A Project Report

submitted by

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under the guidance of **Dr. Jayalal Sarma M.N.**



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THESIS CERTIFICATE

This is to certify that the thesis entitled, submitted by D Akshay Rangasai, to the Indian Institute of

Technology, Madras, for the award of the degree of Master of Technology, is a bona fide record of the

research work carried out by him under my supervision. The contents of this thesis, in full or in parts,

have not been submitted to any other Institute or University for the award of any degree or diploma.

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I want to thank myself for this completely pointless endeavour and my parents for paining me constantly about this. This is in the end, quite depressing.

ABSTRACT

Most materials have two regimes of operation when it comes to the relationship between stress and strain of the material, namely linear and non-linear, while phenomenon and material characterization in the linear regime of operation is pretty well understood, the non-linear regime is not as well understood. This is an intriguing part of the problem as materials that undergo plastic deformation and fatigue loading operate under this non-linear regime, and characterization of these properties help in various manufacturing processes.

This study aims to statistically model and extract relevant parameters to measure non-linearity and its effects on a material by the use of ultrasonic waves, which provide a high strain rate, but very low strain, which is ideal to test the material without changing any of its properties at the current state. We first characterize parameters through harmonics generation and then proceed to non-linear wave mixing, a technique which gives us spatial specificity in our measurements.

The forward model was first built by creating a Finite Difference Time Domain (FDTD) solution to a set of differential equations that represent two dimensional non-linear wave propagation in an isotropic solid medium in a euclidean coordinate system. Wave mixing was simulated using a transverse and a longitudinal wave mixing in collinear path, with a phased array simulated as the transducer. Sensitivity analysis was performed for this solution and this formed the basis of our inverse model that helped predict material parameters.

The inverse model for the forward model was first built using linear regression and the results were compared with a statistical learning technique. We used Gaussian Process modelling to model the predictive model, which we further used to build the inverse model. To evaluate the model, noise was added to the measurements at various Signal to Noise Ratio (SNR) and the error percentage was measured. This model proved to be sufficient for the inverse model. From this, we could effectively estimate model parameters from wave mixing measurements.

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Introduction

The subject of the present work deals with the propagation, non-linear mixing effects of high-frequency shear and longitudinal waves which help us characterize material properties. This section is a brief introduction containing the background, outline and applications of the presented work.

1.1 Background

The stress-strain curve for most ductile materials starts in a linear relationship and moves into a non-linear relationship with a few invariants that define the said relationship. Determining these constants is of great use to characterize the material and predict its behaviour under various conditions and also optimize processes with respect to these constants. While the physical relationship between the linear constants and their estimation has been studied to a great extent, the non-linear constants are more difficult to estimate. Our work aims to estimate these non-linear constants through statistical estimation techniques.

1.1.1 The stress-strain curve

The significant points from fig 1.1.1 are as follows:

- 1. A Proportional Limit
- 2. B Elastic Limit
- 3. y Yield Point
- 4. u Ultimate Tensile Strength
- 5. f Fracture point

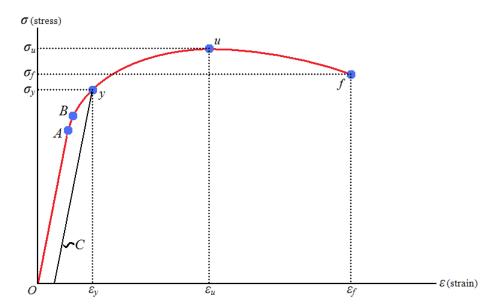


Figure 1.1: The Stress Strain Curve for a Ductile Material

1.1.2 Non-Destructive Testing

There are multiple methods of figuring out the elastic constants of a material, most significant of them being destructive methods, where the material is stressed to its Ultimate Tensile Strength and then, a curve is fit to get the second order constants of the material. This results in the material specimen being destroyed and deemed useless. This method is good for laboratory conditions, but not in a real-world scenario.

To account for this, we employ a method of Non-Destructive testing using ultrasonics. Ultrasonic waves have the characteristic of extremely high strain rates, but the magnitude of strain itself is minimal, and the changes to material properties are thus negligible. These high strain rates result in interesting phenomenon occurring, which in turn helps us estimate parameters of the material, without any physical damage to the specimen.

1.1.3 Wave Propagation and Mixing

One of the main concepts that are used in this study are that of wave propagation in solid media and mixing of waves in linear and non-linear zones. To solve the differential equations involved, we use FDTD simulations. We employed multiple solvers to evaluate the equations and multiple approaches to solve the problem. This will be discussed in detail in upcoming chapters.

1.1.4 Statistical Inversion and Learning

The forward model is inverted by using purely statistical techniques. We employ various techniques from Support Vector Machines (SVM), Gaussian Mixture Models (GMMs), and Gaussian Processes. The mathematics and results will be discussed in detail in the coming chapters.

1.2 Outline of the Report

This report is organized into 6 chapters.

- 1. The current chapter gives a basic introduction to the project and explains very briefly what we hope to achieve and techniques we've employed with a little bit of background information.
- 2. Chapter 2 deals with Literature Review and what we worked on and the subsequent results of the same with reasons as to what method we finally adopted and why with a discussion about the same.
- 3. Chapter 3 describes the construction of the FDTD model for the forward problem and the collinear wave mixing approach that is taken by us and describes the problem and solution in detail.
- 4. Chapter 4 explores the sensitivity analysis of our constructed forward model with respect to various parameters of interest and and exploratory analysis of the inverse model.
- 5. Chapter 5 validates the inverse model and also describes the pitfalls of the model. We make the model more real world friendly and check its performance.
- 6. Chapter 6 summarizes our work and has a section on how this project can be pursued along with suggestions for experimental validation.

1.3 Applications of present work

The present work has wide range of uses from aircraft industry to the shipping industry. A manufacturing specific application of this current technique will be in the estimation of material parameters in forming process and cold working processes where materials undergo plastic deformation.

This technique will help us understand material deformation better and give us a physical insight into what the constants mean and at the same time help improve existing processes and diagnose issues in current processes.

Literature Review

2.1 Introduction

Many papers were reviewed

Description Of Simulations

This chapter presents the description of the simulations used for the current research. The objective of the simulation is to estimate the amplitude and frequency of the resultant generated wave post mixing. This is primarily due to the non-linear behaviour of the material in the mixing zone. The following are the steps followed to achieve this objective.

