocity estimation which is ultimately what is compared to the model results in the following chapter.
Chapter 5

Physics-Based Model for Microstructure Signal in Acoustic Microscopy

In Chapter 3, a rapidly solving model based on physical approximations of eddy current testing over heterogeneous materials was described. This model reduced to a numerical integration over a finite domain above an anisotropic polycrystalline aggregate and thus showed significant run-time advantages over traditional discretization-based methods. In this chapter, a similar model is shown that predicts the estimated velocity in continuous defocus impulse excitation (CDIE) scanning acoustic microscopy (SAM) experiments. The basics of the experimental setup are discussed in Ch. 1, §1.1.3.5. Furthermore, the experimental techniques used to calculate RSW velocity with high fidelity was discussed in Chapter 4. Previous efforts have attempted to relate the estimated velocities to the materials parameters through isotropic assumptions, which led to inaccurate estimates. This chapter shows a numerical model for predicting the estimated velocity in a CDIE experiment and connects the anisotropic material properties and orientations discussed in Ch. 2 to the measurements in the experiment. A novel numerical algorithm for calculating the surface wave velocity in arbitrary directions on arbitrarily oriented crystals is shown in §5.2.
5.1 Theory of the Model

The model assumes that energy propagates in all directions below the transducer in the CDIE experiment and essentially averages the total path length in each grain along the direction of the ray propagating through that grain. To see this, an example focal spot above a single crystal in a polycrystalline aggregate is shown in Fig. 5.1. At each point along the arc of the spot, a surface acoustic wave (SAW) propagates away toward the center of the spot and is detected by the transducer when the wave reaches the opposite side of the arc. The waves propagate at a different velocity based on the anisotropic SAW velocity. Assuming the signal seen at the transducer is a combination of all of these ray paths, the estimated arrival time of the combined surface wave front is the average arrival time of each ray. However, multiple grains are located within the focal spot of the transducer. Thus, the arrival time of each ray will be dependent on the crystallites that the wave travels through. Given the material properties and orientations discussed in Ch. 2, the Euler angles at each point below the transducer are known. This is shown in Fig. 5.2. Thus, for each transducer location, the average ray velocity can be determined by calculating the velocity in each direction for every grain within the focal spot of the transducer.

To obtain an approximation of the response, the velocity curve in each grain is averaged over all 360°, and these are each averaged again to obtain a final estimate of the

Figure 5.1: Problem setup for defocused UT model. The spot is assumed circular and surface waves are assumed to propagate in every direction.
aggregate velocity. This can be written as:

$$\hat{v}_{SW} = \frac{1}{2\pi N} \sum_{i=1}^{N} \int_{0}^{2\pi} v_{SW}(\phi; \psi_{1i}, \theta_{i}, \psi_{2i}) \, d\phi$$  \hspace{1cm} (5.1)$$

where $\hat{v}_{SW}$ is the effective surface wave velocity for that spot, $N$ is the number of data points in that spot, $v_{SW}$ is the directionally dependent surface wave velocity given as a function of the propagation direction on the surface, $\phi$ and the three Euler angles for data point $i$, $[\psi_{1i}, \theta_{i}, \psi_{2i}]$. This is a relatively simplistic approximation of the effective wave velocity, but if the spot lies entirely within a single crystal, the equation reduces to:

$$\hat{v}_{SW} = \frac{1}{2\pi} \int_{0}^{2\pi} v_{SW}(\phi; \psi_{1}, \theta, \psi_{2}) \, d\phi$$  \hspace{1cm} (5.2)$$

which is the averaged wave velocity curve for the grain. This behavior is expected within a single crystal.
5.2 Calculation of Surface Wave Velocities

The governing equation for elasticity was given in §1.1.3.1 by (1.5). In that section, bulk waves propagating as plane waves with wave vector \( k \), were assumed. The plane wave solution was shown and was substituted into the governing equations in (1.5). The resulting equations were reduced to form an eigenvalue problem for calculating the wave velocity known as Christoffel’s equations. For surface waves, the wave vector can not be arbitrarily defined for any given direction due to the fact that the wave amplitude decays into the sample. In other words, the plane wave defined for surface waves is heterogeneous. Furthermore, the stress free boundary condition at the surface of the sample must be satisfied. While authors have solved these equations analytically, the solutions are only for specific symmetry faces or in specific directions. In general, numerical solutions for the eigenvalue problems that arise in surface waves are used for arbitrary orientations and crystal symmetries. This section shows a novel numerical algorithm for computing the phase velocity in arbitrary orientations of crystals and in all propagation directions. The algorithm was tested in multiple different crystal systems and was shown to not only compute the RSW velocity efficiently, but also the supersonic wave velocity when no RSW exists.

5.2.1 Problem Setup

The goal is to find the velocity of a surface wave in arbitrary directions on arbitrary planes of crystals. For the following analysis, it is assumed that the global coordinate system is given by global Cartesian coordinates with axes \([x_1, x_2, x_3]\) corresponding to unit vectors in orthogonal directions in the space so that a vector in that space is expressed as:

\[
x = x_1x_1 + x_2x_2 + x_2x_2
\] (5.3)
The crystal system is assumed to be defined by the elastic moduli $c_{ijkl}$ with $i, j, k, l = 1, 2, 3$ each corresponding to one of the three global coordinates. Next, assume an arbitrary plane with normal vector given by:

$$\mathbf{n} = n_1 \mathbf{x}_1 + n_2 \mathbf{x}_2 + n_3 \mathbf{x}_3$$  \hspace{1cm} (5.4)

This plane represents the crystal surface on which a wave propagates. Any $\mathbf{x}$ for which $\mathbf{n} \cdot \mathbf{x} < 0$ lies within the crystal and any $\mathbf{x}$ for which $\mathbf{n} \cdot \mathbf{x} > 0$ is in the fluid/gas domain above the crystal. Next, the unit vector, $\mathbf{m}$ orthogonal to $\mathbf{n}$ represents the direction of propagation of the wave in the plane. The plane wave solution given by (1.6) is no longer useful as this does not capture the decay of the amplitude as $\mathbf{n} \cdot \mathbf{x} \to -\infty$. The new inhomogeneous plane wave solution is given by:

$$\mathbf{u} = A_0 a \exp \left[-ik(\mathbf{m} \cdot \mathbf{x} + \rho \mathbf{n} \cdot \mathbf{x} - vt)\right]$$  \hspace{1cm} (5.5)

This equation is largely the same as the previous plane wave solution except that the wave is no longer assumed to be uniform. The complex value $\rho$ defines the behavior of the wave in the $\mathbf{n} \cdot \mathbf{x} < 0$ direction. The real component of $\rho$ defines periodic behavior, while the imaginary component defines the decay or growth envelope. Any values of $\rho$ which have positive imaginary component will predict that the wave decays going into the crystal, which is the physically relevant solution.

