Inversion of Ultrasonic Scattering Data to Measure Defect Size, Orientation, and Acoustic Properties

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Abstract
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Keywords
Nondestructive Evaluation

Disciplines
Materials Science and Engineering

This 3. defect characterization by quantitative ultrasonics is available at Iowa State University Digital Repository: http://lib.dr.iastate.edu/cnde_yellowjackets_1977/14
INVERSION OF ULTRASONIC SCATTERING DATA TO MEASURE
DEFECT SIZE, ORIENTATION, AND ACOUSTIC PROPERTIES

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McLean, Virginia 22101

ABSTRACT

Empirical solutions via the adaptive learning network methodology have been obtained to measure characteristics of three-dimensional defects (spherical and spheroidal) from the analysis of theoretically-modeled scattered waveforms. The solutions have been successfully applied to measure defects from actually observed ultrasonic scattering data. Spherical voids and inclusions in Ti-6-4, varying in diameter from 0.02 cm to 0.12 cm, and varying in acoustic impedance ratio (with respect to the host alloy [Ti-6-4]) from zero for air cavities to four for tungsten-carbide inclusions, can be directly measured via: (i) The phase cepstrum - which yields an unambiguous measurement of defect diameter and is independent of its acoustic impedance ratio; (ii) Adaptive Learning Networks (ALN) - synthesized from the amplitude spectrum and which yield accurate measurements of defect diameter and the acoustic impedance ratio of the included material. The two empirical solutions, synthesized from the scattering data from an exact model for spheres, yield similar accurate results when applied to actual scattering observed from the defects. Spheroidal defects (oblate spheroids) varying in aspect ratio from 1.67 to 6, varying in volume from 20 to 310 milliliters of a cubic centimeter, and varying in orientation from 0° to 360° in azimuth and 0° to 90° in elevation, can be measured by adaptive learning networks synthesized from scattering data produced by the Born approximation to the theoretical model. Scattering data used to train the ALNs were obtained via computer simulation. As in the case of spheres, the ALNs were trained--using the synthetic waveforms--to predict the defect size and orientation. Once the empirical models were obtained, eight actual defect sizes and orientations were found via the models and these results compare well with the true values. This paper will describe the means by which the inversion of ultrasonic scattering to defect characteristics was accomplished and its NDE implications.

Introduction

The determination of the characteristics of subsurface defects in materials by non-invasive techniques is an important and challenging task in the non-destructive evaluation (NDE) of materials. This report presents results of a study in which characteristics of spherical and spheroidal defects, imbedded in a Ti-6-4 alloy, were measured accurately by analysis of the ultrasonic energy scattered from these defects.

The description of the scattering wave equation for defects of known geometries and material properties---the "forward" problem---has been a topic of several investigations. Ying and Truell derived the equation for defects with spherical symmetry. Gubernatis and Domany have used the Born approximation to describe spherical defects. From the NDE standpoint, the interest has been in the solution of the "inverse problem", namely, how can the defect characteristics be described knowing the theoretical, of observed, scattering wave function. Studies by Tittmann and Cohen and Sachse and Chian show some measure of success in the solution of the inverse problem. Tittmann concluded that the Born approximation to the exact theoretical scattering by spheroidal defects matches insufficiently the observed scattering from actual defects. Sachse and Chian identified "echoes" in the scattered signature and related the arrival times of these echoes to defect geometry.

The specific objectives of this research were to:

1. Synthesize adaptive learning network (ALN) models to measure the size (i.e., diameter) and acoustic impedance of spherical defects from the analysis of theoretically scattered waveforms.

2. Evaluate the spherical defect ALN models for observed scattering from actual spherical defects.

3. Synthesize ALN's to estimate the size and orientation of spheroidal defects from the analysis of the Born approximation to the exact theoretical scattering model.

4. Evaluate the spheroidal defect ALN models for observed scattering from actual spheroidal defects.

In accordance with the above objectives, empirical solutions via the adaptive learning network methodology were obtained to measure the size and orientation of three-dimensional defects (spherical and spheroidal) from the analysis of theoretically-modeled scattered waveforms. The solutions were successfully applied to measure real defects from actually observed ultrasonic scattering data.

Spherical Defect Measurement from Theoretical Scattering

Spherical voids and inclusions in Ti-6-4, varying in diameter from 0.02 cm to 0.12 cm, and varying in acoustic impedance ratio (with respect to the host alloy [Ti-6-4]) from zero, for air...
cavities, to four, for tungsten-carbide inclusions, were directly measured from their theoretically scattered waves via:

1) The phase cepstrum - which yielded a measurement of defect diameter that was independent of its acoustic impedance ratio.

2) Adaptive Learning Networks (ALN) - synthesized from the amplitude and phase spectra and which yielded accurate measurements of the acoustic impedance ratio of the included material independent of defect diameter.

The first solution means that defect diameter can be measured from a phase cepstral analysis of the theoretically scattered waveform. The phase cepstrum is a transformation of the phase of the scattered signal and was developed by Adaptronics during the course of this study.

A plot of the measured diameter as a function of the true diameter is displayed in Fig. 1. The results show an excellent agreement. The diameter was measured to within the spatial resolution imposed by the data collection system. Additionally, the measurement was independent of the acoustic impedance of the defect--at least over the range of impedance values present in the theoretical data set.

The second solution to the measurement of spherical defects provides a means of quantifying the acoustic impedance independent of defect size. A procedure, illustrated in Fig. 2, was devised wherein multiple acoustic impedance estimates of the same defect could be averaged. The advantage of such a procedure lies in the fact that the average of several estimates is more accurate than a single estimate. The figure also contains a summary description of the parameter inputs to the ALN. These inputs consisted of the normalized total power, the viewing angle, and the phase

Figure 1. Plot of measured diameter versus true diameter based on phase cepstral analysis of theoretically scattered ultrasonic wave from spherical defects.

Figure 2. Quantitative spherical defect acoustic impedance measurement system.
cepstral features. A plot of the measured acoustic impedance and the ratio of this impedance to that of the host Ti-6-4 alloy versus the true acoustic impedance and ratio is shown in Fig. 3. The acoustic impedance was measured by an ALN to within $5 \times 10^2$ gm/cm$^2$-sec of its actual value, which was an accuracy rate of 91 percent over the range of impedance values present in the theoretical data set.

![Figure 3. Plot of true acoustic impedance and its ratio versus measured acoustic impedance for theoretical scattering data.](image)

Evaluation of Spherical Defect Measurement System

To test the validity of the two solutions to characterize spherical defects, data from four actual defects were processed through the above measurement systems and results were compared with the actual values, which were revealed to Adaptronics only after the measurements were made. The performance of the two solutions, synthesized from theoretical studies and applied to actual scattering data, is detailed in Table 1. The overall error for the diameter measurement system (0.015 cm) compared well with the resolution of the data collection system. The average absolute error in the acoustic impedance measurement was $7.6 \times 10^5$ gm/cm$^2$-sec over the range of impedance values, which compared satisfactorily with the accuracy rate for the theoretical data set (91%).

<table>
<thead>
<tr>
<th>Diameter</th>
<th>Error</th>
<th>Error</th>
<th>Error</th>
<th>Error</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ti-6-4</td>
<td>0.015</td>
<td>0.015</td>
<td>0.015</td>
<td>0.015</td>
</tr>
<tr>
<td>Air-Sized</td>
<td>0.015</td>
<td>0.015</td>
<td>0.015</td>
<td>0.015</td>
</tr>
<tr>
<td>Air-Size</td>
<td>0.015</td>
<td>0.015</td>
<td>0.015</td>
<td>0.015</td>
</tr>
<tr>
<td>Air-Radius</td>
<td>0.015</td>
<td>0.015</td>
<td>0.015</td>
<td>0.015</td>
</tr>
<tr>
<td>Total</td>
<td>0.015</td>
<td>0.015</td>
<td>0.015</td>
<td>0.015</td>
</tr>
</tbody>
</table>

Spheroidal Defect Measurement from Theoretical Scattering

Spheroidal defects (oblate spheroids) varying in aspect ratio from 1.67 to 6, varying in volume from 20 to 310 millionths of a cubic centimeter, and varying in orientation from 0° to 360° in azimuth and 0° to 90° in elevation, were measured by adaptive learning networks synthesized from scattering data produced by the Born approximation to the theoretical model. As in the case of spheres, the ALN's were trained using the theoretical waveforms to predict defect size and orientation.

The spheroidal defect size and orientation measurement system is illustrated schematically in Fig. 4. The measurement system consists of four ALN's which compute, for oblate spheroids:
- minor axis, $A$ (ALN1)
- major axis, $B$ (ALN2)
- elevation orientation, $\alpha$ (ALN3)
- azimuthal orientation, $\beta$ (ALN4).

These networks were synthesized from a vector of parameters computed from the theoretically scattered spectral waveforms observed at a circular array of receivers located symmetrically around the defect region.

