

Resonant Ultrasound Spectroscopy of Anisotropic Shale Samples

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ABSTRACT

Resonant Ultrasound Spectroscopy (RUS) is a technique used to determine the material properties of elastic bodies. The normal modes of a sample are measured and the resonant frequencies inverted to calculate the elastic moduli. RUS enables the complete elastic tensor to be calculated from a single measurement, fills an experimental gap between low frequency stress-strain methods and high frequency time-of-flight measurements and can provide a measure of attenuation. We investigate the experimental difficulties associated with RUS, which include sample symmetry and transducer coupling and provide a detailed discussion of the differences between vertical and horizontal transverse isotropy; two symmetries that commonly occur in geological situations. Codes are provided for a forward model and inversion method with the functionality to deal with these and other symmetries. When measured in the frequency domain using RUS and in the time domain with time-of-flight methods, the elastic properties of a shale sample display frequency dispersion.

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Chapter 1

Introduction

1.1 Resonant Ultrasound Spectroscopy

Resonant Ultrasound Spectroscopy (RUS) uses the normal modes of an elastic body to determine its elastic parameters (Migliori et al., 1993). The complete elastic tensor can be inferred from a single measurement of the resonant frequencies (Zadler et al., 2004). It is a non-destructive method that can be used on small, rare or hard-to-obtain samples (Migliori and Sarro, 1997). Schreiber et al. (1970) used resonance methods to measure the elastic moduli of glass spheres from the lunar surface. See Migliori and Sarro (1997) for a comprehensive discussion of RUS methods, covering both theoretical and experimental aspects. While RUS deals with frequencies at the high end of those relevant to geophysics, it fills an experimental gap between low frequency stress-strain measurements and high frequency time-of-flight experiments (Zadler et al., 2004). The frequency domain of the method is partially dependent on the sample size. A 2 cm sample of shale will have a fundamental mode of approximately 35 kHz whereas a 10 cm sample will have a resonant peak at about 7 kHz.

There are significant experimental issues associated with RUS (discussed in Chapter 4 and Appendix A). The effects of loading the sample and the rate of sweep were detailed by Zadler (2005) and are investigated further here. Contacting piezo-electric transducers are used and the effects of transducer location and coupling are shown to be important.

The symmetry of a sample strongly influences the normal modes. We consider isotropic, hexagonal and orthorhombic models of symmetry with a focus on hexagonal symmetry as this is commonly encountered in geological settings. Hexagonal symmetry is seen when a sample has a single axis of rotational symmetry with perpendicular isotropic planes (Tsvankin, 2001). It can result from preferential alignment of particles due to an applied stress, from fine layers formed by deposition or from parallel sets of microfractures. Geological core samples are primarily cylindrical and are often drilled parallel or perpendicular to layering, which is termed horizontal or vertical transverse isotropy respectively. For spherical and cubic samples, horizontal and vertical transverse isotropy can be described with a single model by applying a rotation of 90° . However, for a cylindrical sample the two symmetries are not identical under rotation of 90° . There are fundamental differences between the two as discussed in Chapter 3. In order to model these differences, hexagonal symmetry must be further divided into the two subcases, horizontal and vertical transverse isotropy.

Experimental issues notwithstanding, resonance experiments can be confusing and there is significant potential for the results to be misinterpreted. This is because the raw observations are spectra of signal amplitudes versus frequency from which the normal modes need to be determined and because the resonant frequencies are not coupled to the sample elastic properties in a simple way (Zadler et al., 2004).

1.2 Shales

The 'shale gas revolution' in the United States has generated significant interest in understanding and quantifying the properties of shales. Technological advances and the development of extraction techniques, such as horizontal well drilling and hydraulic fracturing (fracking), have enabled economical recovery of natural gas from shale formations (Horne et al., 2012), which comprise about 75% of the clastic fill of sedimentary basins (Tsvankin, 2001). These developments, combined with favourable geological conditions, have caused US shale gas production to soar from less than 1% of domestic gas production in 2001 to over 20% in 2010 (Stevens, 2012). Shale gas may be able to act as a low carbon fuel reducing carbon emissions today and assisting with the transition to a

renewable energy future. On the back of increased natural gas supply carbon emissions from the United States energy sector have decreased by 700 million tons annually for the past ten years (Nummedal and McCray, 2013).

Shale formations consist of thin layered sequences of aligned microscopic clay platelets (Horne et al., 2012), which are responsible for the inherent anisotropy of shales. Shales can be modeled as transversely isotropic (Tsvankin, 2001) with thin isotropic layers and an axis of symmetry perpendicular to the layering. The degree of anisotropy depends on factors such as porosity, kerogen content and microfractures (Dewhurst and Siggins, 2006) and can be characterized by five elastic constants (Thomsen, 1986a; Tsvankin, 2001). Shale anisotropy has important implications to seismic exploration and imaging (Banik, 1983; Isaac and Lawton, 1999). Information about the elastic moduli of shales is important in order to better exploit shale formations as reservoirs (Blum et al., 2013), to understand the response and distribution of stress (Dewhurst and Siggins, 2006; Holt et al., 2011) and to optimize hydraulic fracturing (Suarez-Rivera et al., 2006).

Shale anisotropy has been studied in the laboratory with a variety of methods (Dewhurst and Siggins, 2006; Sarker and Batzle, 2010; Holt et al., 2011). Here, resonant ultrasound spectroscopy (RUS) is used to determine the complete elastic tensor of a shale sample in the kHz frequency range. The aim of this dissertation is to extend upon the time-of-flight measurements performed by Blum et al. (2013) in the time domain at MHz frequencies. A common cause of anisotropy is periodic thin layering on a scale compared to the dominant wavelength (Tsvankin, 2001). It is hypothesised that measurements at different frequencies will produce different estimates of the anisotropy and elastic moduli as the wave will reveal different scale structures depending on the wavelength. Duranti and Ewy (2005) determined that a West African shale was frequency dispersive whereas Sarker and Batzle (2010) observed no significant dispersion in an organic rich shale sample from Colorado.

Because our samples are measured dry and at room conditions, the anisotropy and attenuation estimates made herein do not represent that of shales in situ (Blum et al., 2013). When core samples are removed from depth the reduction in overlying pressure can create microfractures within the sample causing induced anisotropy. Other members of the Physical Acoustics Laboratory are working towards developing the capacity

to perform similar measurements under in situ stress, both with laser-based methods and contacting transducers.

Chapter 2

Theoretical Description

The underlying principle of resonant ultrasound spectroscopy is that the resonant frequencies of a sample depend on the sample's geometry, density and elastic moduli (Migliori et al., 1993). A larger body will have lower resonant frequencies than a smaller sample. The Earth, for example, has a fundamental mode with a period of 36 minutes (Zadler et al., 2004) while a 5 cm cylinder of shale has a fundamental mode of approximately 15 kHz. An increase in the elastic moduli of a sample will increase the resonant frequencies (Zadler et al., 2004) whereas an increase in the sample density will cause the frequency of the modes to decrease.

In order to determine the elastic moduli the forward problem of calculating the resonant frequencies from the elastic constants and the sample's geometry and density must first be solved. A nonlinear inversion algorithm, derived from the work of Levenberg (1944) and Marquardt (1963), is used to find the elastic constants which correspond to the measured resonant frequencies (Migliori and Sarro, 1997).

Initial resonance measurements in the early twentieth century were restricted to certain geometries such as elongated bars which produced simple patterns of resonances for which the forward problem could be solved analytically. As the length to diameter ratio of a cylindrical sample decreases the resonances become more complicated (Zadler et al., 2004). Advances in computing power and developments in algorithms, such as the discovery by Visscher et al. (1991) that the powers of the Cartesian coordinates work as a flexible and efficient basis for computing the normal modes for arbitrary shaped

bodies, allowed for more complicated geometries to be analysed. See (Maynard, 1996) for a discussion of the history of resonant ultrasound spectroscopy.

Inverse problems are abundant in the field of geophysics and are concerned with making inferences about the properties of a system based on measured data. RUS, where the normal modes are measured and inverted to determine the elastic parameters, is an example of an inverse problem. There are numerous challenges associated with inverse problems; actual measurements of geophysical quantities are never exact (Parker, 1994) and there are almost always many possible answers to an inverse problem which cannot be distinguished by the available observations (Scales et al., 2001). This leads to many geophysical inverse problems being ill-posed with an infinite number of possible models that will fit the available data. Choosing the 'best' model is a significant challenge requiring a misfit function, which quantifies the difference between the observed frequencies and their theoretical counterparts, as well as a tolerance, which is a level of misfit which is considered acceptable (Parker, 1994). An in-depth discussion of inverse theory is outside the scope of this work. Scales et al. (2001) provides a readable introduction to inverse theory, discussing the fundamental ideas and required mathematical framework. Parker (1994) details how almost every geophysical inverse problem can be framed as an optimisation problem and Tarantola (2005) addresses inverse theory from a statistical viewpoint.

2.1 The Forward Problem

The forward problem is to calculate the expected resonances for a given stiffness tensor and known sample geometry and density. It is divided into three sections; variational approximations for resonances, elastic energy and damping, and excitation calculations. Details of the forward problem are discussed in Visscher et al. (1991), Migliori and Sarro (1997) and Zadler et al. (2004). We follow the procedure and terminology of (Zadler et al., 2004).

2.1.1 Variational approximations for resonances

Let ν be a body bounded by a closed, stress-free surface with an elastic stiffness tensor c_{ijkl} and density ρ . Let ω be a non-negative real number and $\mathbf{u}(\mathbf{r})$ be a real-valued function of position $\mathbf{r}$ in ν . $\{\omega, \mathbf{u}\}$ is a free oscillation or resonance if the real-valued displacement field

$$\mathbf{s}(\mathbf{r}, t) = \mathbb{R}(\mathbf{u}(\mathbf{r})e^{i\omega t}) \quad (2.1)$$

satisfies the elastic equations of motion in ν and the stress-free boundary condition on its surface.