The second order spatial derivative from (1.5) can be written as:

$$\frac{\partial^2 u_k}{\partial x_j \partial x_l} = -A_0 a_k \rho^2 (m_j m_l + p m_j n_l + p m_i n_j + \rho^2 n_j n_l) \exp \left[-ik(\mathbf{m} \cdot \mathbf{x} + \rho \mathbf{n} \cdot \mathbf{x} - vt)\right]$$  \hspace{1cm} (5.6)
and the second order time derivative as:

\[
\frac{\partial^2 u_i}{\partial t^2} = -A_0 a_i k^2 v^2 \exp\left[ -i k (m \cdot x + p n \cdot x - vt) \right]
\]  

(5.7)

Substituting into the equation of motion and simplifying gives:

\[
[c_{ijkl}(m_jm_l + pm_jn_l + pm_ln_j + p^2n_jn_l) - \rho v^2 \delta_{ik}] a_k = 0
\]  

(5.8)

This equation is essentially the surface wave equivalent of Christoffel’s equation, (1.7), where the wave solution is allowed to decay as a function of depth. In fact, setting \( p \) to zero in this equation and recognizing that \( m \) is equivalent to the wave vector in this case, the uniformity of the wave front is reestablished and this equation reduces to Christoffel’s equation given earlier. As is often done with Christoffel’s equation for bulk waves, the implied sums over \( i \) and \( j \) are cast as matrix coefficients and the equation rewritten as a \( 3 \times 3 \) matrix problem. To accomplish this, the following matrices are defined:

\[
Q = \{Q_{ik}\} = \sum_{j=1}^{3} \sum_{l=1}^{3} [c_{ijkl}m_jm_l] - \rho v^2 \delta_{ik}
\]

\[
R = \{R_{ik}\} = \sum_{j=1}^{3} \sum_{l=1}^{3} c_{ijkl}m_jn_l
\]

(5.9)

\[
P = \{P_{ik}\} = \sum_{j=1}^{3} \sum_{l=1}^{3} c_{ijkl}m_in_j
\]

\[
T = \{T_{ik}\} = \sum_{j=1}^{3} \sum_{l=1}^{3} c_{ijkl}n_jn_l
\]

The \( P \) matrix is redundant. To show this, the transpose of \( P \) is given by:

\[
P^T = \{P_{ik}\}^T = \sum_{j=1}^{3} \sum_{l=1}^{3} c_{kjil}m_in_j
\]

(5.10)
Because of the symmetry of the elastic modulus tensor, $c_{ijkl} = c_{klij}$ and the equation can be rewritten as:

$$P^T = \sum_{j=1}^{3} \sum_{l=1}^{3} c_{ilkj} m_l n_j$$

(5.11)

Since $j$ and $l$ are dummy indices that are summed over, they can be exchanged in this equation to give $P^T = R$, so that (5.8) can be written as:

$$[Q + p(R + R^T) + p^2T] a = 0$$

(5.12)

This is the eigenvalue problem that results from assuming non-uniform plane waves propagating in the $m$ direction, and the eigenvalues $p$ determine the behavior of the wave in the direction perpendicular to the plane along which the wave propagates. This is a quadratic eigenvalue problem with strictly real coefficient matrices. At any arbitrary velocity, it has 6 solutions, but the nature of these solutions can be determined by the range in which the velocity lies. For instance, for any velocity in the interval $0 \leq v < v_L$, these solutions are complex and come in conjugate pairs [64]. This velocity, $v_L$, is called the limiting velocity and is crucial for calculation of RSW velocity. Surface waves which propagate with velocities below this limiting velocity are called subsonic. Traditional RSW’s lie in the subsonic range. Surface waves which propagate at velocities above the limiting velocity are known as supersonic waves. Two such waves will be discussed in later sections of this chapter in hexagonal and cubic crystals. In the analysis of RSW velocities, the values of $p$ for which the imaginary part is positive (i.e. the values that predict decay in the $n \cdot x < 0$ direction) will be labeled as $p_I$ and their corresponding eigenvectors $a_I$ for $I = 1, 2, 3$. The
total unforced solution can then be written as:

\[ u_{tot} = A Ud \]

\[ A = \begin{bmatrix} a_1 & a_2 & a_3 \\ e^{-ik(m \cdot x + p_1 n \cdot x - vt)} & 0 & 0 \\ 0 & e^{-ik(m \cdot x + p_2 n \cdot x - vt)} & 0 \\ 0 & 0 & e^{-ik(m \cdot x + p_3 n \cdot x - vt)} \end{bmatrix} \]  
(5.13)

with \( d \) an arbitrary vector of combination coefficients.

There are two unknowns in (5.12), \( p \) and the phase velocity, \( v \). Boundary conditions must be applied to completely define the problem and find \( p-v \) pairs that satisfy the physics of the problem. In this case, the boundary at \( n \cdot x \) is assumed to be a traction free boundary.

The stress is expressed as:

\[ \sigma_{ij} = \frac{1}{2} c_{ijkl} \left( \frac{\partial u_k}{\partial x_l} + \frac{\partial u_l}{\partial x_k} \right) \]  
(5.14)

Substituting (5.40) into this expression gives:

\[ \sigma_{ij} = -ik A_0 c_{ijkl} a_k (m_l + p n_l) \exp \left[ -ik(m \cdot x + p n \cdot x - vt) \right] \]  
(5.15)

At the plane \( n \cdot x = 0 \), the tractions at this surface are then given by:

\[ \tau_i = -ik A_0 c_{ijkl} a_k (m_l + p n_l) n_j \exp \left[ -ik(m \cdot x - vt) \right] \]  
(5.16)

This can be rearranged into a \( 3 \times 3 \) matrix by use of (5.9), and the resulting expression for surface tractions is given by:

\[ \tau_i = -ik A_0 b_i \exp \left[ -ik(m \cdot x - vt) \right] \]  
(5.17)
where $b_i$ is an element of the vector:

$$b = (R^T + pT) a$$  \hspace{1cm} (5.18)$$

In this equation, $b$ is the surface traction vector and $a$ was defined in (5.13). The total surface traction at the free surface can then be written as:

$$\tau = BUq$$

$$B = \begin{bmatrix} b_1 & b_2 & b_3 \end{bmatrix}$$  \hspace{1cm} (5.19)$$

$$b_I = (R^T + p_I T) a_I$$

For this expression to be zero at all $x$ and for any arbitrary combination coefficients, the matrix $B$ must be singular, which indicates that the condition:

$$\text{det}[B] = 0$$  \hspace{1cm} (5.20)$$

must be met for a $p$-$v$ pair to satisfy the physics of the problem.