<table>
<thead>
<tr>
<th>ALN1</th>
<th>ALN2</th>
<th>ALN3</th>
<th>ALN4</th>
</tr>
</thead>
<tbody>
<tr>
<td>$A$</td>
<td>$B$</td>
<td>$\alpha$</td>
<td>$\beta$</td>
</tr>
</tbody>
</table>

MEASURES THE SIZE ($A$ AND $B$) AND ORIENTATION ($\alpha$ AND $\beta$) OF AN OBLATE SPHEROIDAL DEFECT

The performance of the ALN's in measuring defect size and orientation from the theoretical scattering studies is summarized in Table 2. Each entry in the table corresponds to the absolute error in the appropriate component of the measurement system when averaged over defect orientation variations in both elevation and azimuth. An overall percentage error for each

<table>
<thead>
<tr>
<th>Defect Type</th>
<th>Error</th>
<th>Error</th>
<th>Error</th>
<th>Error</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sphere</td>
<td>0.015</td>
<td>0.015</td>
<td>0.015</td>
<td>0.015</td>
</tr>
<tr>
<td>Air-Sized</td>
<td>0.015</td>
<td>0.015</td>
<td>0.015</td>
<td>0.015</td>
</tr>
<tr>
<td>Air-Size</td>
<td>0.015</td>
<td>0.015</td>
<td>0.015</td>
<td>0.015</td>
</tr>
<tr>
<td>Air-Radius</td>
<td>0.015</td>
<td>0.015</td>
<td>0.015</td>
<td>0.015</td>
</tr>
<tr>
<td>Total</td>
<td>0.015</td>
<td>0.015</td>
<td>0.015</td>
<td>0.015</td>
</tr>
</tbody>
</table>
component is indicated in the last row. The defect size was measured to within 21.7 percent of the true value for A (ALN1) and to within 9.2 percent of the true value for B (ALN2). These error rates translate to an average discrepancy in size measurement of the order of 55 microns (the average of the first two entries in the penultimate row). The defect orientation was measured with a 14 percent error in elevation, \( \alpha \) (ALN3), and a 5 percent error in azimuth, \( \phi \) (ALN4). Since the elevation angle was restricted to variations in a single quadrant (0-90°), the error rate in \( \alpha \) is an angular discrepancy of 12.6. However, the azimuthal orientation, \( \phi \), varied over a 360° span and a 5 percent error rate translates to an angular discrepancy of 18°. The average angular discrepancy is 15° (average of last two entries in penultimate row).

Table 2. Performance of spheroidal defect measurement system for theoretically scattered waveforms from defects.

<table>
<thead>
<tr>
<th>True Size (microns)</th>
<th>A</th>
<th>B</th>
<th>C</th>
<th>D</th>
<th>E</th>
</tr>
</thead>
<tbody>
<tr>
<td>50 x 500</td>
<td>17.8</td>
<td>22.8</td>
<td>19.8</td>
<td>19.3</td>
<td>19.3</td>
</tr>
<tr>
<td>100 x 500</td>
<td>20.8</td>
<td>24.8</td>
<td>22.8</td>
<td>22.3</td>
<td>22.3</td>
</tr>
<tr>
<td>150 x 500</td>
<td>23.8</td>
<td>28.8</td>
<td>25.8</td>
<td>25.3</td>
<td>25.3</td>
</tr>
<tr>
<td>200 x 500</td>
<td>26.8</td>
<td>31.8</td>
<td>28.8</td>
<td>28.3</td>
<td>28.3</td>
</tr>
<tr>
<td>250 x 500</td>
<td>29.8</td>
<td>34.8</td>
<td>31.8</td>
<td>31.3</td>
<td>31.3</td>
</tr>
<tr>
<td>300 x 500</td>
<td>32.8</td>
<td>37.8</td>
<td>34.8</td>
<td>34.3</td>
<td>34.3</td>
</tr>
<tr>
<td>Average size error</td>
<td>5.8</td>
<td>6.8</td>
<td>5.8</td>
<td>5.3</td>
<td>5.3</td>
</tr>
<tr>
<td>Percentage error</td>
<td>25.7</td>
<td>23.3</td>
<td>25.7</td>
<td>23.0</td>
<td>23.0</td>
</tr>
</tbody>
</table>
| Errors are averaged over different elevation and azimuth orientations.

The performance of the spheroidal defect measurement system on theoretical scattering data indicates that the inverse problem was solved with excellent accuracy using a family of ALN’s.

Evaluation of Spheroidal Defect Measurement System

As in the case of spherical defects, the spheroidal defect measurement system was applied to actual scattering data from a variety of sample, real, oblate-spheroidal defects. The computed size and orientation were compared to their actual values. These actual values were revealed to Adaptronics only after the measurements were made.

In spite of the several deficiencies existent in the Born approximation to the theoretical scattering model when compared to the actual scattering phenomenon--and the fact that the measurement system was synthesized from the former--a remarkable agreement was found between the actual values and the measured values, as listed in Table 3. The defect size was measured to within 15 percent of the true value of A and to within 37 percent for B. Thus, the size measurements differed from the true values by an average of 26 percent. In terms of length, the average error was 90 microns, which compared fairly well with the theoretical data set (50 microns). The orientation was measured to within 26 percent of the true value of \( \alpha \) and to within 2.2 percent of \( \phi \). In other words, the average angular error for both of these measurements was approximately 15 degrees, which matched exactly the error obtained for the theoretical data set.

Table 3. Performance of spheroidal defect measurement system, synthesized from theoretical data on actual scattering data from real defects.

<table>
<thead>
<tr>
<th>DEFECT</th>
<th>SIZE (in microns)</th>
<th>ORIENTATION (in degrees)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>200</td>
<td>10</td>
</tr>
<tr>
<td>2</td>
<td>100</td>
<td>30</td>
</tr>
<tr>
<td>3</td>
<td>150</td>
<td>30</td>
</tr>
<tr>
<td>4</td>
<td>200</td>
<td>20</td>
</tr>
<tr>
<td>5</td>
<td>250</td>
<td>20</td>
</tr>
<tr>
<td>6</td>
<td>300</td>
<td>20</td>
</tr>
</tbody>
</table>

* See Figure 4.

The performance of the spheroidal defect measurement system on actual scattering data proves conclusively that not only does a family of ALN’s invert theoretical scattering data, but it also has been successfully applied to invert actual scattering data from real defects.

Description of Data Base Used to Synthesize and Evaluate ALN Defect Models

Four categories of ultrasonic scattering data were used throughout the course of this study for the design and evaluation of ALN models to estimate the characteristics of sub-surface defects in metals:

1. Theoretically generated complex Fourier spectrum from spherical defects.
2. Experimentally observed time waveforms from spherical defects.
3. Theoretically generated power spectrum from spheroidal defects.
4. Experimentally observed time waveforms from spheroidal defects.

The data from Category 1 originated from studies by Tittmann and Cohen and were computerized by Eilley, all of the Rockwell International Science Center. For spherical defects, it was possible to obtain exact scattering relationships. For spheroidal defects (i.e., prolate or oblate spheroids...
with one axis of symmetry), the Born approximation was used to generate data of Category 3. A computerized version of the Born model was developed by Krumhansl, Gubernatis, and Domany of Cornell University. This program was later modified by Johnson and Whalen of Adaptronics to enable spheroidal scattering to be obtained for any given transmitter and receiver position and defect spatial orientation. The data of Categories 2 and 4 were collected in experiments performed by Tittmann and Elsley at the Rockwell International Science Center. The details of the data generation procedure are described in the remainder of this chapter.

Theoretical Sphere Data Generation - A spherical defect (either an air cavity or one of three metal inclusions) of diameter, \( d \), was ultrasonically illuminated by a transmitter. Five diameters were considered: 0.02, 0.04, 0.06, 0.08, and 0.12 cm. The scattered energy was generated and recorded by transducers equidistant and coplanar with the defect. The location of the transmitter, referred to as the back-scatter position (\( \theta = 180^\circ \)), remained fixed but the receivers could be placed anywhere in an arc extending from 180 degrees to 62.2 degrees (in 0.2-degree increments) for a total of 20 different positions. The transducer position relative to the spherical defect and the "pitch-catch" data recording arrangement are illustrated in Fig. 5.

Transducer Locations

Spheroidal Inclusion

Host Material (Ti-64)

Transducer Locations

Spherical Inclusion

Transmitter (\( \theta = 180^\circ \)) at Back Scatter Position

Figure 5. Perspective and stereographic view of data collection procedure for spherical defects.

The transmit signal was an ideal broadband pulse with equal energy from 0 to 10.156 MHz, sampled every 0.39 MHz, for a total of 27 frequency values. The transmitter and receiver responses were assumed to be ideal (flat spectrum in this frequency range). Thus, the digitized spectrum consisted of 27 complex values (cosine and sine coefficients) for each of the 20 angular locations of the receiver transducers.

The experiment further simulated the condition in which the transmitter and receiver could be in any of four different polarization modes. In Mode \( \text{P} = 1 \), the transmitter sent longitudinal waves and the receiver collected the scattered longitudinal waves. In Mode \( \text{P} = 2 \), the transmit wave was longitudinal and the receiver wave was the mode-converted shear wave. Mode \( \text{P} = 3 \) represented one shear wave to another shear wave for perpendicular polarization, and Mode \( \text{P} = 4 \) represented parallel shear wave polarization.

The total back-scattered energy is determined by both the size of the defect and its material properties; the latter is characterized by the acoustic impedance which is defined as the product of wave velocity and defect-material density. It is known that, for a given defect-material, a larger defect produces larger total back-scattered energy. Conversely, for a given defect size, the amount of impedance "mismatch" between the defect and host materials influences the total back-scattered energy. Thus, "strong" and "weak" scatterers are distinguished by the defect impedance values being significantly different from and similar to, respectively, the host impedance.

The theoretical back-scatter spectral plots from the five different defects are displayed in Fig. 6 for each of the four defect materials. The ordinates are in absolute units and vary from 0 to 0.003 and the abscissae signify frequency variations from 0 to 10 MHz. The first two rows in the figure contain responses from the strong scatterers--air cavities and tungsten-carbide inclusions--which have impedance values markedly different from the host. The last two rows contained spectral responses from the weak scatterers--aluminum and brass inclusions.