The potential energy associated with the displacement field $\mathbf{u}$ is given by the strain energy

$$E_p = \frac{1}{2} \int_{\nu} C_{ijkl} \partial_j u_i \partial_l u_k dV \quad (2.2)$$

where $u_i, i = 1, 2, 3$ are the Cartesian coordinates of $\mathbf{u}$. The corresponding kinetic energy is given by

$$E_k = \omega^2 K \quad K = \frac{1}{2} \int_{\nu} \rho u_i u_i dV \quad (2.3)$$

The quantity I

$$I = \omega^2 K - E_p \quad (2.4)$$

is stationary if and only if ω and $\mathbf{u}$ are a resonance of ν . This is the key to the Rayleigh-Ritz method. We represent $\mathbf{u}$ by a prescribed basis $\{\phi_{\lambda}(\mathbf{r}), \lambda = 1, \dots, N\}$ by defining

$$u_i = a_{i,\lambda} \phi_{\lambda} \quad (2.5)$$

The choice of basis functions ϕ_{λ} is a significant issue when using the Rayleigh-Ritz method. Various trigonometric functions and orthogonal polynomials (Holland, 1968; Demarest, 1969) were used. However, these choices were developed when algebraic and

programming effort was regarded as cheaper than computer time. Substantial effort was required to formulate and programme the integrals for each new sample or geometry (Zadler et al., 2004) and the techniques were not able to keep pace with developments in computing. Visscher et al. (1991) discovered that the products of powers of Cartesian coordinates functioned as a simple and effective basis. The *xyz* algorithm

$$\phi_\lambda = x^{\eta(\lambda)} y^{\zeta(\lambda)} z^{\xi(\lambda)} \quad (2.6)$$

where l , m and n are positive integers, is numerically stable and very flexible. It allows a general anisotropic tensor with any position dependence and any shape with arbitrary density variation (Visscher et al., 1991). The stationary quantity I can be written as

$$I = \omega^2 \alpha \cdot \mathbf{K} \cdot \alpha - \alpha \cdot \mathbf{E} \cdot \alpha \quad (2.7)$$

where α is a vector of the juxtaposed components of $a_{i,\lambda}$. As mentioned previously, I is stationary, meaning that under any perturbation to α I will be unchanged to the first order, provided the values of α are consistent with the stress-free boundary condition. Therefore, $\{\omega^2, \alpha\}$ is a stationary solution if and only if they satisfy

$$\omega^2 \mathbf{K} \cdot \alpha = \mathbf{E} \alpha \quad (2.8)$$

This is the standard form for the generalized symmetric eigenvalue problem. There will be six zero eigenvalues, corresponding to the three degrees of rigid-body translation and the three degrees of rigid-body rotation. The remaining eigenvalues will be positive and correspond to elastic resonances.

2.1.2 Elastic energy and damping

We are interested in how perturbations in the sample's material properties ρ and C affect its resonance frequencies. If we perturb $\mathbf{K}$ and $\mathbf{E}$

$$\mathbf{K} \rightarrow \mathbf{K} + \delta\mathbf{K} \qquad \mathbf{E} \rightarrow \mathbf{E} + \delta\mathbf{E} \qquad (2.9)$$

and the perturbation in the squared frequency of the i th resonance is

$$\omega_i^2 \rightarrow \omega_i^2 + \delta\omega_i^2 \qquad (2.10)$$

then the perturbation in the i th resonance can be computed by

$$\delta\omega_i^2 = \frac{\alpha^{(i)} \cdot (\delta\mathbf{E} - \omega_i^2 \delta\mathbf{K}) \cdot \alpha^{(i)}}{\alpha^{(i)} \cdot \mathbf{K} \cdot \alpha^{(i)}} \qquad (2.11)$$

This equation does not contain terms in the perturbation of the eigenvector saving significant computational time.

2.1.3 Excitation calculations

Not all resonances will be observed with a particular experimental apparatus. It is useful to be able to predict the response of a sample. Consider the experiment where a sinusoidal excitation sweeping across a range of frequencies is applied at some point on the sample and the response is measured at another location. For a force applied at location $\mathbf{r}_s$ with angular frequency ω let

$$\mathbf{f}(\mathbf{r}, t) = \mathbf{f}_0 \delta(\mathbf{r} - \mathbf{r}_s) e^{i\omega t} \qquad (2.12)$$

where $\mathbf{f}_0$ is a constant vector. Define $\mathbf{s}(\mathbf{r}, t)$ as the response of ν to $\mathbf{f}$. As the applied force is sinusoidal we expect the response to be sinusoidal.

$$\mathbf{s}(\mathbf{r}, t) = \mathbf{s}(\mathbf{r}) e^{i\omega t} \qquad (2.13)$$

The resonance displacement eigenvectors

$$\nu^{(i)}(\mathbf{r}) = \alpha_\lambda^{(i)} \phi_\lambda(\mathbf{r}) \qquad (2.14)$$

form a complete basis for the set of all finite elastic displacements in ν . Therefore,

we can find coefficients γ such that

$$\mathbf{s}(\mathbf{r}) = \gamma_i \nu^{(i)} \quad (2.15)$$

It can be shown that

$$\gamma_i(\omega) = \frac{\nu_i(\mathbf{r}_s) \cdot \mathbf{f}_0}{\omega^2 - \omega_i^2} \quad (2.16)$$

which leads to the response $\mathbf{s}(\mathbf{r})$ at any point $\mathbf{r}$ as a function of the frequency ω of the applied force

$$\mathbf{s}(\mathbf{r}) = \frac{\nu_i(\mathbf{r}_s) \cdot \mathbf{f}_0}{\omega^2 - \omega_i^2} \nu^i(\mathbf{r}) \quad (2.17)$$

2.2 The Inverse Problem

The inverse problem is to compute the elastic moduli given the resonant frequencies of the sample. A misfit function, defined by equation (2.18) as the weighted difference between the measured frequencies $f^{(m)}$ and those predicted by the forward model $f^{(p)}$, is minimized using the Levenberg-Marquardt method. This elegant iterative method varies smoothly between the steepest descent method far from the minimum and Newton's method as the minimum is approached (Press et al., 1986). The minimization proceeds iteratively starting from given initial parameter values until F stops (or effectively stops) decreasing. The details of the method are discussed in Fletcher (1980), Migliori and Sarro (1997) and Press et al. (1986). We follow the treatment from Migliori and Sarro (1997).

$$F = \sum_i^N w_i (f_i^{(p)} - f_i^{(m)})^2 \quad (2.18)$$

The resonant frequencies depend nonlinearly on the elastic parameters. Therefore, we consider a model which depends nonlinearly on a set of M unknown parameters $x_\alpha, \alpha = 1, 2, \dots, M$ where M is the number of c_{ij} s. Close to the minimum solution $\mathbf{x}_0$ the misfit function can be approximated as a quadratic function by expanding F as a

Taylor series and truncating the higher order terms. The Taylor expansion of F at the vector of parameter values $\mathbf{x}$ is given by

$$F(\mathbf{x}) \approx F(\mathbf{x}_0) + \sum_{\alpha} (\mathbf{x} - \mathbf{x}_0)_{\alpha} \frac{\partial F(\mathbf{x}_0)}{\partial x_{\alpha}} + \frac{1}{2} \sum_{\alpha, \beta} (\mathbf{x} - \mathbf{x}_0)_{\alpha} \frac{\partial^2 F(\mathbf{x}_0)}{\partial x_{\alpha} \partial x_{\beta}} (\mathbf{x} - \mathbf{x}_0)_{\beta} \quad (2.19)$$

The Taylor expansion in equation (2.19) is only valid for a limited domain about $\mathbf{x}_0$. Therefore, it is important for the initial estimation of the parameters to be as accurate as possible. The Levenberg-Marquardt method is an example of a restricted step method. Far from the minimum the region about $\mathbf{x}$ where the Taylor series expansion is valid does not include a minimiser of the function F . The step from one iteration to the next is restricted by the region of validity of the Taylor series. It is also called a trust region method where the trust region refers to the region where the Taylor series is a good approximation.

If F is a minimum at $\mathbf{x}$ the first derivative in each parameter direction will be zero

$$\frac{\partial F(\mathbf{x})}{\partial x_{\alpha}} = 0, \alpha = 1, \dots, M \quad (2.20)$$

leading to

$$\frac{\partial F(\mathbf{x}_0)}{\partial x_{\alpha}} + \sum_{\beta} \frac{\partial^2 F(\mathbf{x}_0)}{\partial x_{\alpha} \partial x_{\beta}} (\mathbf{x} - \mathbf{x}_0)_{\beta} = 0 \quad (2.21)$$

which can be solved iteratively for $\mathbf{x}$ by Newton's method in M dimensions. Exact expressions for the first and second partial derivatives are shown in equations (2.22) and (2.23).

$$\frac{\partial F}{\partial x_{\alpha}} = \sum_i 2\omega_i \frac{\partial f_i^{(p)}}{\partial x_{\alpha}} (f_i^{(p)} - f_i^{(m)}) \quad (2.22)$$

$$\frac{\partial^2 F}{\partial x_\alpha \partial x_\beta} = \sum_i 2\omega_i \frac{\partial f_i^{(p)}}{\partial x_\alpha} \frac{\partial f_i^{(p)}}{\partial x_\beta} + \sum_i 2\omega_i (f_i^{(p)} - f_i^{(m)}) \frac{\partial^2 f_i^{(p)}}{\partial x_\alpha \partial x_\beta} \quad (2.23)$$

$$\approx \sum_i 2\omega_i \frac{\partial f_i^{(p)}}{\partial x_\alpha} \frac{\partial f_i^{(p)}}{\partial x_\beta} \quad (2.24)$$

In practice, the term proportional to the second derivative of the predicted frequencies in equation (2.23) is often sufficiently small that it can be ignored to save computation time (Migliori and Sarro, 1997). This is acceptable because it is multiplied by the difference between the predicted and measured frequencies $(f_i^{(p)} - f_i^{(m)})$. This term is the random measurement error and the positive and negative terms should largely cancel. Additionally, inclusion of this term can have a destabilising effect on the minimisation if the model fits badly or if the data is contaminated by outliers (Press et al., 1986).