3.1 2D FDTD Simulation in Cartesian Coordinates

Finite Difference Time Domain (FDTD) method is widely used to solve wave propagation problems. In the present work the FDTD algorithm is implemented in 2D Orthogonal Cartesian Coordinates. [3]

3.2 Governing Equations

The primary governing equations for the 2D FDTD simulator are the non-linear wave propagation equations in the material. Let u(y,t), v(y,t) describe the motion of wave propagation for a longitudinal and transverse wave in a solid. The equations can be derived as such from the standard equation of motion in a solid material.

$$\frac{\partial \sigma_{xy}}{\partial u} = \rho \frac{\partial^2 u}{\partial t^2} \tag{3.1}$$

$$\sigma_{xy} = \sigma y x = \frac{\partial u}{\partial y} (\mu + m \frac{\partial v}{\partial y})$$
(3.2)

$$\frac{\partial \sigma_{yy}}{\partial y} = \rho \frac{\partial^2 v}{\partial t^2} \tag{3.3}$$

In terms of the Lame constants λ and μ , and the third order elastic constants l, m, and n (the Murnaghan coefficients), the stress components can be related to the displacement gradients through + [4]

$$\sigma_{yy} = (\lambda + 2\mu)\frac{\partial v}{\partial u} + (l + 2m)\frac{\partial v^2}{\partial u} + \frac{m}{2}\frac{\partial u^2}{\partial u}$$
(3.4)

Substituting the previous two relations to the standard wave equation, we get

$$\frac{\partial^2 u}{\partial t^2} - c_t^2 \frac{\partial^2 u}{\partial y^2} = \beta_t c_t^2 \frac{\partial}{\partial y} \left(\frac{\partial u}{\partial y} \frac{\partial v}{\partial y} \right) \tag{3.5}$$

$$\frac{\partial^2 v}{\partial t^2} - c_l^2 \frac{\partial^2 v}{\partial y^2} = \beta_l c_l^2 \frac{\partial v}{\partial y} \frac{\partial^2 v}{\partial y^2} + \beta_t c_t^2 \frac{\partial u}{\partial y} \frac{\partial^2 u}{\partial y^2}$$
(3.6)

Where, $c_L = \sqrt{(\lambda + 2\mu)\rho}$, $c_T = \sqrt{\mu\rho}$

$$\beta_L = 3 + \frac{2(l+m)}{\lambda + 2\mu} \tag{3.7}$$

$$\beta_T = \frac{\lambda + 2\mu}{\mu} + \frac{m}{\mu} \tag{3.8}$$

3.2.1 Discretization of the wave-equation

This wave equation, can be discretized as a FDTD grid, which using the staggered method of FDTD solver along with the central differencing technique results in a equation similar to this:

$$\frac{u_k^{n+1} - 2 * u_k^n + u_k^{n-1}}{\Delta t^2} = \frac{c_T^2 \frac{u_{k+1}^n - 2u_k^n + u_{k-1}^n}{\Delta y^2}}{+\beta_T c_T^2 \left(\frac{u_{k+1}^n - 2u_k^n + u_{k-1}^n}{\Delta y^2} \frac{v^n k + 1 - v_{k-1}^n}{2\Delta y} + \frac{v_{k+1}^n - 2v_k^n + v_{k-1}^n}{\Delta y^2} \frac{u^n k + 1 - u_{k-1}^n}{2\Delta y}\right)}{(3.9)}$$

$$u_{k}^{n+1} = 2 * u_{k}^{n} - u_{k}^{n-1} + \Delta t^{2} c_{T}^{2} \left(\frac{u_{k+1}^{n} - 2u_{k}^{n} + u_{k-1}^{n}}{\Delta y^{2}} + \beta_{T} \left(\frac{u^{n}k + 1 - u_{k-1}^{n}}{2\Delta y} \frac{u_{k+1}^{n} - 2u_{k}^{n} + u_{k-1}^{n}}{\Delta y^{2}} + \frac{v_{k+1}^{n} - 2v_{k}^{n} + v_{k-1}^{n}}{\Delta y^{2}} \frac{u^{n}k + 1 - u_{k-1}^{n}}{2\Delta y} \right) \right)$$

$$(3.10)$$

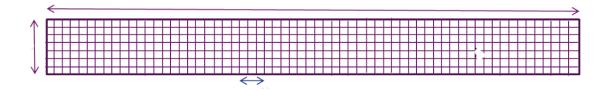


Figure 3.1: Schematic of the solid material as an FDTD grid

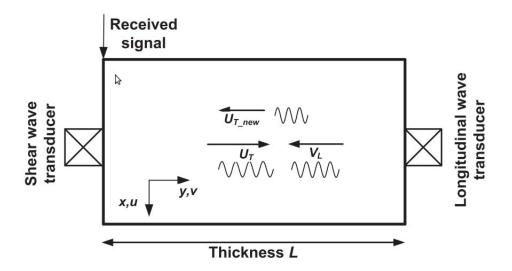


Figure 3.2: Schematic of the setup the FDTD simulation is mimicking

3.2.2 Numerical Considerations

Stability Criteria

A finite difference scheme is stable if the errors made at one time step of the calculation do not cause the errors to increase as the computations are continued. A neutrally stable scheme is one in which errors remain constant as the computations are carried forward. If the errors decay and eventually damp out, the numerical scheme is said to be stable. If, on the contrary, the errors grow with time the numerical scheme is said to be unstable. The stability of numerical schemes can be investigated by performing von Neumann stability analysis. For time-dependent problems, stability guarantees that the numerical method produces a bounded solution whenever the solution of the exact differential equation is bounded. Stability, in general, can be difficult to investigate, especially when the equation under consideration is non-linear.

In the FDTD for sound waves, the main stability criteria is the **Courant** condition. This constraint ensures that the errors in the numerical simulation get damped out to give a fairly accurate estimate of the actual solution.

$$\Delta t \le \frac{1}{C} \frac{1}{\sqrt{\frac{1}{(\Delta x)^2} + \frac{1}{(\Delta y)^2}}} \tag{3.11}$$

$$\Delta x = \Delta y, \Delta t \le \frac{1}{C} \frac{1}{\sqrt{2}} \tag{3.12}$$

Boundary Conditions

The simulation needs a few boundary conditions to be set up, such that there is a solution to the equation that is solved. In this case, we assume the propagation of the wave as equal to the propagation of a wave through any standard wave guide. Since, we are assuming a metal-to-air interface, we have modeled this as a completely reflecting wave guide with no absorption. For other interfaces or absorption in the wave-guide, we could look at a Perfectly Matched Layers (PML) at the boundaries for complete absorption.