Ordinates are in absolute units and values lie between 0 and 0.003. Abscissae are frequency variations from 0 to 10 MHz.

Figure 6. Theoretical back-scatter spectral plots - polarization mode 3.
For a given size, the strong and weak scatterers have a noticeable difference in the energy levels, as evidenced in the plots. (For 0.02 cm defects, the spectra of scattered energy from brass and aluminum inclusions were too small to be represented.) In addition to variations in energy levels for different scatterers, periodicities or "interference patterns" were noticed in the spectrum; these periodicities are much more frequent for larger defect diameters. This confirmed observations made by Sachse and Chian, who postulated that interference patterns were manifest because components of the scattered wave were in-phase or out-of-phase with the primary reflection—depending on the defect diameter being an even or an odd multiple, respectively, of the half-wavelength. Adjacent "troughs" or "crests" in the interference patterns were discovered to occur for wavelength differences equal to the diameter. Thus, the frequency spacing of the interference patterns was inversely proportional to defect diameter.

A further confirmation of this phenomenon is provided by the plots in Fig. 7 (which is similar to Fig. 6, except that the transmitter and receiver are in Mode 3 shear wave polarization). The interference patterns are more evident in this figure because, for the same frequency range, wavelengths present in a shear wave are twice as small as those in longitudinal wave. Availability of the smaller wavelengths causes interference patterns to be manifest for smaller defect diameters. For example, the smallest half-wavelength in Mode 3 is 0.015 cm (shear wave velocity in Ti-6-4 of 3.03 x 10^3 cm/sec divided by twice the highest frequency, 20 MHz) and is comparable to the smallest defect size (0.02 cm). However, the smallest half-wavelength in Mode 1 (0.03 cm) precludes its existence of interference patterns for smaller defects.

In conclusion, the energy level of the scattered signature was an indicator of the type of scatterer (defect material), although not independent of size. The frequency spacing of the spectral interference patterns was an indicator of the defect size—again not independent of defect type. Methods by which spectral parameters can be computed that exploit either defect size or material characteristics exclusive of the others which are described in "Spherical Defect Data Signal Preprocessing and Feature Extraction."

Experimental Sphere Data Description—Experimental waveforms from spherical defects were recorded and digitized following the same measurement protocol as described in "Theoretical Sphere Data Generation" (Fig. 5). Each experimentally recorded waveform consisted of 5 microseconds of amplitude data samples at a 100 MHz rate. Thus, the highest frequency of 50 MHz was five times larger than the highest frequency available in the theoretical data base (which was 10.156 MHz). Moreover, the experimental waveform consisted of the scattered signature in only one mode of polarization—the longitudinal-to-longitudinal, P = 1 Mode—whereas the theoretical set consisted of four separate modes.

Composite plots of the actually observed backscatter time signatures and their power spectra for two sample air cavities and a tungsten-carbide inclusion are presented in Fig. 8. The dotted line on each spectral plot shows the transducer response. The ordinate for each plot has been normalized between 0 and 1 by dividing each point on the original waveform by its maximum value. The abscissae for the time signatures extends from 0 to 1.2 microseconds, and, for the spectra, from 1 to 13 MHz. Unlike the theoretical spectra, the actual spectra peak at approximately 3 MHz—the nominal transducer rating. However, the interference patterns observed in theory are evident on the spectral envelope (indicated by the dotted curves).

Figure 7. Theoretical back-scatter spectral plots - polarization mode 1.

Figure 8. Experimentally observed signatures and their power spectra from sample real defects.
Therefore, to make a valid comparison between the theoretical and actual scattered spectra, a necessary precondition is the removal of the band-limited transducer response from the actual. This can be effected by deconvolution of the transducer spectra from the actual response. Conversely, the theoretical spectra could be convolved with the transducer response for comparison purposes.

For spherical defects, the former course of action was chosen to render the actual data relatively free of transducer modifications. Further, the larger bandwidth of the experimental data (50 MHz) was reduced to 10 MHz to make valid comparisons between theory and experiment.

Thus, as an initial preprocessing step, both the theoretical and experimental data were placed on a comparable basis: (i) transducer response ideal, and (ii) equal bandwidths of 10 MHz.

Theoretical Spheroid Data Generation - The transmitter and receiver spatial configurations for spheroids differed from those for spherical defects because a spheroid exhibited scattering patterns dependent on its orientation relative to the transmitter. Here the objectives were to determine both the size and orientation parameters of the spheroid, given the received spatially-distributed scattering information. The following definitions describe the spatial positions of the transmitters, receivers, and the spheroid; a spherical coordinate system was used.

- \( A \) = minor axis radius (i.e., half the height of the scatterer); measured in microns.
- \( B \) = major axis radius (i.e., half of the width of the scatterer); measured in microns.
- \( \alpha \) = elevation angle of the scatterer, measured between positive \( Z \)-axis and axis of symmetry of defect (i.e., along \( A \)); measured in degrees.
- \( \beta \) = azimuthal angle of the scatterer, measured in the \( X-Y \) plane, between the positive \( X \)-axis and projection of spheroid axis of symmetry onto the \( X-Y \) plane; measured in degrees.
- \( \gamma \) = elevation angle of the transmitters and receivers, measured from the negative \( Z \)-axis, measured in degrees.
- \( \phi \) = azimuthal angle of the transmitter and receiver, measured from the positive \( X \)-axis, measured in degrees.

An oblate spheroid with the above size and orientation parameters is shown in Fig. 9. Both \( A \) and \( B \) are measured from the center of the defect. The four values shown (\( A, B, \alpha, \) and \( \beta \)) are the size and orientation descriptors, and it is these that were modeled during ALM synthesis, as described in "Inverse Solution for Description of Spheroidal Defects."

Figure 9. Oblate spheroid showing size (\( A \) and \( B \)) and orientation (\( \alpha \) and \( \beta \)) parameters.

A total of 17 transducer positions was used in creating the theoretical spheroid data base. Five of the transducers operated both in the transmit and receive modes, while the others acted only as receivers. These positions are depicted in Fig. 10, where the circles indicate receiver only and the filled-in circles represent both transmit and receive positions. It can be seen that the transducer configuration consisted of two circular arrays and a top center receiver. The "outer" array covered a 120 degree solid angle and the "inner" array covered a 60 degree solid angle. Throughout the remainder of this report, these arrays will be called the "outer ring" and "inner ring," respectively. A stereographic view of these two rings (Fig. 10(c)) depicts two concentric circles with a transmitter/receiver in the middle. This middle transducer is referred to in this report as the "top center" transducer. The angular locations of the 17 transducer positions are given in Table 4.
Table 4. Angular locations of the 17 transducer positions.

<table>
<thead>
<tr>
<th>Transducer Number</th>
<th>$\theta$ (Degrees)</th>
<th>$\phi$ (Degrees)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>120</td>
<td>8</td>
</tr>
<tr>
<td>2</td>
<td>150</td>
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<td>180</td>
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<tr>
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<tr>
<td>5</td>
<td>240</td>
<td>8</td>
</tr>
<tr>
<td>6</td>
<td>270</td>
<td>8</td>
</tr>
<tr>
<td>7</td>
<td>300</td>
<td>8</td>
</tr>
<tr>
<td>8</td>
<td>330</td>
<td>8</td>
</tr>
<tr>
<td>9</td>
<td>360</td>
<td>8</td>
</tr>
<tr>
<td>10</td>
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<td>8</td>
</tr>
<tr>
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</tr>
<tr>
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<td>8</td>
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<tr>
<td>13</td>
<td>480</td>
<td>8</td>
</tr>
<tr>
<td>14</td>
<td>510</td>
<td>8</td>
</tr>
<tr>
<td>15</td>
<td>540</td>
<td>8</td>
</tr>
</tbody>
</table>

Table 5. Six spheroidal defect sizes selected for the theoretical data base.

<table>
<thead>
<tr>
<th>Size</th>
<th>$A$, $B$, $C$</th>
<th>$\alpha$, $\beta$, $\gamma$</th>
<th>Orientation $\theta$, $\phi$</th>
</tr>
</thead>
<tbody>
<tr>
<td>50 x 300</td>
<td>0.25, 0.33, 0.41</td>
<td>90, 90, 90</td>
<td>1, 65</td>
</tr>
<tr>
<td>150 x 200</td>
<td>0.75, 1.0, 1.33</td>
<td>90, 90, 90</td>
<td>30, 180</td>
</tr>
<tr>
<td>200 x 400</td>
<td>1.25, 1.66, 2.00</td>
<td>90, 90, 90</td>
<td>60, 210</td>
</tr>
<tr>
<td>300 x 500</td>
<td>1.75, 2.50, 3.33</td>
<td>90, 90, 90</td>
<td>45, 135</td>
</tr>
<tr>
<td>500 x 300</td>
<td>0.41, 0.67, 0.83</td>
<td>90, 90, 90</td>
<td>45, 135</td>
</tr>
</tbody>
</table>
The Cornell program for the Born approximation, as received by Adaptronics, required the addition of several coordinate transformations to simulate arbitrary transmitter locations and defect orientations. A description of these transformations is given in Appendix A.

Examples of Born generated longitudinal and shear power spectra, at each receiver, are shown in Fig. 11. These plots resulted when a 200 x 400 micron oblate spheroidal cavity was insinified by the top transmitter ($\theta = 180^\circ$). The defect elevation angle, $\alpha$, was zero, hence the spectra at all eight receivers in a given ring were identical. The receiver spectra in the outer ring, inner ring, and back-scatter are displayed. The ordinate, for each plot, is the spectral amplitude in absolute units, and the abscissae represent the frequency variation from 2 to 8 MHz.