Equations (5.12) and (5.20) can be consolidated into one $6 \times 6$ eigenvalue problem called Stroh’s eigenvalue problem. Solving for $p a$ in (5.18) gives:

$$p a = -T^{-1} R^T a + T^{-1} b$$  \hspace{1cm} (5.21)$$

Furthermore, solving for $p T a$ in (5.18) and substituting into (5.12) gives:

$$p b = -Qa - pRa$$  \hspace{1cm} (5.22)$$
Substituting (5.21) into this expression gives:

\[ \mathbf{p} \mathbf{b} = (-\mathbf{Q} + \mathbf{R}\mathbf{T}^{-1}\mathbf{R}^T)\mathbf{a} - \mathbf{R}\mathbf{T}^{-1}\mathbf{b} \]  

(5.23)

Equations (5.21) and (5.23) can be combined to give Stroh’s eigenvalue problem:

\[ \mathbf{N}\mathbf{g} = \mathbf{pg} \]  

(5.24)

where:

\[ \mathbf{g} = \begin{bmatrix} \mathbf{a} \\ \mathbf{b} \end{bmatrix} \]  

(5.25)

and

\[ \mathbf{N} = \begin{bmatrix} -\mathbf{T}^{-1}\mathbf{R}^T & \mathbf{T}^{-1} \\ \mathbf{R}\mathbf{T}^{-1}\mathbf{R}^T - \mathbf{Q} & -\mathbf{R}\mathbf{T}^{-1} \end{bmatrix} \]  

(5.26)

\( \mathbf{N} \) is the Stroh matrix and \( \mathbf{g} \) is the Stroh eigenvector. This is a 6 \times 6 eigenvalue problem where the matrix is asymmetric and real. The eigenvalues and eigenvectors, on the other hand, are guaranteed to be complex for any velocity between zero and the limiting velocity. Once again, in general, this problem has no true analytical solution.

### 5.2.2 Numerical Approach

Rayleigh surface wave velocities can be calculated by finding the zeros of equation (5.20) above. The algorithm starts at a certain velocity, assembles the sub-matrices (5.9), calculates the eigenvectors and eigenvalues from (5.24), selects the eigenvectors that predict a decaying solution (i.e. negative imaginary components in the eigenvalues) and assembles the matrix \( \mathbf{B} \) and calculate its determinant. The velocity is then iteratively changed until the zero is found.
5.2.2.1 Calculation of Limiting Velocity

In [64], a relatively simple method of finding the limiting velocity analytically for certain crystallographic orientations was given. This method is also relatively simple to implement numerically so that the limiting velocity can be found in any arbitrary direction in any crystallographic plane of an arbitrary crystal. The method starts by defining an angle, \( \phi \), used to define rotated unit vectors:

\[
\tilde{m}_i(\phi) = m_i \cos(\phi) + n_i \sin(\phi) \\
\tilde{n}_i(\phi) = -m_i \sin(\phi) + n_i \cos(\phi)
\] (5.27)

The vectors \( \tilde{m} \) and \( \tilde{n} \) are the \( m \) and \( n \) vectors, rotated by an angle \( \phi \) about the vector perpendicular to both of them, or \( m \times n \). This basically rotates the plane and direction of propagation about the vector pointing out of the paper.

This technique is used to determine the behavior of the eigenvalues, \( p \), in the subsonic range. It also leads to a relatively simple method to evaluate the limiting velocity numerically. Define the rotated \( Q \) matrix as:

\[
\tilde{Q}_{ik}(\phi) = (c_{ijkl} - \rho v^2 m_j m_l \delta_{ik}) \tilde{m}_j \tilde{m}_l
\] (5.28)

This can be expanded by substituting (5.27) and written as:

\[
\tilde{Q}_{ik}(\phi) = c_{ijkl} (m_j m_l \cos^2(\phi) + (m_j n_l + m_l n_j) \cos(\phi) \sin(\phi) + n_j n_l \sin^2(\phi)) \\
- \rho v^2 \delta_{ik} \cos^2(\phi)
\] (5.29)

Simplifications were made in this expression by recognizing that \( m_i n_i = m \cdot n = 0 \) and that \( m_i m_i = n_i n_i = 1 \). This expression can then be written in equation form by using...
(5.9). This is written as:

\[ \tilde{Q}(\phi) = D(\phi) - \rho v^2 \cos^2(\phi) I_{3 \times 3} \]  

\[ D(\phi) = Q \cos^2(\phi) + (R + R^T) \cos(\phi) \sin(\phi) + T \sin^2(\phi) \]  \hspace{1cm} (5.30)

The matrix \( D(\phi) \) is known as the acoustical tensor. It is shown in Lemma 1.1 of [64] that this matrix is positive definite for all \( \phi \), and thus has 3 real, positive eigenvalues. It can be seen from (5.30) that the eigenvalues of the matrix \( \tilde{Q} \) are then expressed as:

\[ g_i(\phi) = \lambda_i(\phi) - \rho v^2 \cos^2(\phi) \]  \hspace{1cm} (5.31)

where \( \lambda_i(\phi) \) is the \( i^{th} \) eigenvalue of \( D(\phi) \). Lastly, the definition of the limiting velocity is the smallest velocity for which the matrix \( \tilde{Q}(\phi) \) becomes singular for some angle, \( \phi \), and \( \tilde{Q}(\phi) \) is positive definite at velocities below the limiting velocity but greater than or equal to zero. Thus, the smallest velocity for which \( \tilde{Q}(\phi) \) becomes singular is the point at which the smallest eigenvalue of \( \tilde{Q}(\phi) \) is zero. This problem can be written as:

\[ v_L = \min_{\phi \in \{-90,90\}} \sqrt{\lambda_1(\phi)} \frac{1}{\rho |\cos(\phi)|} \]  \hspace{1cm} (5.32)

This is a bounded 1D optimization that requires only one \( 3 \times 3 \) eigenvalue solution per evaluation point. This problem can be solved by using a standard golden section search or any other found in e.g. [136]. On a laptop PC this computation takes roughly 1.7ms, which for comparison is less than an order of magnitude higher than the computation time required for one addition in Matlab.
5.2.2.2 Subsonic Rayleigh Surface Wave Velocity Calculation

Once the limiting velocity is known, the RSW can be calculated by finding a value, \( v \), such that the \((5.20)\) is satisfied. This is a 1D optimization problem that can be written as:

\[
 v_R = \operatorname{argmin}_{v \in (0, v_L)} \left| \mathbf{B} \right| \left| \mathbf{B}^* \right|
\]

where \( \left| \mathbf{B} \right|^* \) is the complex conjugate of the determinant of \( \mathbf{B} \). In cubic crystals, this equation can be solved with a simple bounded 1D optimization routine such as golden section search. The reason is that the equation has exactly 1 minimum and it is located at the RSW. For instance, consider a nickel alloy material where the stiffness matrix is given by:

\[
\mathbf{C} = \begin{bmatrix}
2.41 & 1.47 & 1.47 & 0 & 0 & 0 \\
1.47 & 2.41 & 1.47 & 0 & 0 & 0 \\
1.47 & 1.47 & 2.41 & 0 & 0 & 0 \\
0 & 0 & 0 & 1.26 & 0 & 0 \\
0 & 0 & 0 & 0 & 1.26 & 0 \\
0 & 0 & 0 & 0 & 0 & 1.26
\end{bmatrix} \times 10^{11}\text{Pa.}
\]

The density is assumed to be \( \rho = 8910 \text{kg/m}^3 \). Assuming a wave traveling in the \( x_1 \)-direction along the crystallographic plane given by the Euler angles \([15 \ 45 \ 8]\) in Bunge’s active notation, the velocity of the wave is calculated by solving the determinant equation. This corresponds to propagation direction and plane normal given by:

\[
\mathbf{m} = \begin{bmatrix} 0.9311 & 0.3514 & 0.0984 \end{bmatrix}^T
\]

\[
\mathbf{n} = \begin{bmatrix} 0.1830 & -0.6830 & 0.7071 \end{bmatrix}^T
\]
Plotting this quantity with respect to the velocity gives the curve shown in Fig. 5.3. The RSW velocity is the one minimum in this figure. Any bounded 1D bounded optimization will converge to this point relatively quickly. Given the calculation of the limiting velocity discussed in the previous section, the bounds are set to zero and the limiting velocity and golden section search is used to find the minimum.