We define a vector B and a matrix A by

$$B_\alpha = \frac{1}{2} \frac{\partial F}{\partial x_\alpha} = \sum_i \omega_i \frac{\partial f_i^{(p)}}{\partial x_\alpha} (f_i^{(p)} - f_i^{(m)}) \quad (2.25)$$

$$A_{\alpha,\beta} = \frac{1}{2} \frac{\partial^2 F}{\partial x_\alpha \partial x_\beta} = \sum_i \omega_i \frac{\partial f_i^{(p)}}{\partial x_\alpha} \frac{\partial f_i^{(p)}}{\partial x_\beta} \quad (2.26)$$

The iterative procedure for solving equation (2.21) is then

$$x_\alpha = x_{0\alpha} - \sum_\beta A_{\alpha\beta}^{-1} B_\beta \quad (2.27)$$

This is Newton's method and is only valid for $\mathbf{x}$ values close to the minimum where the Taylor series expansion in equation (2.19) is a good approximation. Far from the minimum the steepest descent method is used to take a step in the direction of the gradient. The new $\mathbf{x}$ value can be calculated by

$$x_\alpha = x_{0\alpha} - k \cdot B_\alpha \quad (2.28)$$

The Levenberg-Marquardt method is a combination of equations (2.27) and (2.28) and can be written as

$$x_\alpha = x_{0\alpha} - \sum_{\beta} G_{\alpha\beta} B_\beta \quad (2.29)$$

where

$$G_{\alpha\beta}^{-1} = A_{\alpha\beta}(1 + \Omega\delta_{\alpha\beta}) \quad (2.30)$$

If $\Omega = 0$ $G_{\alpha\beta} = A_{\alpha\beta}^{-1}$ and the Levenberg-Marquardt method in equation (2.29) reduces to Newton's method shown in equation (2.27). For large Ω G tends to a diagonal matrix and the method becomes similar to the steepest descent method. Therefore, by choosing Ω appropriately a hybrid of the two methods is achieved.

2.3 Computational Methods

The forward and inverse calculations are performed using software developed by Zadler and Le Rousseau (2005) at the Center for Wave Phenomena (CWP) at the Colorado School of Mines. These codes have dependencies on Seismic Unix, a seismic processing and research environment also developed at the CWP.

The forward code *formod-aniso* calculates the predicted resonant frequencies for a sample with given density, geometry and elastic parameters. The inversion *RUS-inverse* uses the Levenberg-Marquardt method to adjust the elastic parameters from a starting estimate to a best-fit model that minimises the difference between the measured and predicted frequencies. *RUS-inverse* requires two files; *freq_data* which contains two columns; the measured resonant frequencies in MHz and the associated weight of each mode, and *param_data* which includes the dimensions, density and initial c_{ij} values for the sample. For more information refer to the Installation and Help Guide by Zadler and Le Rousseau (2005) available at <http://physics.mines.edu/about/downloads/software/mpl/manual.pdf>. The inverse code prints to the terminal the fitted c_{ij} values, the predicted resonant frequencies at the fitted c_{ij} values as computed by a copy of *formod-aniso* nested inside *RUS-inverse*, and χ^2 , a measure of the misfit

between the measured and predicted frequencies defined by

$$\chi^{*2} = F = \sum_i^N w_i (f_i^{(p)} - f_i^{(m)})^2 \times 100 \quad (2.31)$$

where $f_i^{(m)}$ and $f_i^{(p)}$ are the measured and predicted frequencies respectively measured in MHz and w_i is the square of the weight associated with each measured mode, as given in the second column of *freq_data*. The weight is usually taken as one for a measured mode and zero for a missed or repeated peak. For a reasonable fit $\chi^{*2} = O(0.0001)$ depending on the error. Note that equation (2.31) does not account for the number of measured resonances and hence including more resonant frequencies will cause χ^{*2} to increase. In order to calculate a 'true' χ^2 value the standard deviation for each peak must be determined and the number of modes taken into account. Unless stated otherwise the quoted χ^2 values are calculated using the traditional definition given in equation (5.1).

The forward model and inverse code are able to cope with a range of symmetries from isotropic to orthorhombic. However, for hexagonal symmetry there are two sub-cases that are regularly encountered in geophysical measurements; anisotropic samples with a single axis of rotational symmetry and perpendicular isotropy planes in the horizontal or vertical direction termed VTI or HTI respectively (refer to Chapter 3). Previously, no distinction was made between these two cases. For hexagonal models VTI symmetry was assumed. We have extended the functionality of the code to include HTI symmetry. An additional parameter is required in the fourth entry of *param_data*. The value of this parameter is one for VTI symmetry or two for HTI symmetry and for a hexagonal model any other value will cause an error. The value of this parameter does not matter for other symmetries but it needs to be included in order for the other values to be read into the correct parameters. Comments have been added to the code (see Figure 2.1 and 2.2) to provide additional information about the optimisation routines used and aid readability. The updated version of *formod-aniso* and *RUS-inverse* are available at the Physical Acoustics Laboratory webpage <https://www.physics.auckland.ac.nz/research/pal/contrib/>.

```

/* ----- */
/* ----- MRQCOF ----- */
/* ----- */
/* ----- Description from: ----- */
/* ----- Numerical Recipes: the art of scientific computing ----- */
/* --W. H. Press, B. P. Flannery, S. A. Teukolsky, W. T. Vetterling - */
/* ----- */

/* Subroutine MRQCOF(X, Y, SIG, NDATA, A, MA, LISTA, MFIT, ALPHA, BETA,
 * NALP, CHISQ, FUNCS)
 * Used by MRQMIN to evaluate the linearized fitting matrix ALPHA, and
 * vector BETA from (14.4.8), the partial derivatives of chisq wrt to
 * the model parameters A */

/* called by mrqmin each iteration. Computes "chisq" */
void mrqcof(int d,int r,int *itab,int *ltab,int *mtab,int *ntab,
            int *irk,double d1,double d2,double d3,
            double rho,int shape,float freqmin,
            double y[],double sig[],int ndata,double a[],
            int ia[],int ma,double **alpha,double beta[],double *chisq,
            int hextype,
            void (*funcs)(int,int,int *,int *,int *,int *,
                          int *,double,double,double,
                          double,int,float,int,
                          double *, double *, double **, int, int))
{
    int i,j,k,l,m,mfit=0;
    double *ymod,wt,sig2i,dy,**dyda;
    /*sig2i = square of weight from 2nd col of freq_data
     ymod = modeled/predicted freqs
     dy = difference between meas and pred freqs */

    dyda=alloc2double(ndata,ma);
    ymod=alloc1double(ndata);
    for (j=0;j<ma;++j)
        if (ia[j]) mfit++;
    for (j=0;j<mfit;++j) {
        for (k=0;k<j;++k) alpha[j][k]=0.0; /* initialise alpha */
        beta[j]=0.0; /* initialise beta */
    }
    *chisq=0.0;
    /* call the forward model */
    (*funcs)(d,r,itab,ltab,mtab,ntab,
             irk,d1,d2,d3,
             rho,shape,freqmin,ndata,a,ymod,dyda,ma, hextype);
    for (i=0; i<ndata; ++i) {
        sig2i=(sig[i]*sig[i]); /* square weight from 2nd col of freq_data */
    }
}

```

Figure 2.1: Section of the updated version of *RUS-inverse* with additional comments.

```

void mrqcof(int d,int r,int *itab,int *ltab,int *mtab,int *ntab,
           int *irk,double d1,double d2,double d3,
           double rho,int shape,float freqmin,
           double y[],double sig[],int ndata,double a[],
           int ia[],int ma,double **alpha,double beta[],double *chisq,
           void (*funcs)(int,int,int *,int *,int *,int *,
                        int *,double,double,double,
                        double,int,float,int,
                        double *, double *, double **, int))
{
    int i,j,k,l,m,mfit=0;
    double *ymod,wt,sig2i,dy,**dyda;

    dyda=alloc2double(ndata,ma);
    ymod=alloc1double(ndata);
    for (j=0;j<ma;++j)
        if (ia[j]) mfit++;
    for (j=0;j<mfit;++j) {
        for (k=0;k<j;++k) alpha[j][k]=0.0;
        beta[j]=0.0;
    }
    *chisq=0.0;
    (*funcs)(d,r,itab,ltab,mtab,ntab,
             irk,d1,d2,d3,
             rho,shape,freqmin,ndata,a,ymod,dyda,ma);
    for (i=0; i<ndata; ++i) {
        sig2i=(sig[i]*sig[i]);
        dy=y[i]-ymod[i];
        for (j=-1,l=0; l<ma; ++l) {
            if (ia[l]) {
                wt=dyda[l][i]*sig2i;
                for (j++,k=-1,m=0;m<l;m++)
                    if (ia[m]) alpha[j][++k] += wt*dyda[m][i];
                beta[j] +=dy*wt;
            }
        }
        *chisq +=dy*dy*sig2i;
    }

    /* chisq prints from here */
    fprintf(stderr,"chisq=%f\n\n",100.0*(*chisq));
    for (j=1;j<mfit; ++j)
        for (k=0; k<(j-1); ++k) alpha[k][j]=alpha[j][k];
    free2double(dyda);
    free1double(ymod);
}

```

Figure 2.2: Section of the original version of *RUS-inverse*.

Chapter 3

Elastic Properties

The properties of an elastic medium are determined by the stiffness tensor (C_{ijkl}) which relates the stress (σ) applied to a sample with the strain (ϵ) experienced. The stiffness tensor has 81 components. However, for the most general model of anisotropy (triclinic) it has 21 independent parameters. This can be reduced further for higher degrees of symmetry; to five parameters for a hexagonal medium or two parameters for isotropy.

$$\sigma_{ik} = C_{ijkl}\epsilon_{kl} \quad (3.1)$$

Due to the symmetry of the stress ($\sigma_{ij} = \sigma_{ji}$) and strain ($\epsilon_{ij} = \epsilon_{ji}$) tensors the $3 \times 3 \times 3 \times 3$ elastic tensor C_{ijkl} can be expressed as a 6×6 matrix $C_{\alpha\beta}$ by replacing pairs of indices ij or kl using the Voigt recipe (Thomsen, 1986a).

$$\begin{array}{cccccccc} ij & \text{or} & kl & 11 & 22 & 33 & 32 = 23 & 31 = 13 & 12 = 21 \\ \downarrow & & \downarrow : \downarrow & \downarrow & \downarrow & \downarrow & \downarrow & \downarrow & \downarrow \\ \alpha & & \beta & 1 & 2 & 3 & 4 & 5 & 6 \end{array} \quad (3.2)$$

3.1 Isotropy

A medium is isotropic if it has uniform physical properties in all directions. Therefore, seismic waves will travel at the same speed in all directions. Isotropy is the highest possible degree of symmetry and the stiffness tensor for an isotropic medium can be

expressed by two independent parameters (Tsvankin, 2001).