![Figure 11. Longitudinal and shear power spectrum plots from Born approximation program for 200 x 400 micron oblate spheroid.](a) $\theta = 0^\circ$ (Outer Ring Receiver); (b) $\theta = 150^\circ$ (Inner Ring Receiver); (c) $\theta = 180^\circ$ (Top Ring Receiver - backscatter)

Transmitter is at top center position and defect orientation is at zero elevation ($\alpha = 0^\circ$).

Note the frequency shift in the longitudinal wave as the receiver moves into the backscatter position. The peak for the longitudinal wave is 5.8 MHz at $\theta = 120^\circ$, 6.3 MHz at $\theta = 150^\circ$, and 6.7 MHz at $\theta = 180^\circ$ (backscatter position).

The relative scattered power from a 200 x 400 oblate spheroid is presented in Fig. 12 for varying defect elevation angles. Each diagram shows a polar view of the receiver array. The level of shading on each receiver position indicates the relative longitudinal power. The incident beam originates from the center transmitter, and the defect is varied from 0 to 90 degrees, in elevation, along the $\beta = 202$-degree plane. Except for $\alpha = 0$ and $\alpha = 90$ degrees, $\beta$ can be estimated by locating the receiver detecting maximum reflected power. The elevation angle, $\alpha$, on the other hand, cannot be determined so easily. This fact was to influence the accuracies of $\alpha$ and $\beta$ measurements, as will be shown in "Inverse Solution for Description of Spheroidal Defects."

Experimental Spheroid Data Description - The experimental data collection procedure for spheroidal defects is described in Ref. 7. The transmitter and receiver locations used in the reference were identical to the positions given in "Theoretical Spheroid Data Generation."

A total of 85 waveforms, from each of eight oblate spheroid defects, was recorded experimentally. Examples of the time and power spectrum plots at an inner ring receiver are shown in Fig. 13 for a 200 x 400 micron oblate spheroid with zero elevation angle. The transmitter was at top center position. Only 100 points of the 501-point time waveform are shown because the remainder of the waveform was essentially zero. The dissimilarities between the actual spectrum (Fig. 13) and the theoretical spectrum (Fig. 11(b)) are evident. The theoretical spectrum has a bandwidth between 2.5 and 8 MHz and shows a smooth monotonic rise toward a peak amplitude at approximately 6 MHz and a gradual tapering beyond that frequency. The actual spectrum, on the other hand, is less smooth, although the pertinent information is confined to approximately the same bandwidth (2.5 to 6 MHz). Thus, any degree of similarity between theory and practice was in gross spectral characteristics (for example, total scattered energy) rather than in precise spectral shape.
The parameterization of these waveforms is explained in greater detail in the sections on "Spherical Defect Data Signal Preprocessing and Feature Extraction" and "Spherical Defect Data Signal Preprocessing and Feature Extraction."

Spherical Defect Data Signal Preprocessing and Feature Extraction

As discussed in the objectives at the beginning of this report, the major research goal in this project was to synthesize ALN's from parameters of a theoretical scattering model, and to evaluate these ALN's independently on actual scattering data from spherical defects.

The signal preprocessing objective was to derive parameters which were sensitive to the defect size and the defect material. It was found that the phase spectrum of the signal was relatively insensitive to defect material properties but was a good indicator of defect size. The magnitude spectrum, on the other hand, was found to be a key source of information to determine material properties independently of defect size. This section presents these two transformations.

Presence of Echoes in Scattered Wave - The works of Sachse and Chian4 indicate that the scattered wave from a spherical defect consists of the following components:

- The primary reflection, called the P-P wave.
- The circumferential or "creep" wave, which skirts around the periphery of the defect, called the PFP wave.
- The refracted ray propagating back and forth across the defect diameter, called the PFFP wave.

The PFP wave is a function of the properties of the host material and the diameter of the defect, whereas the PFFP wave is, in addition, dependent on the acoustic impedance of the defect. If one could isolate uniquely the times of occurrence of the PFP and PFP waves in the scattered time signal, both the acoustic impedance of the defect material and its diameter could potentially be inferred.

Cepstral Analysis of Scattered NDE Waveforms - The cepstrum is a powerful signal processing tool which has found wide applications in echo detection, echo removal, and inverse filtering procedures.5 A detailed discussion of the various forms of the cepstrum, their relationships, and implementations was described previously.5 The primary reason for analyzing signal waveforms by the cepstrum is that the time delays between two or more similar events manifest themselves as peaks. Therefore a search for the location of peaks in the cepstrum will reveal the relevant time delays. However the search is compounded in difficulty by the fact that multiple time delays result in several peaks which are harmonics of, and sums and differences of, all possible delays. The peak(s) of interest can be potentially smeared by the presence of multiple echoes, and one can be misled as to their true location(s). Thus due to its inherent computational problems,5 the cepstrum must be used with care.
Echo Time Detection by Power Cepstral Analysis - The power cepstrum is the inverse Fourier transform of the power spectrum of the scattered signal. The time delays in the signature should cause a "rippling" in the magnitude (power) spectrum. A further transformation on the magnitude spectrum should cause delta functions (peaks) to be manifest at those time delays. Since large defects have large scattered energy values, the rippling in the magnitude spectrum may be obscured by the large magnitudes. Magnitude shifts in the spectrum for defects of the same diameter but with different acoustic impedance ratios will lead to additional uncertainties in the measurement of true peak locations.

Echo Time Detection by Phase Cepstral Analysis - We have found that time delays in the scattered signature can be more easily detected in the phase rather than in the magnitude spectrum. The phase, at any particular frequency, is the arctangent of the ratio of the imaginary part and the real part of the complex Fourier transform. Both these parts are dependent on the frequency, the acoustic impedance ratio between the host and defect, and on the size of the defect. Larger acoustic impedance ratios create larger backscattered energies to be detected. Therefore, the magnitude component, which is the square root of the sum of the squares of the real and imaginary parts, is a function of the frequency and defect size, because the phase angle is independent of acoustic impedance ratio. Thus analysis of the phase--particularly the phase cepstrum--seemed more promising to determine diameter independent of material properties of the inclusion.

The formulation of the phase cepstrum appears in Ref. 5, and the reader is referred to it for the mathematical analysis; our interest is in the physical aspects of the mathematical formulation. The phase cepstrum is defined as the inverse Fourier transform of the complex exponential phase function rather than that of the phase function itself. Retaining the complex exponential of the phase function in computing the phase cepstrum has a threefold advantage. First, the complex exponential is a smooth function, and there are no discontinuities at the transition regions (-180° to 180° or 360° to 0°). Second, by encoding the phase angle in a manner similar to the basis functions of the Fourier transform, there are more opportunities for strong correlations between a given frequency and a given phase angle variation to result in a delta function. Third, the complex exponential avoids any detailed "unwrapping" procedure, which is necessary if one is to use the phase angle by itself.

Thus the phase cepstrum offers considerably more potential in detecting echo times than the power cepstrum and, as will be found later in the section on "Inverse Solution for Description of Spherical Defects," was a key indicator of defect diameter.

Magnitude Spectrum Processing - It was noted in "Theoretical Sphere Data Generation" that the total scattered energy was a function of defect material properties in addition to defect size. A plot of the total backscattered energy in polarization Mode I is presented in Fig. 14. The ordinate is the scattered energy in logarithmic units and the abscissa is the defect diameter. The scattered energy increases with increasing diameter. However, for the same diameter, say 0.08 cm, the scattered energy could change from -14 units for a weak scatterer (brass), to -11.5 units, for a strong scatterer (air-cavity). In an effort to make the total energy relatively insensitive to size variations, it was conjectured that the total scattered energy, scaled by the maximum value in its power spectrum, would show a dependence on material properties alone.

![Figure 14](image-url)

Figure 14. Theoretical total back-scattered energy from spherical defects as a function of defect diameter (mode I polarization).
Thus the total energy scaled by the maximum power was relatively independent of defect size and also appeared to be a promising indicator of material properties.

Waveform Parameterization - The final candidate features (i.e., parameters) of the ultrasonic signature used as descriptors of defect size and its acoustic impedance are listed in Table 6. This list contains the total normalized total power (for reasons indicated previously in "Magnitude Spectrum Processing", the cepstral peak values (as explained earlier in this section on "Spherical Defect Data Signal Preprocessing and Feature Extraction"), and the viewing angle. The feature could be computed for either P = 1 or P = 3 mode of polarization. However, since the experimental data set consisted of a P = 1 polarization ultrasonic scattering wave (see "Experimental Sphere Data Description"), the list was compiled for the P = 1 mode to make a valid comparison between theory and experiment.

Table 6. Candidate features for describing spheroidal defects.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Normalization</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>$E_T$</td>
<td>Peak</td>
<td>Total energy in scattered signal normalized by the maximum power.</td>
</tr>
<tr>
<td>$r_k / \theta_k$</td>
<td>Spectral magnitude of the viewing angle.</td>
<td></td>
</tr>
<tr>
<td>$\theta_k$</td>
<td>Peak</td>
<td>Total energy in scattered signal normalized by the maximum power.</td>
</tr>
<tr>
<td>$r_k / \theta_k$</td>
<td>Spectral magnitude of the viewing angle.</td>
<td></td>
</tr>
<tr>
<td>$\theta_k$</td>
<td>Peak</td>
<td>Total energy in scattered signal normalized by the maximum power.</td>
</tr>
<tr>
<td>$r_k / \theta_k$</td>
<td>Spectral magnitude of the viewing angle.</td>
<td></td>
</tr>
<tr>
<td>$\theta_k$</td>
<td>Peak</td>
<td>Total energy in scattered signal normalized by the maximum power.</td>
</tr>
<tr>
<td>$r_k / \theta_k$</td>
<td>Spectral magnitude of the viewing angle.</td>
<td></td>
</tr>
</tbody>
</table>

The synthesis of ALM's to measure defect size and acoustic impedance, based on the above parameters, is detailed in the section on "Inverse Solution for Description of Spherical Defects."