Difficulties arise when trying to use this method on hexagonal crystal systems. For instance, consider the hexagonal Zinc system with stiffness matrix:

\[
C = \begin{bmatrix}
1.68 & 0.782 & 0.710 & 0 & 0 & 0 \\
0.782 & 1.68 & 0.710 & 0 & 0 & 0 \\
0.710 & 0.710 & 1.89 & 0 & 0 & 0 \\
0 & 0 & 0 & 0.546 & 0 & 0 \\
0 & 0 & 0 & 0 & 0.546 & 0 \\
0 & 0 & 0 & 0 & 0 & 0.449 \\
\end{bmatrix} \times 10^{11} \text{Pa.} \quad (5.36)
\]

and density \( \rho = 7180 \text{ kg/m}^3 \). When trying to compute the RSW velocity in all directions on the (010) plane, which corresponds to Euler angles \([0 \ 90 \ 0]\), multiple minima are present. An example curve can be seen in Fig. 5.4. There are several different minima in this curve. The last minimum is the value that corresponds to the RSW velocity in this material. The curve could be sampled many times to find all the minimum values, but this leads to computational inefficiencies that are exacerbated when used within an uncertainty propagation algorithm. Thus, it is desirable to find a new method for locating this minimum.

In [137], a result is given that is capable of locating the RSW velocity without relying on the boundary value determinant. In this paper, it is noted that the surface impedance matrix given by:

\[
Z = -iBA^{-1} \quad (5.37)
\]
is positive definite for $0 \leq v < v_R$. This implies that the eigenvalues of $Z$ are all positive until the velocity reaches $v_R$, at which point one of the eigenvalues becomes zero. Furthermore, as observed in [138], there is only one zero eigenvalue at the Rayleigh wave velocity, and the eigenvalues are monotonically decreasing as a function of $v$ in the range
Thus, if the eigenvalues are sorted in ascending order, the first eigenvalue will have a sign change at \( v = v_R \). Again, this leads to a quick and accurate method for obtaining the velocity when the limiting velocity is already known. The drawback to this is that it takes longer to compute the eigenvalues of \( Z \) than simply using the \( b \) vectors to compute the determinant of \( B \). In fact, using the standard algorithms in Matlab’s \textit{fminbnd} function, the RSW velocity required 7ms to compute by using the boundary value determinant, whereas using the \textit{fzero} algorithm on the smallest eigenvalue of \( Z \) required 20ms. Still, this leads to one forward simulation of 180 degrees of orientation taking 3.6 seconds, which is feasible for use in an inversion algorithm or in an uncertainty propagation algorithm.

This definition requires the inverse of \( A \). The inverse exists only if the three eigenvectors used to build it are linearly independent. This is the case if the eigenvalues of (5.12) are distinct. However, in a general sense, this is not the case and degeneracies exist in the eigenvalue problem. In this case, the generalized eigenvectors must be used to build the matrix \( A \). In the case where two of the eigenvalues are equal (called degenerate case \( D1 \)), the third eigenvector can be computed using the relation for Stroh’s eigenvalue problem in Jordan normal form:

\[
\mathbf{N} \left[ \begin{array}{ccc} g_1 & g_2 & g_3 \end{array} \right] = \left[ \begin{array}{ccc} g_1 & g_2 & g_3 \end{array} \right] \begin{bmatrix} p_1 & 0 & 0 \\ 0 & p_2 & 1 \\ 0 & 0 & p_2 \end{bmatrix}
\]

(5.38)

and solving for \( g_3 \). Similarly, for the case when all eigenvalues are equal, the Jordan form of Stroh’s eigenvalue problem can be written as:

\[
\mathbf{N} \left[ \begin{array}{ccc} g_1 & g_2 & g_3 \end{array} \right] = \left[ \begin{array}{ccc} g_1 & g_2 & g_3 \end{array} \right] \begin{bmatrix} p_1 & 1 & 0 \\ 0 & p_1 & 1 \\ 0 & 0 & p_1 \end{bmatrix}
\]

(5.39)
In this case, both \( g_2 \) and \( g_3 \) are solved as the generalized eigenvectors used in building the matrix \( \mathbf{A} \). The eigenvectors and generalized eigenvectors in these two cases form three independent vectors, and thus the inverse of \( \mathbf{A} \) exists. Furthermore, these eigenvectors result in the same form for the displacement and traction expressions at the surface of the anisotropic half-space.

5.2.3 Supersonic Alternate Mode Velocity Calculation

In many crystals, more than one surface wave mode may exist. This computational routine is intended to solve for elastic constants given observed surface wave speeds in multiple directions on a single crystal. Thus it is important to be able to predict velocities of waves that are not fundamentally Rayleigh-like in nature. Two such waves are discussed in this section corresponding to the symmetries shown above.

5.2.3.1 Pseudo-Surface Waves in Cubic Materials

It has been long known that in certain directions on certain surfaces of cubic crystals, pseudo-surface waves will propagate that will dominate the response over RSW’s [139]. A pseudo-surface wave is one which propagates on the surface for a short distance. Portions of the energy propagate into the sample, leading to decay in the propagation direction. Mathematically, the displacements, \( \mathbf{u} \), can be expressed as:

\[
\mathbf{u} = a e^{-ik(qm \cdot x + pn \cdot x - vt)}
\]  

(5.40)

where \( q = 1 + bi \) is a complex constant that indicates decay in the propagation direction. The decay term, \( b \leq 0 \), is now a new constant that needs to be estimated with the surface wave velocity. Carrying this term through the derivations of Stroh’s eigenvalue problem
gives a new N matrix given by:

\[
N' = \begin{bmatrix}
qT^{-1}RT & T^{-1} \\
-Q' + q^2RT^{-1}R^T & -qRT^{-1}
\end{bmatrix}.
\] (5.41)

where

\[
Q' = \{Q'_{i,k}\} = \left\{ \sum_{i,j=1}^{3} q^2 C_{ijkl} - \rho v^2 \delta_{i,k} \right\}.
\] (5.42)

The eigenvalues and eigenvectors of \(N'\) are used in the same way to predict the zeros of the boundary value determinant. However, with the addition of the complex terms in the matrix, the eigenvalues no longer appear in complex conjugate pairs. Furthermore, the third eigenvalue will actually have \(\text{Im}\{p\} > 0\), which would indicate that energy increases as depth approaches infinity. This increase is offset by the decay in the direction of propagation.

When the algorithm encounters a condition where the RSW velocity is near that of the limiting wave velocity, it searches for supersonic solutions to the boundary value problem that are just above the limiting velocity. This condition can be stated as:

\[
\frac{|v_L - v_R|}{v_L} < \varepsilon_s
\] (5.43)

where \(\varepsilon_s\) is a tolerance value that can be adjusted. These solutions may not be zeros, but they are minima of the boundary value determinant. If they are not zeros, the decay term is added to the eigenvalue problem and the search is continued on both \(b\) and \(v\).