$$c_{ij}^{\text{ISO}} = \begin{bmatrix} 2\mu + \lambda & \lambda & \lambda & 0 & 0 & 0 \\ \lambda & 2\mu + \lambda & \lambda & 0 & 0 & 0 \\ \lambda & \lambda & 2\mu + \lambda & 0 & 0 & 0 \\ 0 & 0 & 0 & \mu & 0 & 0 \\ 0 & 0 & 0 & 0 & \mu & 0 \\ 0 & 0 & 0 & 0 & 0 & \mu \end{bmatrix} \quad (3.3)$$

where λ and μ are Lamé's first and second parameters respectively. μ is also referred to as the shear modulus. Lamé's parameters can be related to components of the stiffness tensor by $c_{11} = \lambda + 2\mu$ and $c_{44} = \mu$ and can be converted into P (V_p) and S (V_s) wave velocities using the following equations

$$V_p = \sqrt{\frac{\lambda + 2\mu}{\rho}} = \sqrt{\frac{c_{11}}{\rho}} \quad (3.4)$$

$$V_s = \sqrt{\frac{\mu}{\rho}} = \sqrt{\frac{c_{44}}{\rho}} \quad (3.5)$$

where ρ is the density of the material. The relationships between Lamé's parameters and the more traditional Young's modulus (E), Bulk modulus (K) and Poisson's ratio (ν) are

$$E = \frac{\mu(3\lambda + 2\mu)}{\lambda + \mu} \quad K = \frac{3\lambda + 2\mu}{3} \quad \nu = \frac{\lambda}{2(\lambda + \mu)} \quad (3.6)$$

3.2 Hexagonal

A medium is called anisotropic with respect to a certain parameter if this parameter changes with the direction of measurement (Tsvankin, 2001). Inhomogeneities in physical properties, such as density and stiffness, cause seismic waves to travel faster in some directions than others. An anisotropic medium is called hexagonal if it has a single axis of rotational symmetry with perpendicular isotropic planes (Tsvankin, 2001). The

stiffness tensor for a hexagonal medium can be expressed in five independent elastic constants.

3.2.1 Vertical Transverse Isotropy

Vertical transverse isotropy (VTI) is a special case of hexagonal symmetry (Figure 3.1) where the symmetry axis aligns with the vertical direction (x_3). The VTI model frequently applies to shale formations due to the preferential alignment of clay platelets (Horne et al., 2012) and other sedimentary rocks where layers are deposited horizontally as the rock forms. The stiffness tensor for a VTI medium is defined by five independent parameters, c_{33} , c_{23} , c_{12} , c_{44} and c_{66} (Tsvankin, 2001).

$$c_{\alpha\beta}^{\text{VTI}} = \begin{bmatrix} c_{12} + 2c_{66} & c_{12} & c_{23} & 0 & 0 & 0 \\ c_{12} & c_{12} + 2c_{66} & c_{23} & 0 & 0 & 0 \\ c_{23} & c_{23} & c_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & c_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & c_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & c_{66} \end{bmatrix} \quad (3.7)$$

Seismic wave speeds vary with direction in an anisotropic medium. For a VTI sample the velocity of the P and vertically and horizontally polarized S waves depend on the angle of propagation θ to the symmetry axis. The relationship is given by equations (3.8) to (3.10) (Rüger, 2001).

$$2\rho V_P^2 = (c_{11} + c_{44}) \sin^2 \theta + (c_{33} + c_{44}) \cos^2 \theta + K \quad (3.8)$$

$$2\rho V_{SV}^2 = (c_{11} + c_{544}) \sin^2 \theta + (c_{33} + c_{44}) \cos^2 \theta - K \quad (3.9)$$

$$\rho V_{SH}^2 = c_{66} \sin^2 \theta + c_{44} \cos^2 \theta \quad (3.10)$$

where

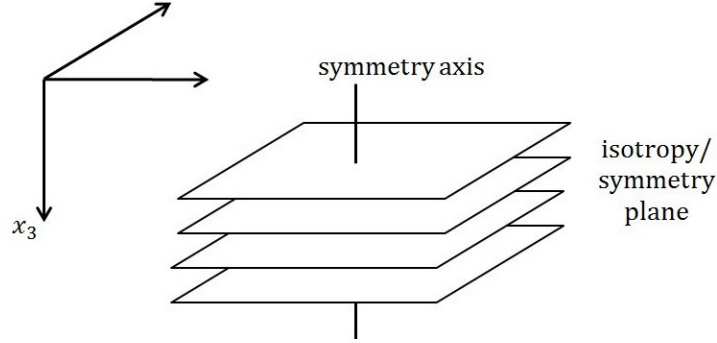


Figure 3.1: Schematic diagram of VTI medium. The symmetry axis is aligned with the vertical (x_3) direction. This geometry can be caused by alignment of clay platelets in shales or horizontal deposition of layers in sedimentary rocks.

$$K = \sqrt{((c_{11} - c_{44}) \sin^2 \theta - (c_{33} - c_{44}) \cos^2 \theta)^2 + 4(c_{23} + c_{44}) \sin^2 \theta \cos^2 \theta}$$

These equations can be evaluated to determine the seismic velocities parallel to ($\theta = 0$) and perpendicular to ($\theta = 90$) along the symmetry axis.

$$V_{P0} = \sqrt{\frac{c_{33}}{\rho}} \quad V_{SV0} = \sqrt{\frac{c_{44}}{\rho}} \quad V_{SH0} = \sqrt{\frac{c_{44}}{\rho}} \quad (3.11)$$

$$V_{P90} = \sqrt{\frac{c_{11}}{\rho}} \quad V_{SV90} = \sqrt{\frac{c_{44}}{\rho}} \quad V_{SH90} = \sqrt{\frac{c_{66}}{\rho}} \quad (3.12)$$

The degree of anisotropy can be characterized by Thomsen's parameters ϵ , δ and γ and the P and S velocities along the symmetry axis defined by equations (3.13) to (3.17). ϵ approximates the fractional difference between the horizontal and vertical P wave velocities. It provides a measure of the P wave anisotropy. γ is similar to ϵ but for the SH wave. ϵ and γ are positive quantities that are commonly quoted as the 'anisotropy' of a material. The meaning of δ is less clear but it is the most significant

term for near-vertical reflection surveys. δ relates to the angular dependence of the P wave velocity in the vicinity of the vertical direction. The velocity increases away from the vertical if δ is positive and decreases if δ is negative. ϵ , δ and γ are dimensionless parameters that go to zero in the isotropic case (Thomsen, 1986a; Tsvankin, 2001).

$$V_{P0} = \sqrt{\frac{c_{33}}{\rho}} \quad (3.13)$$

$$V_{S0} = \sqrt{\frac{c_{44}}{\rho}} \quad (3.14)$$

$$\epsilon = \frac{c_{11} - c_{33}}{2c_{33}} \quad (3.15)$$

$$\delta = \frac{2(c_{23} + c_{44})^2 - (c_{33} - c_{44})(c_{11} + c_{33} - 2c_{44})}{2c_{33}^2} \quad (3.16)$$

$$\gamma = \frac{c_{66} - c_{44}}{2c_{44}} \quad (3.17)$$

Wave speed in a solid depends on how resistant the solid is to deformation. In a stiff solid that is highly resistant to deformation, waves will travel quickly whereas in a less resistant material waves will be slower (Winterstein, 1992). A P wave parallel to the symmetry axis (V_{P0}) compresses the space between layers more easily and hence is slower than the compressional wave parallel to the isotropic planes (V_{P90}). Thomsen (1986b) explained the relative speed of shear waves propagating within a hexagonally symmetric medium using the analogy of a pack of cards. Shear motion is perpendicular to the direction of propagation and can be parallel or perpendicular to the face of the cards (where the cards represent the isotropic planes). By geometric considerations there are three different S waves polarised parallel to the layers and one polarised across the layering. It takes less energy to slides the cards over each other than it does to bend them perpendicular to the face. Therefore, the S waves polarised parallel to the layering are slower than the S wave polarised across the isotropic planes and hence there are three slow S wave polarisations and one fast polarisation. It follows that $c_{11} > c_{33}$ and $c_{66} > c_{44} = c_{55}$, in agreement with the requirement that ϵ and γ are positive.

3.2.2 Horizontal Transverse Isotropy

Horizontal transverse isotropy (HTI) is another special case of hexagonal symmetry (Figure 3.2) commonly encountered in geological settings. The symmetry axis of the sample is aligned with one of the horizontal axes (taken as x_2 in this analysis) while the planes of isotropy are in the vertical direction. HTI symmetry can be caused by near-vertical parallel sets of fractures which can form when the overburden pressure is removed as the rock is brought to the surface. The stiffness tensor for a HTI medium has five independent components, c_{11} , c_{33} , c_{12} , c_{44} and c_{66} (Tsvankin, 2001).

$$c_{\alpha\beta}^{\text{HTI}} = \begin{bmatrix} c_{11} & c_{12} & c_{12} & 0 & 0 & 0 \\ c_{12} & c_{33} & c_{33} - 2c_{44} & 0 & 0 & 0 \\ c_{12} & c_{33} - 2c_{44} & c_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & c_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & c_{66} & 0 \\ 0 & 0 & 0 & 0 & 0 & c_{66} \end{bmatrix} \quad (3.18)$$

HTI symmetry is often treated as a rotation of VTI symmetry. This is appropriate for spherical or cubic samples where the two situations are physically indistinguishable, bar the 90° rotation. The predicted resonant frequencies for VTI and HTI spheres and cubes are identical once the appropriate coordinate transformation, as detailed in equation (3.19), has been applied to account for the rotation. Equation (3.19) assumes that the symmetry axis of the VTI sample is aligned with x_3 and that isotropic planes of the HTI sample are parallel with the x_3 axis.

$$\begin{array}{ccccccc} \text{VTI} & c_{11} & c_{12} & c_{13} & c_{33} & c_{44} & c_{66} \\ \updownarrow & : & \updownarrow & \updownarrow & \updownarrow & \updownarrow & \updownarrow \\ \text{HTI} & c_{33} & c_{23} & c_{12} & c_{11} & c_{66} & c_{44} \end{array} \quad (3.19)$$