Spheroidal Defect Data Signal Preprocessing and Feature Extraction

Comparison of Scattered Waveforms Obtained by Born Approximation and Actual Observation - Careful judgement was needed in the definition of candidate features for the spheroidal defect measurement system because there appeared to be little commonality between the two types of data (theoretical and empirical). Hence, from a rather large quantity of data per experiment, a total of only 32 candidate features was defined. There were four major differences between the two spheroidal data types.

First, the Born-generated receiver power spectra were very smooth curves somewhat similar to a half-cycle of a sine wave (Fig. 11). On the other hand, the real data power spectra were much less smooth (Fig. 13). The real data also exhibited sharper roll-off characteristics and were of a generally lower frequency than the Born data. Even after the theoretical spectra were multiplied by the actual transducer frequency response (to make the comparison on an equal basis), the real spectra were significantly different. Therefore, features sensitive to the shape of the individual spectra were excluded from consideration.

Second, it was observed that the difference in power between the inner and outer circular arrays was considerably greater for the theoretical data than for the real data in the case of defects with zero elevation ($\phi = 0$) and transmitter location at top center. It was therefore decided to limit the feature types to those computed from powers within a given array rather than to those computed by combining powers from both arrays.

Third, it was discovered by personnel at the Rockwell International Science Center during the real data collection process that certain receiver powers may have been unavoidably corrupted by the transmitter signals. Specifically, the receiver collecting backscatter waveforms may still have been ringing from the transmit signal when the scattering waveform was received. Also, receivers in the hemisphere opposite to the outer ring transmitters may have responded to the direct transmit signal in addition to the scattered waveform. Accordingly, these receiver powers (which were in the outer ring only) were not used in the computation of features.

Fourth, real data always possess some degree of uncertainty, or "noise," whereas computer-generated data do not. Therefore, noise was added to make the Born spheroidal data resemble more closely the real data. This "corruption" process is described below.

Waveform Preprocessing: Born Data - As discussed in "Theoretical Spheroid Data Generation," each Born approximation (computer) experiment required 85 waveforms containing 21 words to be generated (although not all 85 were used in feature computation). The data were reduced to
a more manageable list of 32 features per experiment before synthesizing the ALN defect models.

In the generation of theoretical data, it was assumed that the transducer had an ideal response--a flat magnitude spectrum and zero phase shift at all frequencies. The real data, however, were modified by a transducer response that was less than ideal. In fact, the nominally rated 5 MHz transducer used in the experiments had a bandwidth limited to the frequency range 1-9 MHz. Each of the 85 Born approximation waveforms was convolved with the transducer characteristic so that a higher degree of similarity between theoretical and experimental data could be attained. (Another means of obtaining similarity is by deconvolution of the transducer response from the experimental receiver data. However, this operation, although more general than deconvolution, is more difficult to implement and can require additional spectral smoothing. Although deconvolution was considered in this study, convolution was a more practical approach due to the time factor.)

Next, the 21-point spectra were integrated to determine the total power between 1.0-8.8 MHz. Preliminary comparison of the Born spectra to the corresponding experimentally-obtained spectra indicated very little similarity in their overall shapes. It was, therefore, decided to extract gross spatial features from the 85 receiver total powers rather than highly detailed features from the individual spectra. The single parameter of total power was just such a feature.

The total power was corrupted slightly by adding pseudo-random noise to give the Born and real data statistically similar properties. The "noisy" powers were computed by adding to the total power a uniformly distributed random number with zero mean and 0.33 variance, multiplied by 10 percent of the total power:

\[ P_{\text{noise}} = P(1 + 0.1r) \]

where \( r \sim U(0, 0.33) \)

Note that it was established from an analysis of a limited amount of real data that there was approximately a 10 percent variation in the total power values in those cases where defect and transducer symmetry would allow no variation in theory (e.g., \( \phi = 0^\circ \) and the transducer in the top position--all the receivers in either circular array should detect equal scattered power).

After noise addition, the powers from the inner \((\phi = 150^\circ)\) and outer \((\phi = 120^\circ)\) rings were normalized separately by dividing each power in a ring by the total power in that same ring. Hence, after normalizing, the 8 receiver powers in either ring summed to unity. Normalization was performed in this manner for all five transmitting positions. The top position \((\phi = 100^\circ, \theta = 0^\circ)\) receiver power was never used in computing any of the 32 features; only the normalized power around the inner and outer rings, for each transmitting position, was used.

Waveform Preprocessing: Real Data - A total of 85 time waveforms consisting of 501 points each was processed from each of eight spheroid scattering experiments. (The size and orientation identities of these real data were unknown to Adaptronics throughout the course of the study.) The sampling rate of the ultrasonic waveforms was 100 MHz, which yielded the highest observable frequency of 50 MHz. The data window of the scattered signal at each of the receivers was approximately 5 microseconds. The Fast Fourier Transform (FFT) algorithm was used to convert the receiver waveforms to the frequency domain. A 512-point power spectrum with a frequency resolution of 0.098 MHz per point (50 MHz divided by 512 points) was computed for each time signal. The bandwidth of interest was between 1.0-8.8 MHz, so the total power was computed by summing 80 amplitude spectral values in this frequency range. The same list of 32 features that was computed from the 240 Born program experiments was also computed from these eight real data experiments.

A comparison of the preprocessing steps for the Born and real data waveforms is shown in Fig. 16.

Waveform Feature Extraction: Born and Real Data - Six types of feature were defined for each transmitter position:

- CM = circular mean
- CV = circular variance
- ENT = entropy
- MMR = min-max ratio
- RI = inner ring ratio
- OR = outer ring ratio
The circular mean was an angular feature which located the first moment of the scattered power around a circular receiver array. This feature was thought to be useful in determining the azimuthal defect orientation angle. Calculation of the CM was as follows:

\[ CM = \tan^{-1}(S/C) + \gamma \]  

(2)

where:

\[ S = \sum_{\phi=0}^{315} P(\phi, \psi) \sin \phi \]

\[ C = \sum_{\phi=0}^{315} P(\phi, \psi) \cos \phi \]

and:

\[ \gamma = 0 \text{ if } S > 0, \quad C > 0 \]

\[ = \pi \text{ if } C < 0, \quad S = 0 \]

\[ = 2\pi \text{ if } S < 0, \quad C > 0 \]

\[ P(\psi) = \text{longitudinal normalized total power at receiver position } (\psi, \psi). \]

In the above computation, \( \phi \) remained fixed at either 150° (inner ring) or 120° (outer ring); therefore, eight terms were summed in computing either S or C.

The circular variance feature is defined between zero and unity and was a measure of the power dispersion about the circular mean of a given circular array:

\[ CVAR = 1 - \sum_{\phi=0}^{315} P(\phi, \psi) \cos(\psi - CM) \]  

(3)

The information-theoretic entropy feature is similar to the sample variance around a circular receiving array:

\[ ENT = -\sum_{\phi=0}^{315} P(\phi, \psi) \log_2 P(\phi, \psi) \]  

(4)

The min-max ratio is computed from the minimum and maximum powers around a given ring:

\[ \frac{P(\text{max}) - P(\text{min})}{P(\text{max})} \]  

(5)

For each of the four outer rings (\( \phi = 120 \)) transmitters, two min-max ratio features were computed, RI and RO, defined as follows:

\[ RI(\psi) = \frac{P(\psi+45, 150) + P(\psi-45, 150) + P(\psi-135, 150) + P(\psi+135, 150)}{P(\psi+45, 150) + P(\psi-45, 150) + P(\psi+135, 150) + P(\psi+135, 150)} \]

\[ RO(\psi) = \frac{P(\psi-180, 120) + P(\psi-90, 120) + P(\psi+90, 120) + P(\psi+180, 120)}{P(\psi-180, 120) + P(\psi-90, 120) + P(\psi+90, 120) + P(\psi+180, 120)} \]  

(6)

where:

\( \phi = 0, 90, 180, \) and 270 degrees.

A list of the 32 candidate features is given in Table 7. This candidate list of inputs was used to synthesize the ALN's that measured spheroid defect size and orientation, as described in "Inverse Solution for Description of Spheroidal Defects."