The wave guide is modeled as a free waveguide on all ends and the movement is not restricted anywhere. For such a scenario, in the case of plane wave propagation in solids, it is the particle displacement at the boundary which is free, and nothing else. In case the ends are not free to move, the particle displacements at the boundary are trivial. For both these cases, we see reflections, but there is a phase inversion that happens in the latter case. This is not of great importance in this context, but helps

validate simulations.

The conditions for the same implemented in the code is as follows.

$$u_{-1}^n = u_{-2}^n (3.13)$$

$$v_{-1}^n = v_{-2}^n (3.14)$$

Where -1, -2 denote the grid points from the boundaries, with -1 being the last grid point.

Initial condition

Another important component of the boundary layer is basically the initial conditions of the simulation itself. This determines the initial state of the system and the excitement that is given to the system and determines the outcome of the simulation.

For this FDTD simulation, we need to excite the system with one transverse and one longitudinal wave on either end. As the system we have currently taken is collinear, the only criteria is the excitation, and nothing else. The initial wave forms must also be smooth[7] to prevent numerical dispersion and dissipation errors in the simulations [5] [6]

Mesh and Sampling Sampling To further get a more accurate solution, we have to choose a suitable size of mesh for which the solution is acceptable and at the same time not too time consuming. The solution must be approximately right, without too much noise in the data. The solution is also sampled at a rate which is extremely high to prevent aliasing of the data. We sample at a rate that is proportional to the meshing, a criteria we get from the courant condition.

3.3 Simulation

3.3.1 Sources

There are two main sources in the simulations, one is a longitudinal wave with a specific frequency and another is a transverse wave coming in from the opposite direction. These are limited in time, and thus are pulses of waves. The pulses are raised cosine pulses with a pulse width of 10.

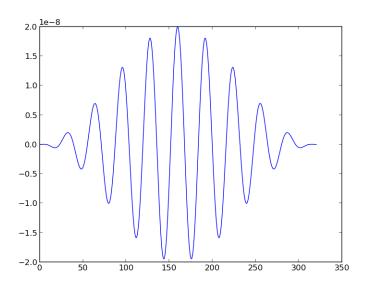


Figure 3.3: Longitudinal Pulse Excited at Source

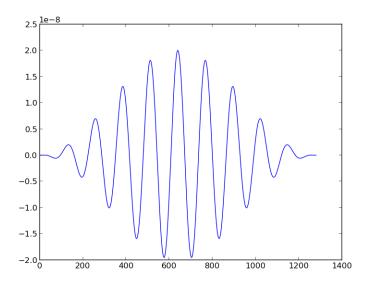


Figure 3.4: Transverse Pulse Excited at Source

3.3.2 Simulation Parameters

Property	Value
Δt	3.125×10^{-09} s
Δx	3.94×10^{-05} m
Sampling Frequency	$3.2 \times 10^8 \text{Hz}$

Table 3.1: General Numerical Properties of Simulation

Property	Longitudinal	Transverse
Number of pulses	10	10
Pulse Frequency	10MHz	2.5MHz
Pulse Amplitude	$2 \times 10^{-8} \text{m}$	$2 \times 10^{-8} \text{m}$
Pulse Duration	10^{-6} s	4×10^{-6} s
Pulse Velocity	$6299.5ms^{-1}$	$3100ms^{-1}$

Table 3.2: Pulse Properties

3.4 Simulation Results

3.4.1 Snapshots of Simulation

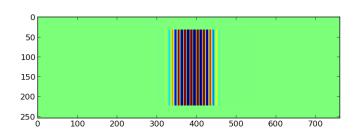


Figure 3.5: Snapshot of the Longitudinal Wave

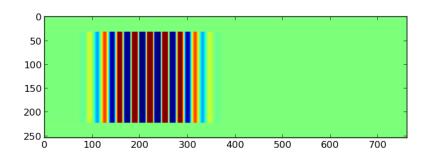


Figure 3.6: Snapshot of the Transverse Wave

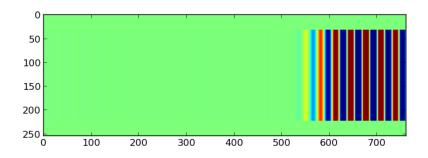


Figure 3.7: Snapshot of the Transverse Wave

3.4.2 Validation of Simulation

The solution from the simulation was obtained from an Amplitude Scan at both the sources. The wave forms and the fourier transforms of the waves after the A-scans were consistent with what is expected from an FDTD simulation. There was minimal dispersion or dissiparion error and thus the simulation parameters were satisfactory. To check if the FDTD simulation is accurate enough to be used for more complex cases with the same solver and engine, we compared the results of our FDTD simulation with the one by Liu Et. al [8] which solved this case by the use of an ODE solver.

From the comparisons of the two solutions, we compared the scale of amplitude as well as the frequency of the generated wave. Due to our input being markedly different from that of the reference paper, the deviations in wave shape are acceptable. All the other criteria match with that of the reference paper. The comparisons and Validation plots are given below.