The velocity equations become

$$V_{P0} = \sqrt{\frac{c_{11}}{\rho}}, \quad V_{SV0} = \sqrt{\frac{c_{66}}{\rho}}, \quad V_{SH0} = \sqrt{\frac{c_{66}}{\rho}} \quad (3.20)$$

$$V_{P90} = \sqrt{\frac{c_{33}}{\rho}}, \quad V_{SV90} = \sqrt{\frac{c_{66}}{\rho}}, \quad V_{SH90} = \sqrt{\frac{c_{44}}{\rho}} \quad (3.21)$$

The subscript 0 indicates a direction of propagation parallel to the symmetry axis while 90 means the wave travels perpendicular to the symmetry axis. Thomsen's parameters transform to

$$V_{P0} = \sqrt{\frac{c_{11}}{\rho}} \quad (3.22)$$

$$V_{S0} = \sqrt{\frac{c_{66}}{\rho}} \quad (3.23)$$

$$\epsilon = \frac{c_{33} - c_{11}}{2c_{11}} \quad (3.24)$$

$$\delta = \frac{2(c_{12} + c_{66})^2 - (c_{11} - c_{66})(c_{33} + c_{11} - 2c_{66})}{2c_{11}^2} \quad (3.25)$$

$$\gamma = \frac{c_{44} - c_{66}}{2c_{66}} \quad (3.26)$$

The same arguments for the relative wave speeds in VTI symmetry can be applied to HTI. Hence, it can be deduced that the P wave parallel to the symmetry axis is slower than the P wave which travels parallel to the isotropic planes and that there are three slow and one fast S wave polarizations. It follows that $c_{33} > c_{11}$ and $c_{44} > c_{66} = c_{55}$, in agreement with the transformation detailed in equation (3.19).

Most geological samples of interest are cylindrical. The resonant frequencies for VTI and HTI cylinders are different and the samples cannot be treated as a simple rotation of each other. For a VTI cylinder, where both S wave polarisations along the symmetry axis have the same wave speed, the fundamental mode is often the reciprocal of two-way travel-time of the S wave that propagates along the length of the cylinder. For HTI the two S wave polarisations have different speeds and the fundamental mode is more complicated and depends on multiple c_{ij} 's. For VTI cylinders flexural modes,

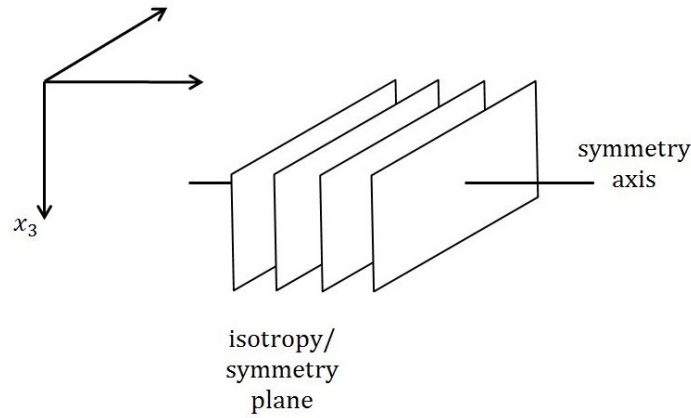


Figure 3.2: Schematic diagram of HTI medium. The symmetry axis is aligned in the horizontal plane (x_1 and x_2 plane) and the isotropic planes are in the vertical (x_3) direction. This geometry can be caused by parallel sets of near vertical fractures.

where energy travels along paths that are tilted with respect to the symmetry axis, occur in pairs, called doublets, with the same resonant frequency (Zadler et al., 2004). Doublets do not appear in the spectra of a HTI cylinder. This may be because a HTI cylinder is not axisymmetric about the cylinder axis. However, the number of resonant modes within a given frequency range is similar for both samples. Therefore, within a given frequency range, for a HTI sample there are more distinct modes that are able to be measured. This provides more information for the inversion but increases the complexity of the spectrum creating challenges for identifying modes consistently between repeated measurements. VTI and HTI symmetries are fundamentally different and cannot be treated as related by a simple rotation, except for spherical or cubic samples that are of little interest to the exploration community.

3.3 Orthorhombic

This is the lowest order of symmetry that we consider. Orthorhombic symmetry consists of three mutually orthogonal planes of mirror symmetry (Tsvankin, 2001) and can be considered as a combination of VTI and HTI. Geologically, orthorhombic symmetry can occur due to a set of parallel near-vertical fractures in a horizontally layered medium.

The elastic tensor is described by nine independent components. If each coordinate plane is a symmetry plane the stiffness tensor can be written as (Tsvankin, 2001)

$$c_{\alpha\beta}^{\text{ORTH}} = \begin{bmatrix} c_{11} & c_{12} & c_{13} & 0 & 0 & 0 \\ c_{12} & c_{22} & c_{23} & 0 & 0 & 0 \\ c_{13} & c_{23} & c_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & c_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & c_{55} & 0 \\ 0 & 0 & 0 & 0 & 0 & c_{66} \end{bmatrix} \quad (3.27)$$

In principle, for a robust inversion code, an orthorhombic model should be able to be fitted to a rock with a higher degree of symmetry, such as hexagonal or isotropic (Migliori and Sarro, 1997). However, this is not always feasible as more data is required to constrain the nine independent parameters.

3.4 Attenuation

Attenuation is a process that dissipates the energy of elastic waves and alters their amplitude and frequency content (Zhu and Tsvankin, 2006). Generally, attenuation varies much more than seismic velocities. However, it is more difficult to measure attenuation than velocities experimentally (Toksöz et al., 1979). Attenuation can be used to supplement velocity information when inferring saturation conditions or pore fluid (Toksöz et al., 1979) and ignoring attenuation effects can lead to errors in amplitude variation with offset (Zhu and Tsvankin, 2006).

Attenuation depends on the saturation and physical properties of a sample. Mechanisms responsible for attenuation include friction on grain boundaries and in thin cracks (Tao and King, 1990), dissipation in a saturated rock due to relative motion of the frame with respect to fluid inclusions, and attenuation due to fluid flow, as well as geometrical effects such as scattering by small pores and large irregularities and selective reflection from thin beds (Johnston et al., 1979). Attenuation for fluid saturated rocks is higher than for dry rocks and decreases with increasing confining pressure (Johnston et al., 1979). Therefore, the attenuation estimates here, measured with dry rocks at

atmospheric pressure, are not representative of what would be observed under reservoir conditions.

Attenuation can be quantified by the quality factor Q defined by

$$Q = \frac{\omega_0}{\Delta\omega} \quad (3.28)$$

where ω_0 is the resonant frequency and $\Delta\omega$ is the full width at half maximum. The quality factor Q of a dry rock is not frequency dependent (Tao and King, 1990). Resonance methods allow the Q factor to be determined easily as ω_0 and $\Delta\omega$ can be read from the measured spectra.

A *MATLAB* or *SciLab* package *fitspectra* (Zadler and Le Rousseau, 2005) can be used to fit a Breit-Wigner model (Breit and Wigner, 1936) to the data:

$$A(f) = B_0 + B_1(f - f_0) + \sum_n^N \frac{C_n + D_n(f - f_0)}{(f - f_n)^2 + \frac{1}{4}\Gamma_n^2} \quad (3.29)$$

where $A(f)$ is the displacement amplitude which is a function of frequency and B_0 and B_1 describe a constant and linear background to the model. Each mode is described by an amplitude C_n , skewness D_n , eigenfrequency f_n and full width at half max Γ_n (Zadler et al., 2004). This assumes that each mode has a Lorentzian shape and that multiple overlapping modes can be considered as a superposition of Lorentzians (Zadler et al., 2004). The Q factor can be calculated from f_n and Γ_n . For more details on *fitspectra* refer to the Installation and Help Guide by Zadler and Le Rousseau (2005).

Chapter 4

Experimental Design and Considerations

A function generator (DS345) sends a sinusoidal signal (10V peak-peak) to a contacting piezo-electric source transducer, sweeping across a range of frequencies. The vibration propagates through the sample and the response, as measured by the receiver transducer, is detected with a DSP (Digital Signal Processing) lock-in amplifier (SR850). The signal is divided into a component x in phase with the lock-in reference signal and a component y out of phase. The magnitude of the two components $R = \sqrt{x^2 + y^2}$ is passed to the computer via a PCI digital oscilloscope card and the resonances determined from this measurement. The experimental setup is shown in Figure 4.1 with a schematic diagram (Figure A.1) included in Appendix A. For more details on the experimental setup and RUS methodology refer to Appendix A.

4.1 Sample Geometry

Sample geometry affects data acquisition. Zadler et al. (2004) computed the theoretical resonances for cylinders with a range of length to diameter ratios for generic soft rock (Figure 4.2). Elongated samples (with a greater length to diameter ratio) have fewer excited modes and a simpler spectra. As the length to diameter ratio decreases more modes are excited and the spectrum becomes more complicated. The bottom spectrum,

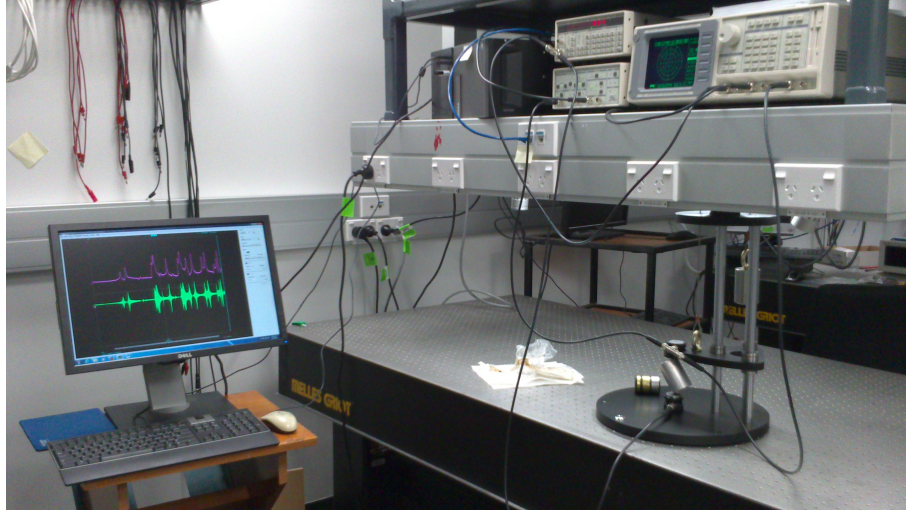


Figure 4.1: Experimental setup. The function generator and lock-in amplifier are shown in the top right corner. Below the function generator is a pre-amplifier (SRS560) that was used in our original setup.

for a squat cylinder, is much more complicated than for the elongated bar in the top plot. The increasing complexity of spectra as the length to diameter ratio decreases is why it took many years of algorithm development and computing advances before the forward problem could be solved efficiently for squat cylinders and for geometries other than elongated bars.