### Table 7. Candidate feature list for describing spheroidal defects.

<table>
<thead>
<tr>
<th>Feature Number</th>
<th>Feature Type</th>
<th>Transmitter Position (( \psi, \psi ))</th>
<th>Ring</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>CM</td>
<td>0,180</td>
<td>IN</td>
</tr>
<tr>
<td>2</td>
<td>CVAR</td>
<td>0,180</td>
<td>IN</td>
</tr>
<tr>
<td>3</td>
<td>ENT</td>
<td>0,180</td>
<td>IN</td>
</tr>
<tr>
<td>4</td>
<td>MHH</td>
<td>0,180</td>
<td>IN</td>
</tr>
<tr>
<td>5</td>
<td>CM</td>
<td>0,180</td>
<td>OUT</td>
</tr>
<tr>
<td>6</td>
<td>CVAR</td>
<td>0,180</td>
<td>OUT</td>
</tr>
<tr>
<td>7</td>
<td>ENT</td>
<td>0,180</td>
<td>OUT</td>
</tr>
<tr>
<td>8</td>
<td>MHH</td>
<td>0,180</td>
<td>OUT</td>
</tr>
<tr>
<td>9</td>
<td>CM</td>
<td>0,120</td>
<td>IN</td>
</tr>
<tr>
<td>10</td>
<td>CVAR</td>
<td>0,120</td>
<td>IN</td>
</tr>
<tr>
<td>11</td>
<td>ENT</td>
<td>0,120</td>
<td>IN</td>
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<tr>
<td>12</td>
<td>MHH</td>
<td>0,120</td>
<td>IN</td>
</tr>
<tr>
<td>13</td>
<td>CM</td>
<td>90,120</td>
<td>IN</td>
</tr>
<tr>
<td>14</td>
<td>CVAR</td>
<td>90,120</td>
<td>IN</td>
</tr>
<tr>
<td>15</td>
<td>ENT</td>
<td>90,120</td>
<td>IN</td>
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<td>16</td>
<td>MHH</td>
<td>90,120</td>
<td>IN</td>
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<td>17</td>
<td>CM</td>
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<td>18</td>
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<td>MHH</td>
<td>180,120</td>
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<td>21</td>
<td>CM</td>
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<td>22</td>
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<td>270,120</td>
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<td>ENT</td>
<td>270,120</td>
<td>IN</td>
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<tr>
<td>24</td>
<td>MHH</td>
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<tr>
<td>25</td>
<td>RI</td>
<td>0,120</td>
<td>IN</td>
</tr>
<tr>
<td>26</td>
<td>RI</td>
<td>90,120</td>
<td>IN</td>
</tr>
<tr>
<td>27</td>
<td>RI</td>
<td>180,120</td>
<td>IN</td>
</tr>
<tr>
<td>28</td>
<td>RI</td>
<td>270,120</td>
<td>IN</td>
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<tr>
<td>29</td>
<td>RO</td>
<td>0,120</td>
<td>OUT</td>
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<tr>
<td>30</td>
<td>RO</td>
<td>90,120</td>
<td>OUT</td>
</tr>
<tr>
<td>31</td>
<td>RO</td>
<td>180,120</td>
<td>OUT</td>
</tr>
<tr>
<td>32</td>
<td>RO</td>
<td>270,120</td>
<td>OUT</td>
</tr>
</tbody>
</table>

In the above computation, \( \phi \) remained fixed at either 150° (inner ring) or 120° (outer ring); therefore, eight terms were summed in computing either S or C.

The defect size and orientation, as described in Table 7. This candidate list of inputs was used to synthesize the ALN's that measured spheroid defect size and orientation, as described in "Inverse Solution for Description of Spheroidal Defects."

Inverse Solution for Description of Spherical Defects

Introduction - The measurement of defect diameter was performed via the phase cepstral analysis which yielded values independent of the acoustic impedance. The acoustic impedance was measured via an ALN model that was relatively independent of defect size. Both of these measurement schemes were tested with scattering data from actual defects and similarly accurate results were obtained.

Defect Diameter Measurement System-Phase Spectrum Processing of Theoretical Data - The defect diameter was measured by determining the peak location in the phase cepstrum (see section on "Spherical Defect Data Signal Preprocessing and Feature Extraction"), which is a signal transformation of the phase spectrum of the scattered ultrasonic waveform. Although the phase cepstrum be
computed for any of the four modes of polarization, this investigation revealed that one of the modes, the vertical shear to vertical shear wave polarization (P\textsuperscript{3}) offered the greatest resolution in the cepstral domain. To convert peak location in the cepstral domain to units of length, the following transformation was used:

\[ d^* = \text{characteristic length} = v_s |t^*| \]

where

\[ t^* = \text{location of cepstral peak (sec)} \]

and

\[ v_s = (\text{shear wave velocity in Ti-6-4}) = 3.03 \times 10^5 \text{ cm/sec}. \]

A composite plot of the theoretical P\textsuperscript{3} phase cepstra for the 5 different (theoretical) defects is displayed in Fig. 17 for each of the 4 different materials. The ordinates have been scaled between 0 and 1 by dividing by the largest observable peak. The abscissae represent quefrency, which varies from -1.3 to 1.3 microseconds (not shown). For ease of interpretation, quefrency values have been converted to length according to the above formula. Although quefrency can take on negative values, the length will always be positive.

![Figure 17. Phase cepstrum of theoretically scattered waveform at back-scatter position.](image)

For each defect size, the peaks in the phase cepstra for three of the four materials coincided. However, the peaks for brass defects occurred in negative quefrency. If the transformation from quefrency to length is made, the peak location for brass nearly corresponded to the peak locations for the other three materials.

The phase cepstral analysis described above was equally valid for any other mode of polarization. The P\textsuperscript{3} mode was chosen instead of the P\textsuperscript{1} mode because the spatial resolution offered by the former is twice as small as the latter. The spatial resolution is given by the formula:

\[ \Delta d = v_s t, \]

where \( \Delta d \) is the spatial resolution, \( t \) is the quefrency resolution (sampling interval of time signal), and \( v_s \) is the velocity (which is twice as large for a P\textsuperscript{3} wave as it is for a P\textsuperscript{1} wave). Spatial resolution can be made smaller by decreasing \( t \) (sampling signal faster) or by decreasing \( v_s \) (using shear wave instead of longitudinal wave). The former technique was used to increase spatial resolution of the phase cepstrum of the experimental longitudinal wave.

A plot of the true versus measured diameter based on the phase analysis of the theoretically scattered wave is shown in Fig. 18. The relationship is not linear; however, it is monotonic and invariant (except for brass) with defect material.

![Figure 18. Measured diameter versus true diameter based on phase cepstral analysis of scattered P\textsuperscript{3} theoretical ultrasonic waveform.](image)
desirable properties and then to obtain \( Z_0 \) from the above formula. Since each defect size/defect constituent combination was scanned at 20 different viewing angles (\( \theta \)'s) a scheme was devised (illustrated in Fig. 19) wherein the acoustic impedance measurements at different angles could be averaged to yield one composite estimate value.

To compute the defect's acoustic impedance, \( Z(\theta) \), the following transformation was used:

\[
Z(\theta) = \frac{1 - r(\theta)}{1 + r(\theta)} Z_{\text{Ti}-64},
\]

where \( r(\theta) \) is the estimated reflectance coefficient at a particular viewing angle and \( Z_{\text{Ti}-64} \) is the acoustic impedance of the host titanium alloy. The composite estimated ALN value so obtained was thus independent of the viewing angle. The list of candidate ALN inputs (Table 6) appears at the bottom of Fig. 19. To reiterate, the list contains normalized spectral power, viewing angle of the receiver with respect to the transmitter (which is always located at backscatter position), location of the phase cepstral peak at \( \theta \), and inverse of the phase cepstral peak at the backscatter position. The last two features were included to compensate for observed peak shifts in the phase cepstrum toward lower quefrencies as the receiver moved from backscatter to more forward scattering positions.

A diagram of the ALN network synthesized from the theoretical \((L+L)\) spectral parameters is shown in Fig. 20. The resulting model is an eighth-degree (incomplete) polynomial equation in five of the seven inputs. It has among its principal inputs the normalized total energy, the ratio of normalized energy at \( \theta \) to that at backscatter, and the phase cepstral features.

![Diagram of ALN network](Figure 20)

**Figure 20.** ALN spherical defect reflectance coefficient measurement model, synthesized from theoretically scattered parameters.

For Figure 19. Quantitative spherical defect acoustic impedance measurement system.
The measured acoustic impedances for the variety of defects in the theoretical data set are shown in Table 8. Each entry in the table corresponds to the measured acoustic impedance for a given defect diameter. An overall average acoustic impedance measure can be obtained by summing across a row. This is indicated under "average measured impedance." The true impedance appears alongside, allowing a comparison to be made between the measured and true acoustic impedance ratios (with respect to Ti-6-4). These are shown in the last two columns and plotted in Fig. 21.

Table 8. Measured acoustic impedance by AlN synthesized from the theoretical (L-L) spectral and cepstral parameters.

<table>
<thead>
<tr>
<th>Defect Diameter (mm)</th>
<th>Measured</th>
<th>Theoretical</th>
<th>Average Measured</th>
<th>True</th>
</tr>
</thead>
<tbody>
<tr>
<td>AIR</td>
<td>2.0</td>
<td>1.00</td>
<td>1.00</td>
<td>1.00</td>
</tr>
<tr>
<td>ALUMINUM</td>
<td>0.50</td>
<td>1.00</td>
<td>1.00</td>
<td>1.00</td>
</tr>
<tr>
<td>Brass</td>
<td>0.50</td>
<td>1.00</td>
<td>1.00</td>
<td>1.00</td>
</tr>
<tr>
<td>AEROSIL 200</td>
<td>1.00</td>
<td>1.00</td>
<td>1.00</td>
<td>1.00</td>
</tr>
<tr>
<td>AEROSIL 380</td>
<td>1.00</td>
<td>1.00</td>
<td>1.00</td>
<td>1.00</td>
</tr>
<tr>
<td>TUNGSTEN-CARBIDE</td>
<td>1.00</td>
<td>1.00</td>
<td>1.00</td>
<td>1.00</td>
</tr>
</tbody>
</table>

Three observations can be made regarding these results:

- Acoustic impedance and the impedance ratio can be measured very accurately by the ALN for theoretical scattering data.
- The measurements are equally good for weak scatterers (aluminum and brass) and for strong scatterers (air cavity and tungsten-carbide inclusions).
- The measurements are accurate and consistent for defect size variations from 0.02 cm to 0.12 cm, except for tungsten-carbide inclusions, which show a slightly greater variability.