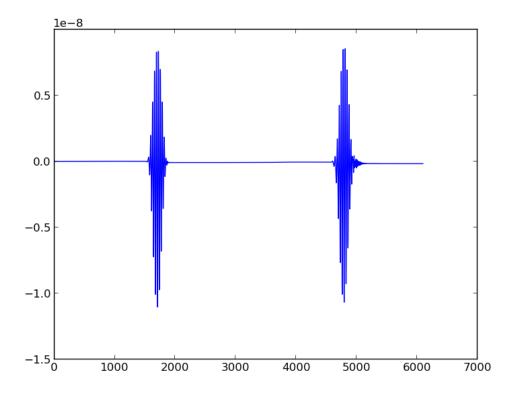


Figure 3.8: A-scan of the longitudinal wave

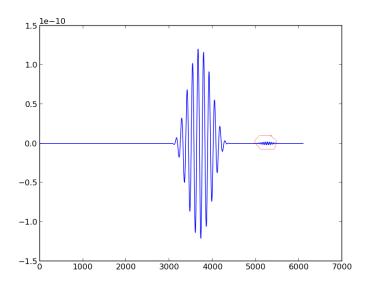


Figure 3.9: A-scan of the transverse wave

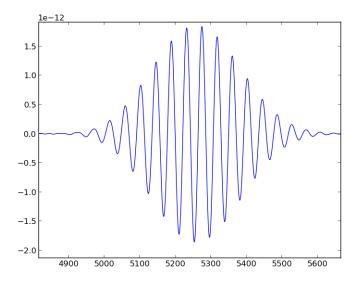


Figure 3.10: Zoomed A-scan of transverse wave

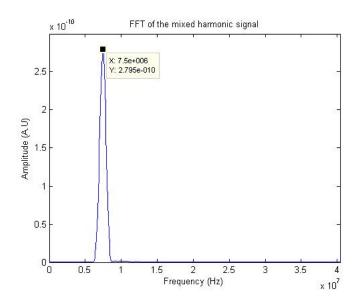


Figure 3.11: Fourier Transform of the New Wave Generated

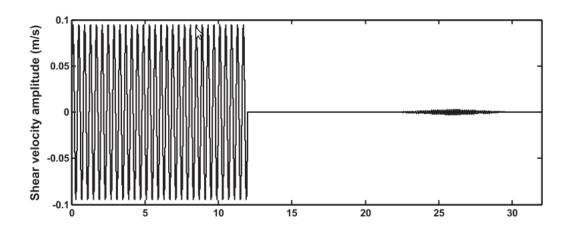


Figure 3.12: Simulation Results From DE solver[8]

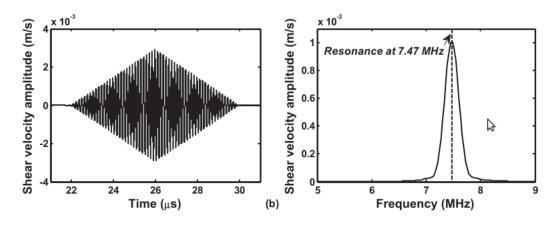


Figure 3.13: Zoomed solution and Fourier Transform of the solution from DE solver [8]

Sensitivity Analysis

Inverse Model

Summary and Future Work

APPENDIX A

Appendix

A.1 Solver Code

```
1 import numpy as np
2 import scipy as sp
3 import defaults as df
4 from math import sin, pi, cos
5 from matplotlib.pyplot import imshow, plot, show, draw, pause, clim,
      \hookrightarrow
           figure
6 import sys
7 from constants import *
8 transverse = []
9 \quad longi = []
10
   _{transverse} = 0
11
   longi = 0
12
13 #from matplotlib import figure
  class Solver:
14
15
        _{transverse} = 0
        longi = 0
16
17
18
        Simulation = None
19
        Location = None
20
        Width = None
        #Create a Movie Variable to calculate number of movies and plots
21
           \hookrightarrow , to bring them up when necessary. add arguments to put it
           → in grid, instead of what's happening here. This is
           \hookrightarrow hardcoded waste.
```

```
def putMovie(self, pauseTime):
22
            data = np.reshape(self.Simulation.Grid[:,:,0,1], (self.
23
                → Simulation . ElementSpan [0] , self . Simulation . ElementSpan
               \hookrightarrow [1]))
            figure ("Wave_Movie_Transverse")
24
25
            imshow (data)
            clim([-1e-8,1e-8])
26
27
            draw()
28
            pause ( pauseTime )
29
30
            data = np.reshape(self.Simulation.Grid[:,:,1,1], (self.
               → Simulation . ElementSpan [0], self . Simulation . ElementSpan
               \hookrightarrow [1]))
                                #
            figure ("Wave_Movie_Longitudinal")
31
            imshow (data)
32
33
            clim([-1e-8,1e-8])
            draw()
34
            pause(pauseTime)
35
36
37
38
39
        def putSource (self, i, frequency, index, waveType = 0):
40
            #Multiply with gaussian to remove edge effects.
41
            #Adding default Source
42
43
            #waveType 0 - Transverse. 1 - Longitudinal
44
45
46
            X_S = round(self.Location[0])
47
            Y_S = slice (round (self.Simulation.ElementSpan [0]/2) - round (

→ self. Width [1]/2), round (self. Simulation. ElementSpan

                \hookrightarrow [0]/2) + round(self.Width[1]/2))
```