At least five resonant frequencies should be measured for each parameter to be determined (Migliori and Sarro, 1997). Compared to a short squat sample, measurements must be made across a wider range of frequencies for an elongated sample in order to measure the same number of normal modes. For the same frequency band displayed in Figure 4.2 nine modes are measured for the squat bar in the bottom plot while only three are observed for the elongated bar in the first plot. For an anisotropic sample more data is needed in order to rigorously invert for the greater number of independent components of the elastic tensor.

Geological samples of interest often have a low quality factor Q . Low Q materials have fewer observable resonance frequencies than high Q materials (Ulrich et al., 2002). A squat sample has a more complicated spectra providing more data for the inversion. However, the complexity of identifying peaks consistently between repeated measure-

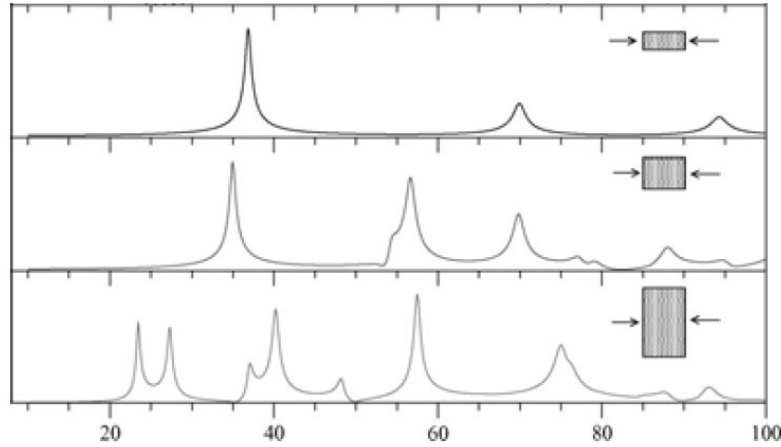


Figure 4.2: The theoretical resonance response of a generic soft rock ($\rho = 2.5 \text{ gm cm}^{-3}$, $V_P = 3.000 \text{ km s}^{-1}$, $V_S = 1.400 \text{ km s}^{-1}$) sample for several length to diameter ratios. Frequency is plotted on the x-axis and amplitude of the response on the y-axis. The spectra is simpler for elongated samples than for samples with reduced length to diameter ratios. Adapted from Zadler et al. (2004).

ments increases as the closely spaced modes can become distorted by neighbouring resonant modes, especially in geological materials with low Q factors and broad peaks.

4.2 Transducer Location

Measurements are made using contacting transducers. The coupling of the transducer to the rock influences which modes are measured. When the sample is pinned on its edges more modes are excited and the modes are better defined than when the transducers are placed on the ends of the cylinder (Figure 4.3) The experimental apparatus is set up so that the sample is balanced edge on between the transducers (Figure 4.4) in order to excite the maximum number of resonances possible for a fixed geometry.

4.3 Loading

The derivation of the forward problem assumes a stress-free boundary condition on the surface of the sample (Zadler et al., 2004). The sample is lightly pinned between

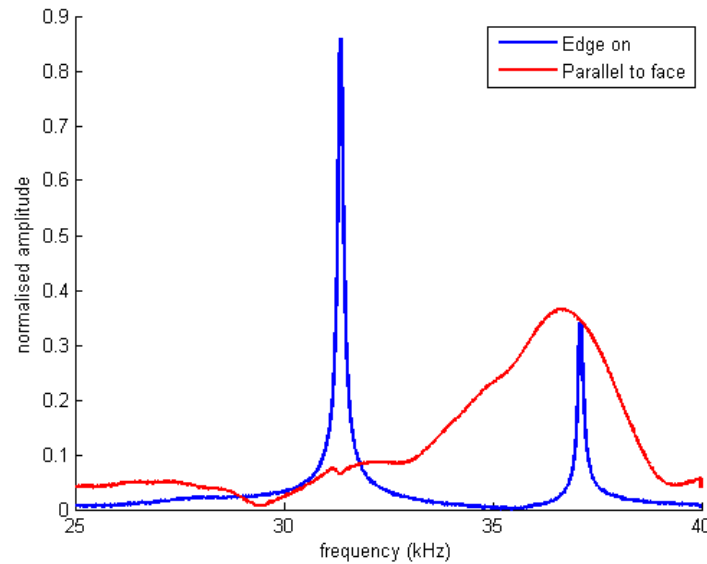
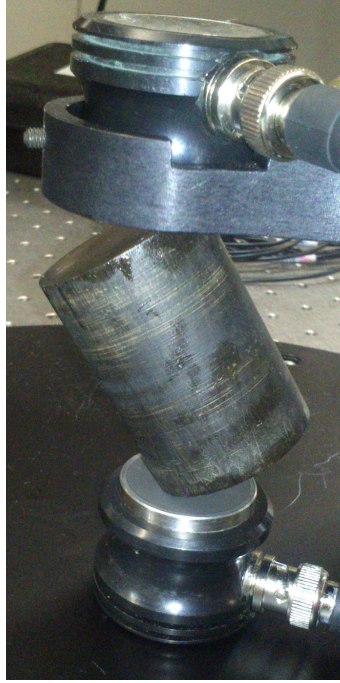


Figure 4.3: The effect of transducer coupling for a sample of aluminum. If the sample is pinned edge on between the transducers (Figure 4.4) more modes are excited and the peaks are more clearly defined. If the transducers are pinned parallel to the flat ends of the cylinder the resonances are weaker and less defined.

the source and receiver transducers in order to approximate this boundary condition. However, the loading (the mass of the top transducer that rests on the sample) is non-negligible and must be corrected for. The effect of loading is to increase the resonance frequencies (Zadler, 2005). Measurements are made for different values of loading in order to determine a relationship between the loading mass on the sample and the change in resonant frequencies. The relationship can be extrapolated to determine the resonance frequencies that would be measured with zero loading.

Flexural modes occur in pairs called doublets or degenerate modes. Excess loading can cause the two members of the doublet to experience different frequency shifts so that a single peak can be distorted into two distinct peaks in a loaded sample. This can also occur due to poor sample preparation or inhomogeneities such as cracks or inclusions (Ulrich et al., 2002).



(a) Pinned edge-on between transducers



(b) Pinned flat between transducers

Figure 4.4: Samples are pinned edge on to the transducers as shown in (a) and not with the flat face of the cylinder parallel to the transducer surface (b) in order to excite the maximum number of modes possible.

4.4 Sensitivity of modes

The low frequency resonances are strongly dependent on the S wave and only weakly sensitive to the P wave moduli. Therefore, RUS experiments constrain the S wave related c_{ij} 's more than those associated with the P wave speed (Migliori et al., 1993; Ulrich et al., 2002). The frequency of the first mode which is substantially sensitive to V_P can be decreased by reducing the length to diameter ratio of the sample. Hence, squat samples enable the c_{ij} 's associated with the P wave speed to be determined at lower frequencies.

Zadler et al. (2004) computed the sensitivities of each mode to perturbations in V_P and V_S for a sample of generic isotropic soft rock ($\rho = 2.5 \text{ gm cm}^{-3}$, $V_P = 3.000 \text{ km s}^{-1}$, $V_S = 1.400 \text{ km s}^{-1}$, height = 3.099 cm, radius = 0.635 cm). The lowest frequency

mode which is significantly sensitive to V_P is at approximately 150 kHz, well above the upper frequency limit of our experimental apparatus. However, doubling the radius of the sample decreases the frequency of this mode to 80 kHz, which is observable with our equipment.

Chapter 5

Results: Aluminum

5.1 Aluminum

In order to test the quality of our apparatus and the accuracy of our methodology we first tackled the problem of determining the elastic parameters of an aluminum cylinder which is 5 cm high with a diameter of 3.82 cm and a density of 2.71 g/cm³. Aluminum is a good test material as it is well studied, with reliable results available in the literature to which our inversion results can be compared. Aluminum is an isotropic material requiring only two independent elastic parameters (λ and μ or equivalently c_{11} and c_{44}) to describe the material. Fewer resonant peaks are required to confidently estimate the elastic tensor for an isotropic material than for a sample with a lower degree of symmetry as the elastic tensor has fewer independent components. Additionally, aluminum has a high Q factor so most resonances are well defined and the amplitude decreases rapidly away from the eigenfrequency. Therefore, resonant peaks do not contribute significantly to neighbouring modes reducing issues associated with mode identification.

18 resonant modes were recorded between 30 and 100 kHz. This was more than enough information to accurately fit the two independent elastic parameters (Migliori and Sarro, 1997; Ulrich et al., 2002). The sample was rotated, remounted and measured six times with a loading of 30.6 ± 1.4 g in order to determine the frequency of each mode and the associated error. Three sweeps were performed with V101 transducers and three with V151 transducers. The V101 transducers are designed for P wave

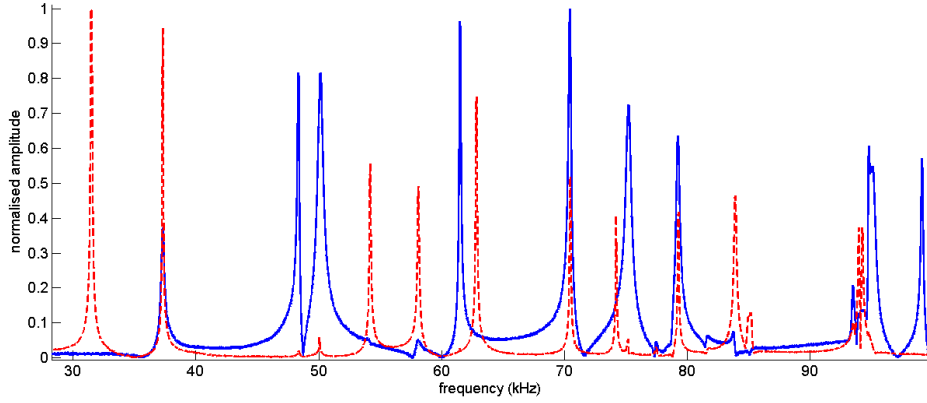


Figure 5.1: Resonant spectra of aluminum cylinder from 30 to 100 kHz. Blue solid line is measured with V101 transducers and red dashed line with V151.

detection while the V151 transducers excite shear motion. Figure 5.1 shows how using both types of transducers enabled more resonances to be observed than is possible with only one transducer type.