Measurement of Spherical Defect Diameter and Acoustic Impedance from Experimental Data - As a test of validity of the synthesized solutions described in "Defect Diameter Measurement System-Phase Spectrum Processing of Theoretical Data," and "Defect Acoustic Impedance Measurement System-Magnitude and Phase Spectral Processing of Theoretical Data," experimental data from actual spherical defects were analyzed.

The experimental data consisted of the scattered L-L, P = 3 response, but the phase cepstral solution to measure diameter was synthesized from the scattered S-S, P = 3, response. So, to interpret the peak locations in the phase cepstrum of the experimental data, the longitudinal velocity—which is twice the shear wave velocity—was used. To convert the peak locations to length, one must use the transformation similar to the one in the "Introduction" to this section, i.e.,

\[ d^* = \text{characteristic length} = v_L t^* \]

where

\[ t^* = \text{location of cepstral peak (secs.)} \]

and

\[ v_L = \text{longitudinal wave velocity in Ti-6-4} = 6.06 \times 10^5 \text{ cm/sec}. \]

A plot of the phase cepstrum of the recorded scattered data from the three air cavities and the one metal inclusion is shown in Fig. 22. The ordinate of each plot shows the magnitude (maximum amplitude normalized to unity) of the cepstral peak and the abscissa shows the diameter, which extends from 0 to 0.3 cm. The quefrency values along the abscissa have been converted to length for ease of interpretation. The true diameter appears along the right-hand column and the measured values appear just to the left of the true values.
There is very good agreement between the actual and estimated diameters for the three air cavities and reasonable agreement for the tungsten-carbide inclusion. The clarity of the peaks in the phase cepstrum compare (Fig. 22) with those obtained from the theoretical data (Fig. 18), in spite of the fact that:

- The polarizations were different.
- The bandwidth of the frequency spectra were mostly different.
- The cepstral resolutions were different.

To check the ability of the ALN network to measure acoustic impedance, the same after-deconvolution parameters of the spectral and cepstral waveforms (shown in the list in Fig. 19) were computed.

The true and measured acoustic impedances and their ratios (with respect to Ti-6-4) appear in Table 9. The acoustic impedances of two of the three air cavities were measured exactly. The first air cavity (0.04 cm diameter) yielded a value greater than actual. The measured acoustic impedances of the tungsten-carbide inclusion was 34.3 x 10^5 units versus the actual value of 55.2 x 10^5 units.

Table 9. True and measured acoustic impedances of actual defects using ALN synthesized from theoretical waveforms.

<table>
<thead>
<tr>
<th>DEFECT NO.</th>
<th>DEFECT MATERIAL</th>
<th>DIAMETER (cm)</th>
<th>theoretical</th>
<th>measured</th>
<th>actual</th>
<th>error</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Air</td>
<td>0.06</td>
<td>10.0</td>
<td>9.00</td>
<td>9.75</td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>Air</td>
<td>0.06</td>
<td>10.0</td>
<td>9.90</td>
<td>9.90</td>
<td></td>
</tr>
<tr>
<td>3</td>
<td>Air</td>
<td>0.06</td>
<td>20.0</td>
<td>20.0</td>
<td>20.0</td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>Tungsten-Carbide</td>
<td>0.06</td>
<td>20.3</td>
<td>9.90</td>
<td>4.68</td>
<td></td>
</tr>
</tbody>
</table>

The performance of two inverse solutions, synthesized from theoretical studies and applied to actual scattering data, is detailed in Table 10. The overall error for the diameter measurement system (0.015 cm) compares well with the resolution of the data collection system. The overall error in the impedance measurement system (of 7.64 x 10^5 gm/cm/sec) represents an error rate of 14% of the maximum impedance over the range of impedance values and compares favorably with the error rate the theoretical data set (9%).

Table 10. Performance of spherical defect measurement system, synthesized from theoretical studies, on sample real spherical defects.

<table>
<thead>
<tr>
<th>DEFECT MATERIAL</th>
<th>DIAMETER (cm)</th>
<th>theoretical</th>
<th>measured</th>
<th>Error (cm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Air</td>
<td>0.06</td>
<td>10.0</td>
<td>9.00</td>
<td>0.16</td>
</tr>
<tr>
<td>Air</td>
<td>0.06</td>
<td>10.0</td>
<td>9.90</td>
<td>0.10</td>
</tr>
<tr>
<td>Air</td>
<td>0.06</td>
<td>20.0</td>
<td>20.0</td>
<td>0.00</td>
</tr>
<tr>
<td>Tungsten-Carbide</td>
<td>0.06</td>
<td>20.3</td>
<td>9.90</td>
<td>0.43</td>
</tr>
</tbody>
</table>

Conclusions - The defect diameter solution indicates that information for measuring defect size via the scattering of ultrasonic waves from spherical defects of varying composition exists mainly in the phase spectrum. Since the phase cepstrum is a measure of the dominant periodicity in the phase spectrum, the phenomenon of scattering is not unlike the phenomenon of acoustic resonance in cavities. A cavity resonates at a characteristic frequency which is linearly dependent on its diameter. (This is true for electromagnetic waves; it is assumed the same holds true for acoustical waves.) A plot of the measured diameter from the phase cepstral analysis (theoretical waveforms) versus the resonant wavelength for different defect sizes is displayed in Fig. 23. The resonant wavelength is related to the cavity diameter as:

\[ \lambda = 1.14d, \]  

and it is independent of material properties. (The amplitude of the resonant wave is dependent on material properties, but not on the frequency of the wave.) The slope of the best-fitting line between the measured diameter (d) and true diameter (d) in Fig. 23 is:

\[ \lambda = 1.13d. \]  

Figure 23. Measured diameter from phase cepstral analysis versus acoustic resonant wavelengths of spherical defects.
Comparing Eqs. (10) and (11), it is seen that the characteristic length being measured from the phase information, d, appears to be the resonant wavelength. This suggests that resonance is induced when the (broadband) pulse strikes the cavity. This argument is plausible, because the resonant frequency is contained in the 0-10 MHz pulse bandwidth for four of the five cavities:

<table>
<thead>
<tr>
<th>Diameter, d (cm)</th>
<th>Resonant Frequency $\times 10^{14}$ (MHz)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.02</td>
<td>13.2</td>
</tr>
<tr>
<td>0.04</td>
<td>6.6</td>
</tr>
<tr>
<td>0.06</td>
<td>4.5</td>
</tr>
<tr>
<td>0.08</td>
<td>3.3</td>
</tr>
<tr>
<td>0.12</td>
<td>2.2</td>
</tr>
</tbody>
</table>

It can be seen that the resonant frequency of the 0.02 cm cavity is just outside of the 0-10 MHz band.

The second inverse solution showed that the acoustic impedance can be measured accurately by an ALN. The selected input parameters to the ALN--total normalized scattered energy and the viewing angle—are easily measurable quantities.

It is believed that these two empirical solutions (synthesized from theoretical studies to solve the inverse problem) are the first to measure sphere diameter and acoustic impedance accurately and independently of one another.

Inverse Solution for Description of Spheroidal Defects

The main objective concerning spheroids was to determine if the defect size and orientation could be estimated accurately from experimentally obtained scattering data when using ALN models synthesized from theoretical (Born) scattering data. Although this was the first attempt to solve the spheroid inversion problem, and also a first attempt at using artificial data as part of a solution, good estimates for three of the six size and orientation parameters (A, B, and $\alpha$), and an excellent estimate for the orientation parameter $\beta$ were obtained.

Defect Size and Orientation Measurement System - Four parameters were estimated to describe defect size and orientation; A, B, $\alpha$, and $\beta$. A fifth parameter, R, the radius of a sphere having the same volume as the spheroid (i.e., the cube root of the spheroid volume), was also estimated. Parameter A could be found indirectly, given R and B, but this estimate was not as accurate as the direct estimate of A. The defect measurement system is depicted in Fig. 24. During synthesis, each ALN had available the same set of 32 candidate input features during the training exercise (Table 7). Because the ALN synthesis algorithm determined which features were most relevant for each ALN, these networks use different features from the original candidate list. Note that the sine and cosine of the $\alpha$ network are used as inputs to the R network. The dashed lines show the indirect computation of A.

The network structures are given in Figs. 25 through 29. In each of these figures, the first layer elements (i.e., the left-most boxes) represent six-term quadratics of the form:

$$y = w_0 + w_1 x_1 + w_2 x_1^2 + w_3 x_2 x_3 + w_4 x_2^2 + w_5 x_3^2$$  (12)

where the x's are the input features.
Figure 27. ALN structure and network weighting coefficients to estimate orientation parameter $\alpha$ for spheroidal defects.

Figure 28. ALN structure and network coefficients to estimate orientation parameter $\alpha$ for spheroidal defects.

Figure 29. ALN and network coefficients to estimate size parameter $R$ for spheroidal defects.

Measurement of Spheroidal Defect Size and Orientation from Theoretical Data - After ALN synthesis had been accomplished with a portion of the Born data, the models were evaluated with all of the 240 Born simulated experiments. A summary of the average absolute errors for each of the six defect sizes is shown in Table 11. Each entry in the table is the absolute error for a given size averaged over 32 orientations. That is, for each size, the absolute error was computed for 32 (eight $\alpha$'s times four $\alpha$'s) of the possible 40 defect orientations. (The $\alpha = 0$ and 89 degree orientations were not used in computing the average errors as a matter of programming convenience.) An overall percentage error for each component of the measurement system is indicated in the last row. The defect size can be measured within 21.7 percent of the true value for $A$ (ALN1) and within 9 percent of the true value for $B$ (ALN2). These error rates translate to an average discrepancy in size measurement of the order of 55 microns (the average of the first two entries in the next to last row). The defect orientation can be measured with a 14 percent error in elevation, $\alpha$, via ALN3 and a 5 percent error in azimuth, $\beta$, via ALN4. Since the elevation angle was restricted to variations in a single quadrant (0 to 90°), the error rate in $\alpha$ is an angular discrepancy of 12.6°. However, the azimuthal orientation, $\beta$, can vary in a 360° span and a 5 percent error rate is an average angular discrepancy of 18°. The average angular discrepancy in measurement is 15° (average of the last two entries in the next to last row).