48

```
49
            #Raised Cosine Pulse.
50
             self. Simulation. Grid [Y_S, index, waveType, 2] = (1-\cos(2*pi*)
51

    frequency * i * self . Simulation . Dt/ self . Simulation . Pulses ) )
                → *cos(2*pi*frequency*i*self.Simulation.Dt)*1e-8
52
             return (1-\cos(2*pi*frequency*i*self. Simulation. Dt/self.
                → Simulation. Pulses))*cos(2*pi*frequency*i*self.
                \hookrightarrow Simulation. Dt) *1e-8
53
54
            #Sine Pulse. Trying to recreate the paper
            \#self. Simulation. Grid[Y_S, index, waveType, 2] = sin(2*pi*
55
                \hookrightarrow frequency * i * self. Simulation. Dt) * 1e-8
56
            \#print\ self.\ Simulation.\ Grid[X_S],\ round(self.\ Simulation.
57
                \hookrightarrow ElementSpan [1]/2) - round(self. Width [0]/2) + 1,0,2]
58
59
        #Line Sources only, currently. Multiple Sources must be
           → accounted for, Must think of a matrix solution. So much
           → fight for something that might not even work. Pain.
60
        def setSource(self, Location = None, Width = None, Theta = None)
           \hookrightarrow :
61
62
             if Location is None:
                 self. Location = [df.LOCATION*self.Simulation.Dimensions
63
                    \hookrightarrow [0]/self.Simulation.Dx]
             else:
64
65
                 self. Location.append(Location*self.Simulation.Dimensions
                    → [0]/self.Simulation.Dx)
66
             if Width is None:
67
                 self. Width = [(df.WIDTH/self.Simulation.Dx)*D for D in
68
                    → self. Simulation. Dimensions]
69
             else:
```

```
70
                  self. Width.append((Width/self.Simulation.Dx)*D for D in

    self. Simulation. Dimensions)
71
72
             if Theta is None:
                  self.Location = [df.THETA]
73
74
             else:
                  self. Location.append(Theta)
75
76
77
78
79
        def Solve (self):
80
             #First Equation We'll be solving will be the standard wave
                \hookrightarrow equation.
             self.setSource()
81
82
             #Setting the Source first. Now, let's solve the DE like a
                \hookrightarrow boss
             #
83
             X = \text{slice}(0, \text{self}. \text{Simulation}. \text{ElementSpan}[0] - 2)
84
             X = slice(1, self. Simulation. ElementSpan[0]-1)
85
86
             X_{-} = slice(2, self. Simulation. ElementSpan[0])
87
             _{Y} = slice(0, self. Simulation. ElementSpan[1]-2)
88
89
             Y = slice(1, self.Simulation.ElementSpan[1]-1)
             Y_{-} = slice(2, self.Simulation.ElementSpan[1])
90
91
             \#\_X indicates previous X coordinate and X\_ indicts the one
92
                \hookrightarrow after
             r_var = round(self.Simulation.Time/self.Simulation.Dt)
93
94
             \#print "Total Iterations are", r_{-}var
95
             c_t2 = pow(self.Simulation.MaterialProperties.WaveVelocityT
                \hookrightarrow ,2)
             c_12 = pow(self.Simulation.MaterialProperties.WaveVelocityL
96
                \hookrightarrow ,2)
```

```
97
98
             \# sdata = sp.zeros((r_var, 1))
99
               for i in range(1,int(r_var)):
100
                    dv_y = (self.Simulation.Grid[X, Y_-, 1, 1] - self.Simulation
                       \hookrightarrow . Grid [X, Y, 1, 1]) /(2 * self . Simulation . Dx)
101
                    d2v_y = (self.Simulation.Grid[X,Y_1,1] - 2*self.
                       \hookrightarrow Simulation. Grid [X, Y, 1, 1] + self. Simulation. Grid [X,
                       \hookrightarrow Y, 1, 1]) /pow(self. Simulation. Dx, 2)
102
                    du_y = (self.Simulation.Grid[X, Y_-, 0, 1] - self.Simulation
                       \hookrightarrow . Grid [X, Y, 0, 1]) /(2* self . Simulation . Dx)
103
                    d2u_y = (self.Simulation.Grid[X, Y_-, 0, 1] - 2*self.
                       \rightarrow Simulation. Grid [X, Y, 0, 1] + self. Simulation. Grid [X,
                       \hookrightarrow Y,0,1])/pow(self.Simulation.Dx,2)
104
105
                   #Solving for Displacements in the X directio
106
                    self.Simulation.Grid[X,Y,0,2] = 2*self.Simulation.Grid[X]
107
                       \rightarrow ,Y,0,1] - self. Simulation. Grid [X,Y,0,0] + pow(self.
                       \hookrightarrow Simulation. Dt,2)*(c_t2*d2u_y + self. Simulation.
                       → MaterialProperties.BetaT*c_t2*(dv_y*d2u_y + du_y*
                       \hookrightarrow d2v_y))
108
                    self. Simulation. Grid [X, Y, 1, 2] = 2 * self. Simulation. Grid [X, Y, 1, 2] = 2 * self.
                       \hookrightarrow ,Y,1,1] - self. Simulation. Grid [X,Y,1,0] + pow(self.
                       \hookrightarrow Simulation. Dt,2)*(c_12*d2v_y + self. Simulation.
                       → MaterialProperties.BetaL*c_12*dv_y*d2v_y + self.
                       → Simulation. Material Properties. BetaT*c_t2*du_y*d2u_y
                       \hookrightarrow )
109
110
111
                    self. Simulation. SourceSignal[i,0] = sum(self. Simulation.
112
                       \hookrightarrow Grid [:, -2,0,2]) / self. Simulation. Grid. shape [1]
```

113

```
114
115
                   self. Simulation. SData[i,0] = sum(self. Simulation. Grid
                      \hookrightarrow [:,1,1,2]) / self. Simulation. Grid. shape [1]
116
117
                   \#self.Simulation.SData[i,0] = sum(self.Simulation.Grid)
                      \hookrightarrow [:,1,0,2])/self. Simulation. Grid. shape[1]
118
119
                   #print self. Simulation. Grid[15,15,0,2]
120
121
                   #Boundary COnditions. Making the ends soft reflections.
                      → Let's see how that works out.
122
                   , , ,
123
                   if self. Simulation. Mixing is not True:
124
                        self. Simulation. Grid[-1,:,0,2] = self. Simulation.
125
                           \hookrightarrow Grid[-2,:,0,2]
126
                   else:
127
                         self. Simulation. Grid[:, 0, 1, 2] = self. Simulation.
                      \hookrightarrow Grid[:,1,1,2]
128
                        self. Simulation. Grid[:,0,0,2] = self. Simulation.
                      \hookrightarrow Grid[:,1,0,2]
129
                        self. Simulation. Grid[:, -1, 0, 2] = self. Simulation.
                           \hookrightarrow Grid[:, -2,0,2]
                         self. Simulation. Grid[:, -2, 1, 2] = self. Simulation.
130
                      \hookrightarrow Grid[:, -1,1,2]
131
132
                    #Updates go Here
133
134
135
                   if(i <= round(self.Simulation.Pulses*(1.0/(self.</pre>
                      → Simulation. WaveProperties. Frequency))/self.
                      → Simulation.Dt)):
136
                        transverse.append(self.putSource(i, self.Simulation.
```

```
→ WaveProperties. Frequency, 0, TRANSVERSE))
137
                   else:
                        if ( self . _transverse == 0):
138
139
                             plot(transverse)
140
                             show()
141
                             self._transverse = 1
142
                        self. Simulation. Grid [:,1,0,2] = self. Simulation. Grid
                           \hookrightarrow [:,0,0,2]
143
                        self. Simulation. Grid [:, -2, 0, 2] = self. Simulation.
                           \hookrightarrow Grid [:, -1,0,2]
                        \#self.Simulation.Grid[:,0,1,2] = self.Simulation.
144
                           \hookrightarrow Grid[:,1,1,2]
145
146
147
                   if self. Simulation. Mixing == True:
148
                        if (i <= round (self. Simulation. Pulses *(1.0/(0.997*4*
149

→ self. Simulation. WaveProperties. Frequency))/self
                           → . Simulation.Dt)):
150
                             longi.append(self.putSource(i,0.997*4* self.
                                \hookrightarrow Simulation. WaveProperties. Frequency, -1,

→ LONGITUDINAL ) )

151
                        else:
                             if(self.longi == 0):
152
                                  plot (longi)
153
154
                                  show()
155
                                  self._longi = 1
                             self. Simulation. Grid [:, -1, 1, 2] = self. Simulation
156
                                \hookrightarrow . Grid [:, -2, 1, 2]
157
                             self.Simulation.Grid[:,0,1,2] = self.Simulation.
                                \hookrightarrow Grid [:,1,1,2]
                             \#self.Simulation.Grid[:,-1,0,2] = self.
158
                                \hookrightarrow Simulation. Grid[:, -2,0,2]
```

```
159
160
                   self. Simulation. Grid [:,:,1,0] = self. Simulation. Grid
                       \hookrightarrow [:,:,1,1]
161
                   self. Simulation. Grid [:,:,1,1] = self. Simulation. Grid
                       \hookrightarrow [:,:,1,2]
162
163
                   self. Simulation. Grid [:,:,0,0] = self. Simulation. Grid
                       \hookrightarrow [:,:,0,1]
164
                   self.Simulation.Grid[:,:,0,1] = self.Simulation.Grid
                       \hookrightarrow [:,:,0,2]
                    print i
165 #
                   if i\%round (0.05*r_var) == 0:
166
167
                        #print i
                        if self. Simulation. ViewMovie == True:
168
169
                             self.putMovie(0.01)
170
                        sys.stdout.write('=='*int(round(i/round(0.1*r_var)))
                            \hookrightarrow )
171
                        #p. plot. show()
172
173
              #print self. Simulation. Material Properties. BetaL, self.
                  \hookrightarrow Simulation. Material Properties. BetaT, self. Simulation.
                  \hookrightarrow Material Properties. Wave Velocity L, self. Simulation. Dt
174
175
176
              figure ("Source Signal")
177
              plot (self. Simulation. Source Signal)
178
              pause (0.01)
179
180
              figure ("Non Linear Signal")
181
              plot(self.Simulation.SData)
182
              show()
          , , ,
183
184
```

```
185 #
              np. save("TotalSignal", self. Simulation. SourceSignal)
186 #
              np. save ("LinSignal", sdata)
        def __init__(self, Simulation = None):
187
             if Simulation is None:
188
                 raise ValueError ("Simulation _ Cannot _ be _ None . _ Please _
189
                     → Initialize _a _New _ Simulation _to _proceed")
190
             else:
                  self. Simulation = Simulation
191
192
                 self.Solve()
193
    if __name__ == "__main__":
194
195
         raise Exception ("Cannot_run_file_as_a_standalone_file._Please_

→ run _through _proper _initialized _channels")
```