5.2.3.2 Alternate Surface Wave Modes in Non-Cubic Materials

Surface waves propagating on the basal plane of hexagonal crystals do not behave like typical Rayleigh waves. The dominant surface wave mode on this specific crystallographic plane is a supersonic, 2-component wave (according to the classification system from
The velocity of this wave was predicted analytically by [141]. As the cut-plane tilts away from the basal plane, this supersonic mode eventually gives way to the traditional subsonic RSW with all three components. In the configuration in which the free surface normal lies in the Basal plane, the surface waves that propagate in any direction are purely traditional Rayleigh waves and their velocities have been predicted in certain directions by many authors (e.g. [142]). The condition for the existence of this alternate propagation mode in hexagonal crystals is the same as that for the PSW in cubic crystals, and the method of finding the velocity is also the same. The calculations were verified on a hexagonal crystal analyzed previously in [143]. In that work, the authors performed computations for a number of different crystals with the reference plane of the surface wave coincident with a plane of symmetry of the crystal system. Their plots show propagation of surface waves along a surface with the angle between the surface normal and the main axis, or c-axis, of the hexagonal material varying between 0 and 90 degrees. The algorithms from the current work were used to calculate this curve for Cadmium Telluride, and the data is shown in Fig. 5.5. This plot shows the same surface wave velocity as “Figure 11” from [143].

To test this algorithm on more complex material systems, a monoclinic material was analyzed as well. In [144], the authors discussed propagation of surface waves when the plane of symmetry in monoclinic materials was spanned by the normal to the free surface as well as the direction of propagation, \(n\) and \(m\), in the notation used in this paper. They gave an in-depth analysis of the theory of wave propagation in this special case and showed a number of numerical examples. For the purpose of this work, one crystal that they analyzed, Aegirite-Augite, was used to calculate the surface wave velocity and compare with the results shown in this previous work. The curves shown in that work were calculated by keeping \(n\) and \(m\) in the plane of symmetry and rotating them by an angle, \(\alpha\), about the vector normal to them, essentially changing the angle of inclination of the stress free boundary relative to the crystal system. The results of the computation are shown in Fig. 132.
5.6. Once again, the predicted surface wave velocity is the exact same curve as that shown in the paper by Chadwick and Wilson.

5.3 Verification of the Numerical Scheme

The algorithms for calculating surface wave velocities discussed in the previous section were validated using data previously collected by other researchers. This section shows these results as well as verification in the context of inverse algorithms for calculation of the elastic constants.
Figure 5.6: Plot of the surface wave velocity, the limiting velocity, and the fast and slow shear wave velocities for Aegirite-Augite with the surface waves propagating in the plane of symmetry.

5.3.1 Calculation of Surface Wave Velocity on Certain Cut-Planes

A large set of experimental data sets on multiple different cut planes in a cubic nickel crystal was given in [2]. For this work, two specific planes from [2] were picked to determine the agreement with experimental data. In their paper, Li et al. gave the crystallographic planes as Miller indices, so the indices were converted to Euler angles for use in the code. The same material properties as those found in the paper were used to generate the curves ($c_{11} = 235\, GPa$, $c_{12} = 142\, GPa$, $c_{11} = 131\, GPa$, and $\rho = 8720\, kg/m^3$). The velocities generated by the code discussed previously are given in Fig. 5.7. The first plot, Fig 5.7a shows the velocities on the plane (0.28 0.1 1) and the second is for the plane (0 0.25 1). While the tilt in plane is different, the calculated velocities are the same as those shown in the paper, which also matched the experiments that were performed in that work. These figures take an average of $\sim$3s to generate on a laptop computer with an Intel Core™ i7-3630QM processor and 16GB of DDR3 RAM.
Figure 5.7: Polar plots showing the RSW velocity and the PSW velocity on the nickel crystal used in \[2\]. (a) shows the velocity on the \((0\ 0.25\ 1)\) plane and (b) shows the velocity on the \((0.28\ 0.1\ 1)\) plane.

5.3.2 Verification of the Inverse Problem on Cubic Materials

The inverse problem was tested with simulated data to verify convergence and test the sensitivity to the initial guess of the elastic constants. Velocity curves were generated using the elastic constants given in \(\S 5.2.2.2\) on the cubic crystal given there for the plane described by the Euler angles \([15\ 45\ 8]\). Noise was added to the data and the inverse problem was run for multiple initial guesses of elastic constants to determine the convergence of the algorithm with increasingly poor starting points. The velocity profile at this orientation is shown in Fig. 5.8.

In an experiment, the velocity of sound is typically not measured directly. Instead, often the arrival time of a wave is measured at one point on a sample surface and then again on a different point separated by a distance, \(\Delta d\). Thus, the noise in the experiment will likely be on the measured arrival time. In lieu of this, synthetic data was generated by adding independent and identically distributed (IID) noise to the calculated change in
The calculated arrival time, $t_{i}^{calc}$, is determined by calculating the velocity in the $i^{th}$ direction, $v_{i}^{calc}$ and dividing an assumed spacing between measurement points by this velocity. The assumption that the noise in the data is IID and normal is assumed to be valid in the experiment, though possible deviations should be addressed if the assumptions do not appear valid from analysis of the data. This allows the algorithm to take advantage of the typical nonlinear least squares estimates:

$$\arg\min_{c_{ij}} \sum_{m=1}^{n} \left( t_{m}^{synth} - \frac{\Delta d}{v_{m}(c_{ij})} \right)^2$$

subject to $c_{ij}^{lower} \leq c_{ij} \leq c_{ij}^{upper}$

The change in arrival time for the plane used in this section at a separation distance of $0.01m$ is given in Fig. 5.9. The simulated data is plotted on top of the calculated arrival times. In this study, a standard deviation of $3 \times 10^{-8}s$ was used to generate the noise in the data.
This number was chosen based on previous experience with peak fitting for finding the time of arrival of Rayleigh surface waves. The experimental setup in the lab was discussed in Ch. 4. Though no number was given there for the standard deviation of time of arrival, \(3 \times 10^{-8}\) s has been typical for this experiment.

Two aspects of the forward problem make the inverse problem more challenging. Scaling is important factor in any optimization problem. For instance, the results of the simulation are in seconds, but the time of flight of waves in an ultrasound experiment are generally on the order of \(\mu s\). Therefore, the objective function shown in (5.45) is multiplied by a factor of 1e6. Furthermore, elastic constants are generally on the order of 1e11, so the parameters of the inverse function are divided by this factor. This ensures that the scales of the objective function and parameters are similar. Another confounding factor is that the
gradients of the problem with respect to the elastic parameters are not currently calculated analytically. Furthermore, the objective function is itself a minimization problem which is subject to non-negligible noise due to the convergence criteria of the inner optimization problem. Finite difference methods for gradient computation tend to enhance the strength of this noise to the point that derivative calculation with finite difference is very unreliable. A combination of finite difference for the eigenvalue problem and analytical derivatives for the optimization/root finding algorithm can be used to reliably compute the sensitivities, but this is at considerable computational cost. Thus, for this work, a non-gradient based Nelder-Mead optimization algorithm was used to perform the optimization in the inverse problem.