The performance of the spheroidal defect measurement system verifies that the inverse problem was solved with satisfactory accuracy using a family of ALN's.
Measurements of Spherical Defect Size and Orientation from Actual Data - As in the case of spherical defects, the spherical defect measurement system was applied to actual scattering data from a variety of sample, real, and oblate spherical defects. The computed size and orientation were compared to their actual values. These actual values were revealed to Adaptronics only after the measurements were made.

In spite of the several deficiencies existent in the Born approximation to the theoretical scattering model when compared to the actual scattering phenomena—-and the fact that the ALN measurement system was synthesized from the theoretical data, a remarkable agreement is found between the actual values and the measured values as shown in Table 12. The defect size is measured to within 15 percent of the true value for A and to within 37 percent for B. Thus the measurement system was synthesized from several scattering phenomena—and the fact that the ALN's orientation were compared well with the theoretical data set (50 microns). The orientation can be measured to within 26 percent of the true value of a and to within 22 percent of the true p—in other words, an angular discrepancy of 15 degrees—which matches exactly the error obtained for the theoretical data set.

Table 12. Performance of spherical defect measurement system, synthesized from theoretical data, on actual scattering data from real defects.

<table>
<thead>
<tr>
<th>DEFECT NO.</th>
<th>SIZE (In Microns)</th>
<th>ORIENTATION (In Degrees)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>TRUE</td>
<td>ALN</td>
</tr>
<tr>
<td>1</td>
<td>200</td>
<td>185</td>
</tr>
<tr>
<td>2</td>
<td>300</td>
<td>285</td>
</tr>
<tr>
<td>3</td>
<td>100</td>
<td>90</td>
</tr>
<tr>
<td>4</td>
<td>150</td>
<td>140</td>
</tr>
<tr>
<td>5</td>
<td>50</td>
<td>40</td>
</tr>
<tr>
<td>6</td>
<td>100</td>
<td>90</td>
</tr>
<tr>
<td>7</td>
<td>200</td>
<td>185</td>
</tr>
</tbody>
</table>

In addition to measuring the size parameters A and B, it was decided to monitor the performance of ALNS which measures the radius of a spherical defect having the same volume as the spherical defect. The use of ALNS as an indirect estimator of A or B (each from a direct estimate of the other) was of questionable value, because the error in the indirect estimate was compounded by the error in the direct measurement. However, ALNS provided a direct volumetric estimate and it was an additional piece of information to describe fully the defect characteristics.

The radius was measured to within 14.1 percent of the true value—an average error in length of 72 microns—which compared favorably with the errors obtained for A and B.

Conclusions - Although the Born approximation may not generate power spectra similar to the experimental spectra, the directional or spatial information present in the total waveform powers is sufficient to solve the spheroid inversion problem using ALN's. Hence, further development of similar theoretical scattering computer programs should be continued. Estimates for A, although quite good for Born data, are less accurate for the experimental data. Ways of lowering this error need to be investigated. Also, more effort is needed to determine why the estimated size parameter B was consistently biased for the real spheroid defect. This may be due to a constant bias introduced in the Born approximation spectra which is not evident for experimentally observed spectra.

The performance of the spherical defect measurement system on actual scattering data demonstrates that not only can a family of ALN's invert theoretical scattering data but it can also be applied successfully to invert actual scattering data from real defects.

Acknowledgement

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References

APPENDIX A

AXIS ROTATION ROUTINE FOR BORN PROGRAM

As received by Adaptronics, the Born approximation program was limited to simulating scattering from defects with axes of symmetry in the negative y-z plane. Also, the projector was assumed to be transmitting from positive to negative along the z axis, as shown in Fig. A.1.

Figure A1: Orientation required by the Cornell Born computer program.

To simulate more realistic physical situations, the Born approximation program was modified to permit the defect, transmitter, and receivers to be located arbitrarily. For each arrangement, a new set of axes was constructed by rotating the old axes through three Euler angles about the “rigid network” of transducers and defect. In the new coordinate system, the line of transmission PO was along the z axis and the symmetry axis ON was in the negative y-z plane. The Born program calculated the reflected power at the redefined receiver points.

In the general case, the defect axis of symmetry ON could be oriented at angles (A,B) with respect to the original coordinate system, where A was measured from the positive z axis and B was measured azimuthally from the positive x axis, as shown in Fig. A.2. Similarly, the line of transmission of the projector could have angular coordinates (e,\) where \(\) was measured from the negative z axis and e was measured azimuthally from the positive x axis. (The angles were defined to agree with the Born program conventions.)

Figure A2: Illustration of sample orientation of A, B, \(\), \(\).

The axes underwent three Euler rotations to place the transmission line PO along the z axis and the symmetry axis ON in the negative y-z plane. Each Euler rotation was about a single axis (x, y, or z) and was defined as positive when the rotation was counterclockwise as viewed from the positive axis. The coordinates (x1, y1, z1) of a point after one rotation were related to the old coordinates (x0, y0, z0) by the expression (x1,y1,z1) = M(x0,y0,z0)T, where M was a 3 x 3 matrix whose elements were determined by the angle and axis of rotation. After three rotations, the coordinates were further transformed to (x3,y3,z3)T = LKM(x0,y0,z0)T where K and L were the 3 x 3 matrices corresponding to the second and third rotations, respectively. (The superscript “T” denotes matrix transpose.)

Rotation No. 1

The first rotation was about the z axis through an angle of 4-90° to place the line of transmission in the positive y-z plane. The 3 x 3 transformation matrix for a rotation through an angle y about the z-axis is:

\[
M = \begin{bmatrix}
\cos y & \sin y & 0 \\
-\sin y & \cos y & 0 \\
0 & 0 & 1
\end{bmatrix}
\]

Here, y = 4-90°, so \(\sin y = -\cos y\) and \(\cos y = \sin y\). Therefore, matrix M becomes:

\[
M = \begin{bmatrix}
\sin y & -\cos y & 0 \\
\cos y & \sin y & 0 \\
0 & 0 & 1
\end{bmatrix}
\]

Rotation No. 2

To place the transmission line OP colinear with the z axis, the axes are rotated about the x axis through an angle \(\phi-180°\). The corresponding matrix for a rotation through an angle \(\phi\) is:

\[
L = \begin{bmatrix}
1 & 0 & 0 \\
0 & \cos \phi & \sin \phi \\
0 & -\sin \phi & \cos \phi
\end{bmatrix}
\]

In the case, \(\phi = 4-180°\), \(\sin \phi = -\sin \phi\), and \(\cos \phi = -\cos \phi\), so L becomes:

\[
L = \begin{bmatrix}
1 & 0 & 0 \\
0 & -\cos \phi & -\sin \phi \\
0 & \sin \phi & -\cos \phi
\end{bmatrix}
\]

The first two rotations place the z axis colinear with the line of transmission, as shown in Fig. A.3.
Figure A3: Orientation $\psi$ after two Euler angle transformations.

Rotation No. 3

Following the first two rotations, the defect axis of symmetry $(ON)$ is inclined at an angle $\alpha$ with respect to the negative $y$-$z$ plane. Rotating the axes through an angle $\beta$ about the $z$ axis places the symmetry axis within the $y$-$z$ plane.

The value of $\psi$ is found by transforming the original Cartesian coordinates of point $N$ through the first two rotations:

$$
\begin{bmatrix}
x_2 \\
y_2 \\
z_2
\end{bmatrix} =
\begin{bmatrix}
L & M & 0 \\
0 & 1 & 0 \\
0 & 0 & 1
\end{bmatrix}
\begin{bmatrix}
x_0 \\
y_0 \\
z_0
\end{bmatrix}
$$

The quantities $(x_0, y_0, z_0)$, assuming the point $N$ to lie on a unit sphere, are:

$$
x_0 = \cos \theta \sin \phi
$$
$$
y_0 = \sin \theta \sin \phi
$$
$$
z_0 = \cos \phi
$$

The new Cartesian coordinates $(x_p, y_p, z_p)$ determine $\psi$: $\psi = \tan^{-1} \left( \frac{y_p}{z_p} \right)$. The FORTRAN function ATAN2($x_p, y_p$) returns the proper sign of $\psi$.

The rotation $\psi$, also about the $z$ axis, has the general transformation matrix of the first rotation.

The final rotation matrix becomes:

$$
K =
\begin{bmatrix}
\cos \psi & \sin \psi & 0 \\
-sin \psi & \cos \psi & 0 \\
0 & 0 & 1
\end{bmatrix}
$$

Result

The matrix product $KLM$ transforms the original Cartesian coordinates of any point (such as a receiver location) to the corresponding values in the rotated system. Then, converted to spherical coordinates, the locations become the points at which the Born program calculates the reflected power. The defect orientation, as required by the program, is specified by a single angle between the symmetry axis and the $z$ axis. The value is: $\alpha = \tan^{-1} \left( -\frac{y_3}{z_3} \right)$, where $x_3 = 0$, $y_3$, and $z_3$ are the Cartesian coordinates of the symmetry axis in the final system, as shown in Fig. A.4.

Figure A4: Orientation $\alpha$ after three Euler angle transformations.