A.2 Problem Formulation Code

```
1 from data import waveProperties, materialProperties
2 import numpy as np
3 import scipy as sp
4 import matplotlib as mp
5 import defaults as df
6 import sys
7 from solver import Solver as sl
8 import scipy.io as sio
9 from matplotlib.pyplot import plot, figure
10
11
12 #
     13 #Rules of code: Class elements always begin with a capital letter.
     → Defaults are always allcaps. Arguments to functions to mimic
     \hookrightarrow class members.
14 #
     \hookrightarrow
15
16
  class simulation:
17
      def save(self, filename):
18
19
          sio.savemat(filename, {"SData": self.SData, "SourceSignal":

    self.SourceSignal })
20
21
      def setMixing(self, val):
22
          self. Mixing = val
23
      def setStep(self, Dx):
24
```

```
#Courant Condition check
25
             return (Dx/self. Material Properties. Wave Velocity L)/2
26
27
        def setMesh(self):
28
29
30
             if self.Mesh == 0:
                 return (float) (self. WaveProperties. WaveLength/8.0)
31
             elif self.Mesh == 1:
32
33
                 return (float)(self. WaveProperties. WaveLength/12.0)
34
             elif self. Mesh == 2:
                 return (float)(self. WaveProperties. WaveLength/64.0)
35
             elif self. Mesh == 3:
36
37
                 return (float) (self. WaveProperties. WaveLength/128.0)
38
39
        #Time is of type float; Dimensions is a list of floats.
40
41
        def setParam(self, paramName, value):
42
43
44
             if paramName == '1':
45
                 self. Material Properties. 1 = value
46
                 \#self.Material Properties.BetaT = (self.
                    \hookrightarrow Material Properties. Lambda + 2*self.
                    → Material Properties. Mu)/self. Material Properties. Mu +
                    \hookrightarrow self. Material Properties.m/self. Material Properties.
                    \hookrightarrow Mu
47
                 self. Material Properties . refresh Params ()
             if paramName == 'm':
48
49
                 self. Material Properties.m = value
50
                 self. Material Properties.refresh Params()
51
             if paramName == 'BetaT':
52
53
                 self. Material Properties. BetaT = value
```

```
54
55
        def getParam(self, paramName):
56
            if paramName == '1':
57
                return self. Material Properties. 1
58
59
            if paramName == 'm':
60
                return self. Material Properties.m
            if paramName == 'BetaT':
61
62
                return self. Material Properties. BetaT
63
            return 0
64
65
66
        def __init__(self, MaterialProperties = None, WaveProperties =
67
           → None, Reflections = None, Dimensions = None, WaveGuide =
           \hookrightarrow None, Mesh = None, Pulses = None):
68
            if Material Properties is None:
69
70
                self.MaterialProperties = materialProperties()
71
            else:
72
                self. Material Properties = Material Properties
73
74
            if WaveProperties is None:
                self.WaveProperties = waveProperties()
75
76
            else:
77
                self. WaveProperties = WaveProperties
78
            if Reflections is None:
79
                self.Reflections = df.REFLECTIONS
80
81
            else:
                self. Reflections = Reflections
82
83
            if Dimensions is None:
84
```

```
85
                 self. Dimensions = df. DIMENSIONS
             else:
86
                 self. Dimensions = Dimensions
87
88
             if WaveGuide is None:
89
                 self. WaveGuide = df. WAVEGUIDE
90
             else:
91
                 self. WaveGuide = WaveGuide
92
93
94
             if Mesh is None:
95
                 self.Mesh = df.MESH
96
             else:
97
                 self.Mesh = Mesh
98
99
             if Pulses is None:
                 self.Pulses = df.PULSES
100
101
             else:
102
                 self.Pulses = Pulses
103
104
             self. Time = 2*self. Reflections*self. Dimensions[1]/self.
                → MaterialProperties. WaveVelocityL
105
106
             #1D, 2D or 3D
107
             self.DimensionCount = len(self.Dimensions)
108 ##
               self. WaveProperties. WaveVelocity = self. MaterialProperties
       → . WaveVelocity
109
             self. WaveProperties. WaveLength = (float) (self.
                → Material Properties. Wave Velocity L/self. Wave Properties.
                → Frequency)
110
             self. Mixing = False
             self.Dx = self.setMesh()
111
             self.Dt = self.setStep(self.Dx)
112
113
```

```
114
            #print self.Dx
115
            ##List of elementsb
116
             self.ElementSpan = [round(X/self.Dx) for X in self.
                → Dimensions ]
117
118
            #Append Dimensions
             self. ElementSpan.append(3)
119
120
            #Append Times
121
             self. ElementSpan.append(3)
122
123
             self.Grid = sp.zeros(tuple(self.ElementSpan), float)
             self.NLGrid = sp.zeros(tuple(self.ElementSpan), float)
124
125
             self.SourceSignal = sp.zeros((round(self.Time/self.Dt),1))
             self. SData = sp. zeros ((round(self.Time/self.Dt),1))
126
             self. ViewMovie = False
127
             self.viewPlot = True
128
129
130
    def __init__():
131
        args = sys.argv
132
        args = [arg.replace('--','') for arg in args]
133
        names = []
134
        sim = simulation()
135
        print sim.Dt, sim.Dx, sim.MaterialProperties.WaveVelocityL, sim.
           → WaveProperties. WaveLength
136
        if 'mixing' in args:
137
            sim.setMixing(True)
138
        if 'movie' in args:
             sim. ViewMovie = True
139
140
        solution = sl(sim)
141
        if 'noplot' in args:
142
143
            pass
144
        else:
```

```
145
             figure (5)
             plot (sim. SData)
146
147
        if 'save' in args:
148
149
             try:
                 ind = args.index('savenames')
150
                 names.append(args[ind+1])
151
                 names.append(args[ind+2])
152
153
             except:
                 print "Using Default File names to save data"
154
                 names.append("TotalSignal")
155
                 names.append("NLinSignal")
156
             sio.savemat(names[0], {names[0]:sim.SourceSignal})
157
             sio.savemat(names[1], {names[1]:sim.SData})
158
159
160
161
162
    if __name__ == "__main__":
         __i n i t __ ()
163
```