Another important observation is that the inverse problem is generally more well behaved for cubic crystals when the parameter estimates are performed on the alternative but equivalent parameterization:

\[
E = \frac{(c_{11} + 2c_{12})(c_{11} - c_{12})}{c_{11} + c_{12}} \\
\nu = \frac{c_{12}}{c_{11} + c_{12}} \\
\alpha = \frac{2c_{44}}{c_{11} - c_{12}}
\]  

\tag{5.46}

This parameterization is essentially the Young’s modulus, Poisson ratio, and the Zener anisotropy ratio of the material, respectively. The sensitivity of the velocity with respect to these two parameterizations were computed at the known elastic constants and are plotted in Fig. 5.10. It can be seen in these plots that the sensitivity to \(c_{11}\) and \(c_{12}\) are both very similar for all the directions of propagation, which would tend to indicate identifiability issues with these two parameters. This is not an issue with the \(E, \nu,\) and \(\alpha\) parameterization. An alternative parameterization could be to use the eigenvalues of the stiffness matrix as
the parameters for the inverse problem, or:

\[
\begin{align*}
\lambda_1 &= c_{11} - c_{12} \\
\lambda_2 &= c_{11} + 2c_{12} \\
\lambda_3 &= 2c_{44}
\end{align*}
\]  

This parameterization has the added advantage of simply being able to place bounded constraints on the optimization to keep the eigenvalues positive, thus enforcing positive definite stiffness matrices. However, the sensitivities (shown in Fig. 5.11) have similar issues as those from the usual \(c_{ij}\) parameterization between \(\lambda_2\) and \(\lambda_3\). Thus, the \(E, \nu, \) and \(\alpha\) parameterization was used in the inverse problem, and the results of the inverse were converted back to the usual \(c_{ij}\) after an optimal solution was found.

The inverse problem was run with multiple different initial design points. The known values of the elastic constants that generated the data were \([2.41, 1.47, 1.26] \times 10^{11}\) Pa. Initial design points were selected randomly by assuming a uniform distribution in a reasonable range of \(E, \nu\) and \(\alpha\). The table of the initial design points is shown in Tbl. 5.1.
The final converged results are shown in Tbl. 5.2. It is clear that the initial designs all underestimated the values of $c_{ij}$, the most egregious of which are points 4-7. However, the only design points that did not converge to the correct minimum are points 2, 3, and 8. These initial designs were actually relatively close to the true values, with 3 being the closest out of all the initial designs. This strange behavior is likely due to the algorithm used for the optimization not being able to effectively linearize the problem around these design points. This is because of the numerical error in the inner optimization loop from (5.20). However, the values of the objective function are three orders of magnitude lower for points 1, 4-7, and 9-10 than they are for the troubled values, and it is clear that the algorithm can actually be used effectively in the inverse problem provided multiple initial designs are sampled. Strides should be taken to improve the gradient estimation so that a gradient-based approach for the inverse problem can be used rather than the linearized simplex algorithms.
Table 5.1: Starting Points Attempted for Inverse (1e11 Pa)

<table>
<thead>
<tr>
<th>Point Number</th>
<th>$c_{11}$</th>
<th>$c_{12}$</th>
<th>$c_{44}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1.9201</td>
<td>1.0669</td>
<td>0.9903</td>
</tr>
<tr>
<td>2</td>
<td>2.0366</td>
<td>0.9923</td>
<td>1.1760</td>
</tr>
<tr>
<td>3</td>
<td>2.3138</td>
<td>1.3255</td>
<td>1.1245</td>
</tr>
<tr>
<td>4</td>
<td>1.5680</td>
<td>0.7683</td>
<td>1.0896</td>
</tr>
<tr>
<td>5</td>
<td>1.5746</td>
<td>0.7735</td>
<td>1.0384</td>
</tr>
<tr>
<td>6</td>
<td>1.5329</td>
<td>0.7445</td>
<td>0.9812</td>
</tr>
<tr>
<td>7</td>
<td>1.4871</td>
<td>0.7323</td>
<td>0.8413</td>
</tr>
<tr>
<td>8</td>
<td>1.8068</td>
<td>0.8971</td>
<td>1.0227</td>
</tr>
<tr>
<td>9</td>
<td>1.9947</td>
<td>0.9992</td>
<td>1.0723</td>
</tr>
<tr>
<td>10</td>
<td>2.1144</td>
<td>1.1001</td>
<td>1.3895</td>
</tr>
</tbody>
</table>

Table 5.2: Final Values for Each Starting Point (1e11 Pa)

<table>
<thead>
<tr>
<th>Point Number</th>
<th>$c_{11}$</th>
<th>$c_{12}$</th>
<th>$c_{44}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>2.3365</td>
<td>1.3942</td>
<td>1.2683</td>
</tr>
<tr>
<td>2</td>
<td>4.2637</td>
<td>3.3114</td>
<td>1.1234</td>
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<td>3</td>
<td>4.1307</td>
<td>3.1769</td>
<td>1.1174</td>
</tr>
<tr>
<td>4</td>
<td>2.3365</td>
<td>1.3941</td>
<td>1.2683</td>
</tr>
<tr>
<td>5</td>
<td>2.3364</td>
<td>1.3940</td>
<td>1.2683</td>
</tr>
<tr>
<td>6</td>
<td>2.3399</td>
<td>1.3976</td>
<td>1.2681</td>
</tr>
<tr>
<td>7</td>
<td>2.3365</td>
<td>1.3941</td>
<td>1.2683</td>
</tr>
<tr>
<td>8</td>
<td>4.8179</td>
<td>3.8537</td>
<td>1.0951</td>
</tr>
<tr>
<td>9</td>
<td>2.3364</td>
<td>1.3940</td>
<td>1.2683</td>
</tr>
<tr>
<td>10</td>
<td>2.3365</td>
<td>1.3941</td>
<td>1.2683</td>
</tr>
</tbody>
</table>
5.4 Comparison to Experiment

The algorithm was run to compute the approximate CDIE estimated velocities over the Ti64-plate1 sample shown in Fig. 2.3. Equation (5.1) was used to compute the average RSW velocity at each point in a scan given the velocities calculated with the results in the previous section. A 50 MHz focused transducer was used to collect data at multiple defocus levels, and the SAW velocity was calculated using (1.10). The results of the experiment and the simulation are shown in Fig. 5.12. These results agree well in certain areas, but there are regions in which agreement is very poor. The explanation for this is similar to that given in §4.4. A map of the second Euler angle can be seen in Fig. 5.13. From these images it seems that the poorest agreement happens when the tilt of the c-axis falls below the 55-60 degree range. Again, this phenomenon has not been explained at this point, but the agreement in the other areas of the image is promising.