18 of the first 24 modes were observed and the missing six resonances were filled in by the forward code. They were given zero weighting and acted as placeholders, not contributing to the final misfit value. χ^2 , the misfit between the measured and predicted frequencies, is defined by

$$\chi^2 = \frac{1}{N} \sum_i^N w_i \left(\frac{f_i^{(\text{obs})} - f^{(\text{pre})}}{\sigma_i^{(\text{obs})}} \right)^2 \quad (5.1)$$

where N is the number of measured modes, $f^{(\text{obs})}$ and $f^{(\text{pre})}$ are the measured and predicted frequencies respectively, $\sigma^{(\text{obs})}$ is the observed uncertainty in each mode and w is the weight of the mode. w is included in the χ^2 definition so that placeholder modes with a zero weighting do not contribute. A curious feature of RUS measurements is that the first one or two modes always give a bad fit, regardless of the apparatus, transducer type, sample, or other experimental considerations (Migliori and Sarro, 1997). Therefore, the first mode, which makes a significant contribution to the variance, is given a weight of zero.

The measured and predicted frequencies and the observed error are shown in Table

5.1. χ^2 is calculated as 32.2 which is higher than expected for convergence ($\chi^2=1$). For each resonant peak the measured frequency is the average of the frequencies observed in the repeated measurements and the error is the standard deviation. Not all peaks are observed in all measurements. For some resonant peaks the standard deviation is calculated using a smaller data set which is likely to underestimate the error and overestimate χ^2 . An average error is computed from the resonant peaks that were observed in five or more sweeps. This results in χ^2 decreasing to 8.3 which is closer to unity.

Aluminum					
$f^{(obs)}$ (Hz)	$f^{(pre)}$ (Hz)	$\sigma^{(obs)}$ (Hz)	$(\frac{f^{(pre)}-f^{(obs)}}{\sigma^{(obs)}})^2$	# peaks obs.	freq. #
31468	31356	16	49.00	3	1
37321	37450	47	7.53	6	2
48345	48774	42	104.33	3	3
50128	49773	95	13.96	5	4
54160	54159	46	0.00	3	5
58076	58236	62	6.66	3	6
61508	61555	21	5.01	5	7
62822	62712	21	27.4	2	8
70454	70257	16	151.60	5	9
74198	74095	18	32.74	3	10
75248	75127	38	10.14	3	11
77423	77788	35	108.76	2	12
79189	79292	159	0.42	6	13
81572	81550	89	0.06	2	15
83811	83708	85	1.47	5	16
93498	93307	30	40.53	4	19
94767	94808	13	9.95	4	23
99125	99285	31	26.64	4	24

Table 5.1: Comparison of measured ($f^{(obs)}$) and predicted ($f^{(pre)}$) resonant frequencies of aluminum. $\sigma^{(obs)}$ is the uncertainty in each frequency calculated from repeated measurements, $(\frac{f^{(pre)}-f^{(obs)}}{\sigma^{(obs)}})^2$ is the relative contribution of $f^{(obs)}$ to the total χ^2 , # peaks. obs is the number of measurements that each mode was observed in and freq. # is the number of the identified mode.

The fitted c_{ij} values are shown in Table 5.3 and are similar to those quoted in the

literature (Scruby and Drain, 1990; Zadler and Le Rousseau, 2005). Uncertainty in the c_{ij} values was estimated from the inversion procedure. For a wide range of starting c_{44} values the inversion will converge to the same value. However, depending on the initial value of c_{11} the iterations will converge to a wider range of possible c_{11} solutions. The uncertainty is greater for c_{11} than c_{44} because the low frequency modes are only weakly sensitive to V_P (Zadler et al., 2004) but depend strongly on the shear moduli. Reducing the error in c_{11} would require extending the work to higher frequencies (we were limited by the 102 kHz upper operating limit on the lock-in amplifier) or changing the sample geometry to have a greater diameter to height ratio.

The Q factor for the first peak is 115. This is significantly larger than for the shales and is reflected in the sharper peaks observed in Figure 5.1.

5.2 Aluminum with Foil Jacket

Other members of the Physical Acoustics Laboratory are measuring the elastic properties of core samples under pressure. In order to do this the rock needs to be encased so that the pressurising fluid does not seep into the pore space of the rock and distort its properties. A significant number of the rock samples available in the lab were covered, or partially covered by various foils. Many exploration companies coat samples in wax as they are removed from depth in order to preserve the sample. The wax is removed while experiments are carried out and promptly reapplied. Understanding the effect of a layer of wax on the resonant modes may enable RUS measurements to be made without removing the coating. Understanding the effect of the foil jacket on measurements is a preliminary step in this direction as well as towards making RUS measurements under pressure. The aluminum cylinder with the foil jacket is shown in Figure 5.2. The jacket consists of thin layers of foil approximately 1 mm thick which partially cover the curved face of the cylinder.

Acquisition was performed using the same parameters as for the aluminum sample without the foil jacket. Six sweeps were made with the sample remounted and rotated between measurements. The loading was 37.8 ± 3.7 g, 7 g greater for the sample without the jacket. The excess loading should cause the observed frequencies to be higher for the jacketed sample by ~ 10 Hz (Zadler, 2005). The measured and predicted frequencies and the observed error are shown in Table 5.2 and the fitted c_{ij} values in

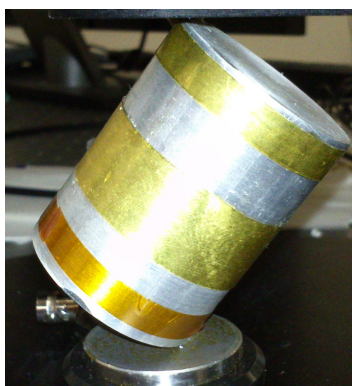


Figure 5.2: Aluminum sample with the foil jacket.

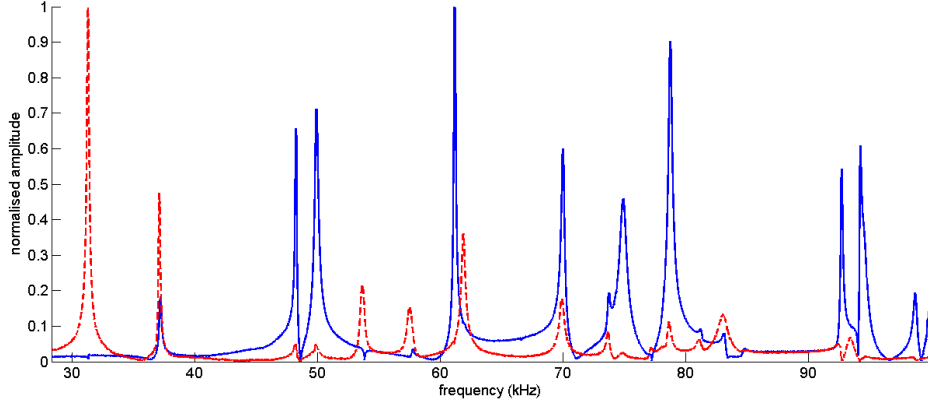


Figure 5.3: Resonant spectra of aluminum cylinder with the foil jacket from 30 to 100 kHz. Blue solid line is measured with V101 transducers and red dashed line with V151.

Table 5.3.

The variance is dominated by modes one and eight. The first mode is given a weight of zero as the first mode in RUS measurements is often a poor fit (Migliori and Sarro, 1997). Peak eight has a very small uncertainty term (23 Hz) that may be underestimated as the result of the mode only being observed in three sweeps. χ^2 is calculated as 6.7 using equation (5.1), with the first mode assigned a weighting of zero and using an average error of 68 Hz. The average error is determined from the seven resonances which are observed in all six sweeps.

The foil jacket makes a clearly measurable difference to the resonances as illustrated in Figure 5.4. The effect of the jacket is to decrease the frequency of the resonant modes by 425 ± 230 Hz. If the loading was the same between measurements the difference would be ~ 10 Hz greater.

The effect is observable in the results of the inversion. The sample with the foil jacket has a lower shear modulus. For the aluminum without the jacket c_{44} is calculated as 26.6 ± 0.1 and for the sample with the jacket $c_{44} = 26.3 \pm 0.1$. The c_{11} values are the same within errors bars. Extending the work to higher frequency modes with greater sensitivity to c_{11} may result in observable differences in c_{11} . However, within our range of investigation, despite the resonant frequencies being higher for the sample without the jacket for all modes only c_{44} differs between the jacketed and non-jacketed samples.

Aluminum with foil jacket					
$f^{(obs)}$ (Hz)	$f^{(pre)}$ (Hz)	$\sigma^{(obs)}$ (Hz)	$(\frac{f^{(pre)}-f^{(obs)}}{\sigma^{(obs)}})^2$	# peaks obs.	freq. #
31301	31150	15	128.88	3	1
37168	37238	50	0.12	6	2
48237	48475	29	77.75	5	3
49886	49455	67	41.05	6	4
53691	53805	32	17.62	5	5
57661	57867	119	3.54	6	6
61144	61156	46	3.01	6	7
62010	62300	23	294.76	3	8
69966	69818	43	5.60	6	9
73671	73631	56	1.20	6	10
74833	74663	75	5.60	4	11
77234	77351	43	5.45	3	12
78759	78632	47	27.74	3	13
81287	81110	94	7.89	4	15
83101	83233	44	0.09	4	16
92618	92710	99	1.51	6	19
94292	94214	90	0.13	3	23
98712	98777	45	0.48	3	24

Table 5.2: Comparison of measured ($f^{(obs)}$) and predicted ($f^{(pre)}$) resonant frequencies of aluminum with foil jacket. $\sigma^{(obs)}$ is the uncertainty in each frequency calculated from repeated measurements, $(\frac{f^{(pre)}-f^{(obs)}}{\sigma^{(obs)}})^2$ is the relative contribution of $f^{(obs)}$ to the total χ^2 , # peaks. obs is the number of measurements that each mode was observed in and freq. # is the number of the identified mode.