A.3 Material Data Setting Code and Constants

```
1 import defaults as df
2 from math import sqrt
3
4
5 ## These classes are created to create a default set of elements. I
      → will implement a file reader to get elelment data later.
      → createing a new object of this type ensures that we get a nice
      → default simulation. Let's hope this works. Solver is yet to be
      → implemented. Sigh
6
7
   class waveProperties:
       def __init__(self, Frequency = None):
8
9
            if Frequency is None:
                self.Frequency = df.FREQUENCY
10
            else:
11
12
                self.Frequency = Frequency
13
            self.WaveLength = None
14
15
16
   class material Properties:
17
       def __init__(self, Mu = None, K = None, Rho = None, A = None, B
18
          \rightarrow = None, C = None, 1 = None, m = None, Lambda = None):
19
           ##Initialize All defaults if none.
20
21
            if Mu is None:
22
                self.Mu = df.MU
23
24
            else:
                self.Mu = Mu
25
26
```

```
27
           if K is None:
              self.K = df.K
28
29
           else:
              self.K = K
30
31
           if Rho is None:
32
               self.Rho = df.RHO
33
34
           else:
35
              self.Rho = Rho
36
37
           if A is None:
              self.A = df.A
38
39
           else:
              self.A = A
40
41
           if B is None:
42
              self.B = df.B
43
44
           else:
              self.B = B
45
46
47
           if C is None:
              self.C = df.C
48
           else:
49
              self.C = C
50
51
52
           if 1 is None:
              self.1 = df.1
53
54
           else:
              self.1 = 1
55
56
           if m is None:
57
              self.m = df.m
58
59
           else:
```

```
60
                 self.m = m
61
             if Lambda is None:
62
                 self.Lambda = df.Lambda
63
             else:
64
65
                 self.Lambda = Lambda
66
67
             self.WaveVelocityL = sqrt((self.Lambda + (2*self.Mu))/self.
                \hookrightarrow Rho)
             self.WaveVelocityT = sqrt(self.Mu/self.Rho)
68
             self.BetaL = 3 + 2*(self.1 + 2*self.m)/(self.Lambda + 2*self
69
                \hookrightarrow . Mu)
70
             self.BetaT = (self.Lambda + 2*self.Mu)/self.Mu + self.m/self
                \hookrightarrow . Mu
71
72
        def refreshParams(self):
73
74
75
             self.WaveVelocityL = sqrt((self.Lambda + (2*self.Mu))/self.
                \hookrightarrow Rho)
76
             self.WaveVelocityT = sqrt(self.Mu/self.Rho)
77
             self.BetaL = 3 + 2*(self.1 + 2*self.m)/(self.Lambda + 2*self
                \hookrightarrow . Mu)
             self.BetaT = (self.Lambda + 2*self.Mu)/self.Mu + self.m/self
78
                → .Mu
79
80
   class waveGuide:
81
82
83
        def __init__(self , Boundary = None):
             if Boundary is None:
84
                 self.Boundary = df.BOUNDARY
85
86
             else:
```

```
87 self.Boundary = Boundary
```

88

- 89 ## Boundary Legend
- 90 ## 0 All reflecting
- 91 ## 1 Sides Reflecting Ends PML
- 92 ## 2 Sides PML Ends Reflecting
- 93 ## 3 Everything PML
 - 1 LONGITUDINAL = 1
 - 2 TRANSVERSE = 0