One potential issue with the model could be in the calculation of supersonic surface waves in hexagonal crystals. It has been noted [143] that in certain symmetry planes there is a smooth transition between the propagation of typical RSW and supersonic surface waves. However, in planes that are off tilt from the symmetry plane, this transition is not as smooth and the behavior of the surface wave is extremely sensitive to the tolerance value in the condition given in (5.43). To improve the agreement, it may be necessary to adjust this parameter to more appropriately handle these conditions. Furthermore, this may provide insight into the nature of wave propagation in these materials when the reference plane is not coincident with a plane of symmetry.
Figure 5.12: Comparison between the (a) experimental data and the (b) model results for RSW calculations in the sample.

Figure 5.13: Map of the second Euler angle, indicating the plunge of the c-axis of the hexagonal crystal.

5.5 Summary

In this chapter, a model was shown that calculates the predicted surface wave velocity in a material during a continuous defocus impulse excitation scanning acoustic microscopy experiment. The model was developed to handle arbitrary orientations in the crystallites as well as heterogeneity in the material. To compute the surface wave velocities on the surface of a sample, a new algorithm was shown that calculates both the RSW velocity as well as the pseudo-surface wave velocities in arbitrary directions on arbitrary crystallographic
planes. This algorithm was verified and validated on multiple different crystal symmetries including transversely isotropic, cubic, and monoclinic materials. The model itself was compared with experimental data and found to be within good agreement for regions where the surface wave behavior is well understood. There are still areas in the experiment where wave propagation is not fully understood, and this could provide an avenue for further research that could elucidate the nature of wave propagation in these crystallographic planes.
Chapter 6

Summary, Conclusions, and Future Work

The goal of this work was to create quickly solving approximate nondestructive evaluation models for uncertainty propagation when heterogeneous material properties have a significant impact on NDE signals. Heterogeneous materials can often result in a source of noise that acts as the most confounding factor in an NDE inspection, and a computational method for quantifying this noise before the material system is manufactured would have substantial benefit in a design of materials framework. Furthermore, having a computational tool for determining the sensitivity of an NDE inspection due to various material parameters is crucial for computational design of materials when the inspectability of the material system is to be considered in the design process. However, this uncertainty propagation framework does not currently exist due to a lack of rapidly solving forward models and effective sampling methods for the underlying microstructure. These developments were the focus of this dissertation.

The Karhunen-Loeve (KL) method was explored as a potential method to sample the underlying statistics of the microstructure and generate samples of at least one Euler angle. This method was applied with the assumption that the microtexture in the sample could be described by Poisson statistics, an assumption that has been made in the past for this type of material. This led to very efficient computation of the eigenvalues and eigenvectors of the
random process due to the availability of an analytical eigendecomposition. This eigendecomposition was used to generate expansions of varying fidelity to analyze the convergence of the KL method. It was found that for a large field-of-view and for a relatively small correlation length, a large amount of terms (at least 250) were required for convergence of the estimated correlation length of the random samples. However, using a transformation based on the inverse CDF of the standard normal distribution, the samples from the KL expansion were shown to contain the correct correlation function as well as the correct cumulative distribution function. Thus, a mathematical expression was derived that could be sampled repeatedly, with each sample containing the correct first and second order statistics given orientation data available from a real physical experiment or from a processing model in a digital design of materials framework. The high number of terms needed for convergence should be analyzed further using a reduced field of view and by possibly continuously stitching multiple patches together. This would result in a feasible uncertainty propagation problem if the number of expansion terms needed were significantly reduced. Future work on this algorithm should be directed at this aspect.

Rapidly-solving models were developed and validated for two of the more commonly used eddy current probes in practice. The first model was developed assuming that the average conductivity below the coil could be used as an approximation of the effective conductivity in an analytical calculation of the impedance of the coil. This model was shown to be relatively accurate compared with numerical computations using the finite element method as well as the volume integral method, but it was found to reduce the computational complexity dramatically. The numerical complexity of averaging is $O(n)$, whereas the computational complexity of the discretization-based methods such as FEM is much higher. The second model was based on a derivation of the impedance equations by applying the Born approximation. This model resulted in a 2D integration using the trapezoidal rule, which again is an $O(n)$ operation. These models were verified for accuracy using analytical solutions for simplified problems, effectively determining the range of
conductivity change where the Born approximation holds. Furthermore, the integral-based model was tested for accuracy using experimental data for absolute coils as well as reflection differential probes. The validation showed very promising results when the data and the model results were compared qualitatively. The major improvement with these models comes from the computational efficiency, but results from the verification and validation steps were crucial in building confidence in the approximations that were made to achieve this efficiency. Any improvements or modifications to the models should be vetted with the results of the verification and validation in this dissertation or with similarly rigorous analysis.

A model was also developed for a Rayleigh surface wave acoustic microscopy experiment that is subjected to significant noise from microstructure. The model was based on averaging the effective velocity below the transducer, which again is a very inexpensive procedure. However, the computational complexity of this model was drastically reduced by improving the calculation of surface wave velocity. A new numerical algorithm for calculating the surface wave velocity was developed which reduced the computation time of a full surface wave velocity curve from 3 minutes to 3 seconds. This algorithm combines the traditional brute force numerical optimization with the elegance of the analytical solutions that have been proposed for specific crystallographic orientations to drastically improve the computational efficiency of surface wave velocity computations. Overall, incorporation of this algorithm into the model results in significantly improved computation times over what would be required from a finite element model as a full time-dependent model would be required to calculate the response of the transducer. The algorithm was verified and validated for 3 different crystal systems, and the entire model was compared with an experiment and found to be in good agreement. Thus, rapidly solving forward models for uncertainty propagation were developed for both eddy current and ultrasound inspections. The contributions to the state-of-the-art are discussed in the following section, followed by a section discussing the avenues for further investigation in this research.
6.1 Research Contributions

In the course of this research, several contributions were made to advance the state-of-the-art:

1. A new model for eddy current testing of heterogeneous materials was developed [1, 132, 145]. This model is based on the assumption that the change in the conductivity of each grain is small, leading to efficient and accurate integral approximations to the actual response of the eddy current probe. The model was verified and validated extensively, and the model was also applied to multiple different probe types. The accuracy of the model was verified while also showing the computational efficiency gained by using the model. It was applied to titanium alloys with large grains and the model results matched the experiments very well. It was also tested on materials with significant amounts of microtexture, and the estimated statistics of the experiments matched well with the model results. This model is crucial for application of an uncertainty propagation routine for computational design of materials when grain noise in eddy current testing is a design parameter. Further, it could help in design of new eddy current probes and inspections.

2. A new model for continuous defocus impulse excitation acoustic microscopy scans over materials where the grain size is smaller than the spot size of the transducer was developed [134]. The model is based on calculating the effective velocity of the material in the presence of multiple crystallites, resulting in an efficient tool for estimating CDIE velocity measurements. The model was tested against experimental data and found to be within reasonable agreement, though it was noted that more could be done to improve the model agreement. This model is important for interpretation of the signals seen during these experiments as current state-of-the-art assumes that the material is effectively isotropic below the transducer. A model such
as this could greatly improve the estimate of the material parameters when looking at anisotropic materials.