A.4 Code for Automating Simulations

```
1 from formulation import simulation
2 from solver import Solver as sl
3
4 #Limit of L and M in terms of percentages. How do we combine this?
      → We need to run experiments, check correlations and all. Let's
      → see if it has any effect:w
5
6 \quad \_LIMIT = 10
7 \quad \_STEP = 1
8 for percent in range(-int(round(__LIMIT)), int(round(__LIMIT))+1,
      \hookrightarrow __STEP):
9
       sim = simulation()
10
        old1 = sim.getParam('BetaT')
        print percent/100.0
11
12
        new1 = old1*(1 + (percent/100.0))
        print oldl, newl
13
14
        sim.setParam('BetaT', newl)
        sim.setMixing(True)
15
16
        sl(sim)
        sim.save("%d.mat"%percent)
17
18
19
   , , ,
   for percent in range(-int(round(__LIMIT)), int(round(__LIMIT))+1,
      \hookrightarrow __STEP):
       sim = simulation()
21
        oldl = sim.getParam('m')
22
        print percent/100.0
23
        newl = oldl*(1 + (percent/100.0))
24
25
        print oldl, newl
       sim.setParam('m', newl)
26
       sim.setMixing(True)
27
```

A.5 Code to Analyse Sensitivity

```
1 import numpy as np
2 import scipy.io as sp
3 from matplotlib import pyplot as plt
4 import os
5
  __DIR = "./data/sensitivity/tentoten"
7 \quad \text{\_TOTALLENGTH} = 2048
8 \quad \_STARTINDEX = 4900
9 _ENDINDEX = 5600
10 __PADDING = __TOTALLENGTH - (__ENDINDEX - __STARTINDEX)
11 __FILE = "amplitude_BetaT1010.txt"
  files = [os.path.join(__DIR,f) for f in os.listdir(__DIR)]
12
13
   fi = open(_-FILE, 'w+')
14
15
16
17
   def fft(signal):
       fftsignal = np.zeros(_TOTALLENGTH)
18
       #fftsignal[0:(_TOTALLENGTH - _PADDING)] = signal[_STARTINDEX:
19

→ __ENDINDEX ]

       fftsignal_2 = signal[_STARTINDEX:_ENDINDEX]
20
21
       ftp = abs(np.fft.fft(fftsignal_2))
22
       plot = plt.plot(ftp)
       return plot
23
24
   def ampcalc(data):
25
       return abs(min(data) - max(data))
26
27
   for f in files:
28
       print f.split('/')
29
       datafile = sp.loadmat(f)
30
```

```
fftplot = fft(datafile['SourceSignal'])
amplitude = ampcalc(datafile['SourceSignal'])

plt.savefig("%s.png"%f.split('/')[4])

plt.close()

fi.write('%s_-_%.25f\n'%(f.split('/')[4], amplitude))
```

A.6 Inverse Model Code

```
1 from sklearn.gaussian_process import GaussianProcess as GMM
2 #from sklearn.svm import SVR as GMM
3 import numpy as np
4 import matplotlib.pyplot as plt
5 import scipy as sp
6 FILE = 'data/sheet.csv'
7 dataset = np.vstack(set(map(tuple,np.genfromtxt(FILE, delimiter=',')
      \hookrightarrow )))
8
   def addNoise(snr):
10
       signal = dataset[:, -1]
       #print signal
11
       signalstd = np.std(signal)
12
13
       noisestd = signalstd/np.sqrt(snr)
14
       noise = np.random.normal(0, noisestd, len(signal))
       datasetnoisy = dataset
15
       datasetnoisy[:,-1] = datasetnoisy[:,-1] + noise
16
17
       return datasetnoisy
18
   def ensemble (value, noise):
19
20
       \#mixture = GMM(C = 100)
21
22
       mixture = GMM()
23
       newdataset = addNoise(noise)
24
       temp = np.copy(newdataset[:, -1])
       \#newdataset[:,-1] = newdataset[:,2]
25
       \#newdataset[:,2] = temp
26
27
       \#print\ newdataset[:,-1],\ newdataset[:,3]
28
       for ensemble in range (0, value):
29
            np.random.shuffle(newdataset)
            train = np.copy(newdataset[0:-10,:])
30
```

```
31
            test = np.copy(newdataset[-10:-1,:])
32
            test_pred = np.copy(test)
33
            mixture. fit (newdataset [0:-10,0:-2], newdataset [0:-10,-1])
            preds = mixture.predict(newdataset[-10:-1,0:-2])
34
            test_pred[:,-1] = preds
35
            errorabs = abs(dataset[-10:-1,-1]-preds)/(dataset
36
               \hookrightarrow [-10:-1,-1]
37
            meanerrorabs = np.mean(errorabs)
            stderrorabs = np.std(errorabs)
38
39
            #print errorabs
            print meanerrorabs, stderrorabs
40
            \#plt.plot(abs(dataset[-10:-1,-1]-preds))
41
42
            #plt.ylim(-5e-12,5e-12)
            \#plt.scatter(dataset[-10:-1,0], dataset[-10:-1,-1])
43
44
            #plt.plot(preds)
45
            #plt.show()
46
            np.savetxt('data/forward_train_%d_snr_%d.csv'%(ensemble,
               → noise), train, delimiter=',')
47
            np.savetxt('data/forward_test_%d_snr_%d.csv'%(ensemble, noise
               → ), test, delimiter=',')
            np.savetxt('data/forward_test_predict_%d_snr_%d.csv'%(
48

    ensemble, noise), test_pred, delimiter=',')

49
            #sp.io.savemat('data/train_%d_snr_%d.mat'%(ensemble, noise),
               \hookrightarrow train)
50
            #sp.io.savemat('data/test_%d_snr_%d.mat'%(ensemble, noise),
               \hookrightarrow test)
51
            #sp.io.savemat('data/test_predict_%d_snr_%d.mat'%(ensemble,
               \hookrightarrow noise), test_pred)
52 for noise in range (2,20,2):
53
        ensemble(1, noise)
```

A.7 Defaults Code

 $19 \quad 1 = -38.75e10$

20 m = -35.8 e 10

1 FREQUENCY = 2.5 e6 $2 A = -3.1*(10^{1})$ 3 B = 04 C = 05 BOUNDARY = 0 # Purely Reflecting6 DIMENSIONS = [.010, 0.030] #metres 7 MESH = 2 # 0, l, 2, 3 Coarse, Medium, fine and extrafine mesh l/8, l \hookrightarrow /12, l/64, l/1288 MU = 2.68 e 109 Lambda = 5.43 e1010 K = 76e911 RHO = 271912 TIME = 1.5 # seconds13 WAVEGUIDE = 1 14 LOCATION = 0.515 THETA = 016 WIDTH = 0.2517 PULSES = 1018 REFLECTIONS = 2

APPENDIX B

Material Properties Used in Simulations

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- [8] Liu Et, Al