3. A new numerical technique for prediction of the surface wave velocity on arbitrary crystallographic planes in arbitrary directions was developed [146]. The numerical technique predicts both the Rayleigh surface wave velocity and also automatically detects regions in which the typical RSW could give way to supersonic/pseudo surface wave behavior. This is important for the prediction of the response of the material in SAM experiments as well as experiments where the surface wave slowness curve would be used for estimation of the full elastic tensor of the material. If this prediction is not performed quickly and accurately, the estimates of the material properties could be extremely poor.

4. A new computational method for analyzing the results from CDIE SAM experiments was developed [147]. This computational method greatly increases the fidelity of the data during the experiment and improves the images obtained. Furthermore, it allows for true characterization of the reliability of the technique, and improves the reliability over previous iterations of the technique. This method has been crucial for analysis of the data for the purpose of verification and validation of the models. This method was used to perform an in-depth analysis of the experiments in Ti64 and has led to the identification of a new behavior where the wave amplitudes decay drastically in certain crystallographic planes. This has not been observed previously in these materials.

5. An expansion used to represent material noise in NDE models was improved to include arbitrary first order distributions and the convergence was analyzed for accuracy in the NDE model [123]. Previous implementations of the Karhunen-Loeve transform for propagation of material uncertainty through NDE models relied on very strong assumptions about the first order distribution of the underlying random pro-
cess being Gaussian. Furthermore, the convergence of the expansion was analyzed in terms of the eigenvalues only. In this work, the assumption of Gaussian random processes was alleviated using the inverse CDF transform and the convergence of the expansion was shown in terms of the correlation lengths of the samples from the expansion. This led to a new convergence criteria which was more stringent than those used previously.

6.2 Future Work

While significant progress has been made in the course of this dissertation research, there are several avenues that could be pursued for further investigation. These topics are listed here.

1. The work in this dissertation was focused on propagation of uncertainty from the microstructure through forward models of NDE inspections. This is vitally important for design of new materials when inspectability and its impact on sustainment is of interest in the design optimization process. However, one application of these methods that has not been addressed in any literature to date is characterization of microtexture region statistics with low-frequency electromagnetic techniques. The vast majority of work on microstructure characterization using NDE techniques has been focused on a combination of backscatter, velocity, or attenuation measurements using ultrasound. Ultrasound has an advantage in that the resolution is typically finer than that of eddy current and the signals propagate in bulk, giving the potential for 3-D characterization of the microstructure. As discussed in §1.1.2.3, the work on characterization of microstructure using eddy current methods has been either on large scales (1-10mm) or on very small scales (50-100nm). Microtexture characterization falls between these size scales. Furthermore, the methods developed on large scales were applied to characterization of the statistics of the microstructure, but they did
not include spatially dependent information. The microtexture problem is distinctly spatially dependent, as the goal of characterization would be in estimating the spatial correlation length. To this end, the modeling techniques in this dissertation as well as the expansions discussed in Ch. 2 could be used to develop a rapid characterization technique given spatially registered eddy current data. Similar efforts have been undertaken for characterization of surface roughness in eddy current inspections, as discussed in §2.3. This area of research could be fruitful and provide a much needed rapid characterization tool to the quality control and sustainment communities.

2. Computational tools for design of materials when inspectability is of interest would benefit from the forward uncertainty propagation scheme outlined in this dissertation. However, while the connection between the statistical representation of the microstructure and the NDE response was made theoretically, this connection has not been made in practice. One aspect that needs to be addressed with future work is reducing the number of terms required for convergence in the K-L expansion. As it stands, the number of random variables to propagate through the forward model is not feasible in an uncertainty propagation framework. One method of doing this would be to reduce the range of view and patch multiple instances of the material together to create one large effective material. This creates discontinuities in the sample which would need to be smoothed using kernel smoothing, but it would effectively reduce the number of terms needed by at least an order of magnitude. Even if this is not feasible, using tools such as DREAM.3D or the other kernel-regression techniques discussed in §2.3.1.4, the significant aspects of the microstructure that have the most impact on an NDE inspection can be determined by essentially performing a sensitivity study. With the computational tools developed in this dissertation, this can be done entirely digitally, enabling high throughput digital experimentation to determine the most significant factors for NDE sensitivity. To this end, the algorithms could be implemented directly as a DREAM.3D filter to keep all computations in one
environment. Furthermore, a major breakthrough would be in determining how the information from this type of model should be incorporated in the optimal design of materials process. For instance, microstructure noise becomes a limiting factor in the inspection, and thereby contributes to the sustainment costs of a structure. This could be incorporated in the optimization process by adding it as an objective function or as a constraint if a design-to spec is determined a priori. However, this needs to be coupled with the geometric information. The overall inspectability of a system will be a function of the geometry and the material properties. Research toward determining the inspectability of a structure given its geometry and microstructure would provide a useful tool in design optimization.

3. The behavior of surface waves on certain crystallographic planes of the Ti64 material that was analyzed in this work should be studied in more detail. This could have high impact on any technique that seeks to estimate the elastic tensor from observed surface wave data, such as traditional scanning acoustic microscopy and laser-based techniques. Essentially, as shown in Ch. 4, there are crystallographic planes where the amplitude of the SAM transducer is very low. If there are areas where surface waves do not propagate in these materials or if the wave propagation changes from subsonic to supersonic in a discontinuous way, the estimates of wave velocity in those directions would be completely incorrect and potentially lead to poor estimates of the elastic properties. This issue has not been noted in the literature, to the author’s knowledge. One potential explanation is that the surface waves have a very low out-of-plane component in the specific crystallographic orientation where the wave amplitude is low. This could be verified by using the computational tools discussed in this dissertation, but extending them to calculate the wave displacement components in arbitrary directions on arbitrary planes. Another explanation is that the Ti64 material is not actually a single phase system, and that the $\beta$-phase laths could be causing significant attenuation of the waves in certain crystallographic planes. This
could be verified by running the CDIE experiments on other single-phase hexagonal crystals that have similar elastic constants as the Ti64 material. Lastly, a full numerical simulation solved with FEM, for example, could be used to verify the behavior by modeling both the material and the transducer and calculating the received signals in the transducer, rather than simply aggregating the velocities in the material. All of these things would provide a more thorough understanding of the nature of wave propagation in the material as well as the signals received in the CDIE experiment.

4. The eddy current models developed in Ch. 3 are embarrassingly parallel and could definitely benefit from implementation on the graphics processing unit (GPU). This would require some finesse in handling the memory transfers to and from the card, as well as making sure the operations on each thread in the GPU are themselves efficient. The primary computational burden is the interpolation that must be done in each iteration, as this interpolation typically involves large data sets. If this operation could be performed in parallel, it would greatly enhance the speed of the routine. Furthermore, if each scan point could be run in parallel, there could be upwards of 50% increase in the speed of the algorithm. The ultrasound numerical codes could be parallelized as well, but they would require an eigenvalue solver on each thread. However, the ultrasound solvers would benefit greatly from computation of gradients with respect to the elastic constants. These computations could be made analytically, as was partially shown in this dissertation, but there are steps in the derivation of the gradients that require a new mathematical derivation as the results do not currently exist, to the author’s knowledge. More work on this subject would be beneficial to both the inverse problem as well as the uncertainty propagation problem.
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