Sample	c_{11}	c_{44}	χ^2
Aluminum	109.8 ± 2.0	26.6 ± 0.1	8.3
Aluminum with foil jacket	110.0 ± 2.0	26.3 ± 0.1	6.7

Table 5.3: Summary of elastic moduli (GPa) and χ^2 (dimensionless) for aluminum with and without a foil jacket.

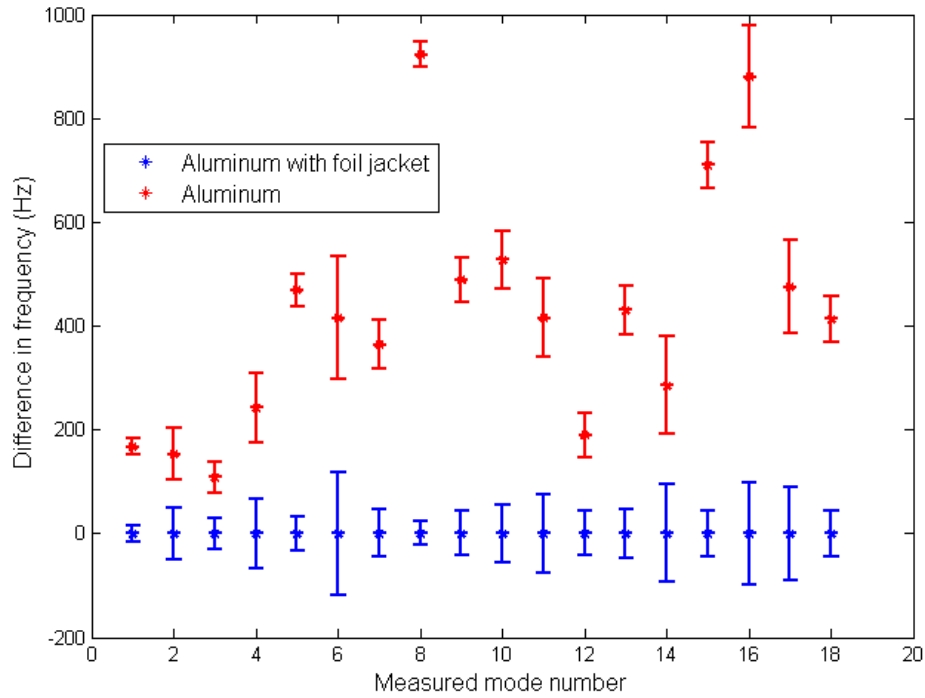


Figure 5.4: Effect of foil jacket on the resonant frequencies of an aluminum cylinder. The number of the measured mode is plotted on the x axis (the absolute frequency of the mode increases to the right) against the difference between the resonant frequencies with and without the foil jacket. All modes are higher in frequency for the sample without the foil jacket. The average difference is 425 ± 230 Hz.

Chapter 6

Results: Shale

Shale MSH is an oil shale from an outcrop in Montana (Blum et al., 2013). We measured two mutually perpendicular cores drilled within centimeters of each other. The shale displays considerable heterogeneity. The density of the VTI core is 2.1 g/cm^3 and for the HTI core is 1.7 g/cm^3 . Therefore, the two cores do not provide complementary information that can be used to constrain the inversion of the other.

6.1 Horizontal Transverse Isotropic (HTI) Sample

Shale MSH (HTI) is 5.39 cm high with a diameter of 3.76 cm and a density of 1.70 g/cm^3 . 25 resonant modes were measured between 10 and 50 kHz with a rate of sweep of 0.0005 Hz. Six measurements were performed, three with V101 and three with V151 transducers, with the sample rotated and remounted between sweeps. The loading of the sample was kept at $9.9 \pm 1.5 \text{ g}$. Table 6.1 compares the measured and predicted frequencies and the relative error contribution of each mode.

The resonant frequencies were determined from each measurement and the uncertainty for each mode was calculated as the standard deviation of the measured data set. Not all modes were measured in every sweep and hence for some peaks the standard deviation was calculated using less data points. It is expected that this would result in an underestimation of the errors and hence an overestimation of χ^2 . Further work is required to improve the error estimation. The first mode dominates the relative uncer-

tainty contributions. This is a common feature of RUS measurements in which the first one or two modes do not fit well regardless of the apparatus, sample geometry or other experimental considerations (Migliori and Sarro, 1997). Therefore, in the inversion the first and second modes are assigned a weighting of zero and do not contribute to the calculation of χ^2 .

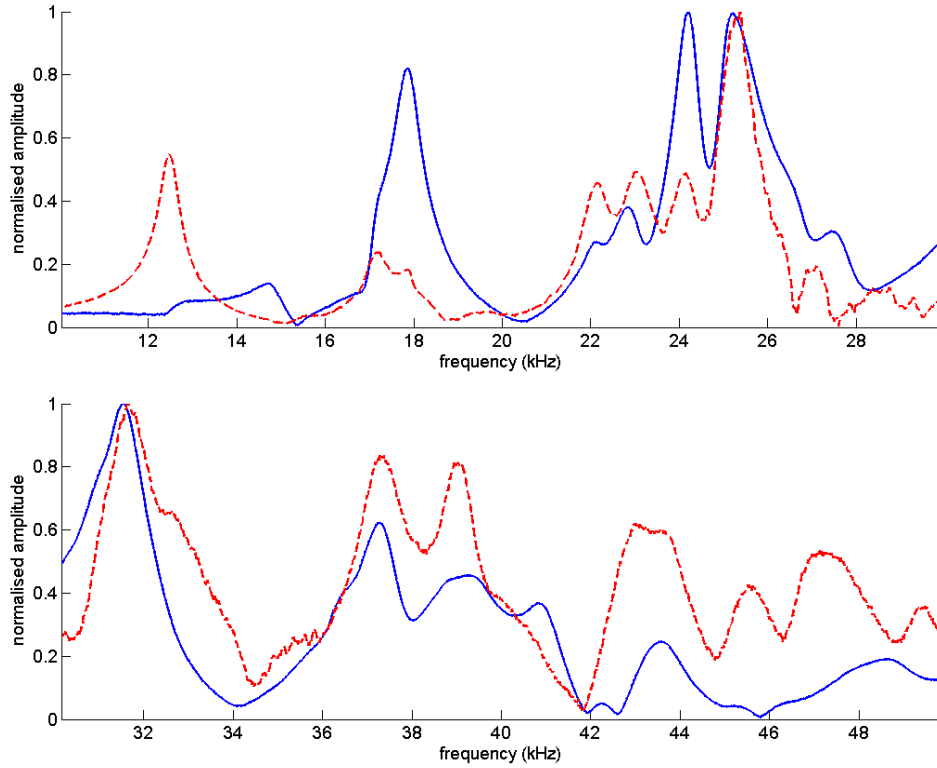


Figure 6.1: Measured spectra of shale MSH HTI from 10 to 30 kHz (top) and 30 to 50 kHz (bottom). The blue solid line is the response using V101 transducers which excite and recorded compressional motion. The red dashed line is the measured spectra using V151 transducers which measure the shear motion preferentially.

The final c_{ij} values and Thomsen's anisotropy parameters for a horizontally transverse isotropic model are shown in Table 6.2. The χ^2 value is 6.5 calculated from equation (5.1) and is a significant improvement over an isotropic fit with a χ^2 of 154. To partially account for the effect of the missing modes in some sweeps an average error can be calculated from the peaks which were observed in most measurements. Using

an average error of 186 Hz calculated from the thirteen modes which were observed in four or more sweeps gives $\chi^2 = 1.6$.

The P and S wave speeds parallel to the symmetry axis are $V_{P0} = 2590 \pm 110 \text{ ms}^{-1}$ and $V_{S0} = 1110 \pm 30 \text{ ms}^{-1}$ respectively. Perpendicular to the symmetry axis $V_{P90} = 2920 \pm 100 \text{ ms}^{-1}$ and the fast S wave speed is $1590 \pm 40 \text{ ms}^{-1}$. ϵ and γ are positive indicating that the P wave and a polarisation of the S wave increase in velocity away from the symmetry axis. The negative value of δ shows that in the near-vertical the velocity of the P wave decreases away from the vertical. δ has a larger error as more operations are required to compute δ from the c_{ij} values (nine operations) than for ϵ or γ (two operations) and the errors are amplified as they are propagated through the calculations.

The attenuation can be calculated from the amplitude spectrum (Section 3.4) using equation (3.28). For shale MSH HTI the first normal mode occurs at 12473 Hz with a full width at half maximum of 790 Hz. Therefore, the Q factor is 15.8 which, as expected, is substantially less than for the aluminum.

Time-of-flight measurements were used to provide initial estimates for the c_{ij} values and to investigate the effect of frequency on the observed elastic moduli. In the time-of-flight measurements a pulse generator excited a contacting transducer which sent a pulse propagating through the rock. The response, as measured by another piezo-electric transducer, was displayed on an oscilloscope (Tectronix TDS 380). The pulse has a dominant frequency of 500 kHz. The travel time and wave speed were determined from the oscilloscope output. The use of contacting transducers enabled the S wave speed to be measured, providing additional information to that determined by Blum et al. (2013). However, the contacting source and receiver introduce coupling issues and uncertainty if phase or group velocity is measured.

The velocities calculated from the time of flight measurements are $3080 \pm 90 \text{ ms}^{-1}$ and $2690 \pm 100 \text{ ms}^{-1}$ for the fast and slow P waves respectively and $1680 \pm 60 \text{ ms}^{-1}$ and $1420 \pm 70 \text{ ms}^{-1}$ for the fast and slow S wave polarisations. These correspond to c_{ij} values of $c_{11} = 12.3 \pm 0.9 \text{ GPa}$, $c_{33} = 16.1 \pm 0.9 \text{ GPa}$, $c_{44} = 4.8 \pm 0.3 \text{ GPa}$ and $c_{66} = 3.4 \pm 0.3 \text{ GPa}$. The time-of-flight measurements were a rough experiment to provide initial estimates of the c_{ij} 's. Errors in seismic velocities and c_{ij} values are estimated from the range of

Shale MSH HTI						
$f^{(obs)}$ (Hz)	$f^{(pre)}$ (Hz)	$\sigma^{(obs)}$ (Hz)	$(\frac{f^{(pre)}-f^{(obs)}}{\sigma^{(obs)}})^2$	# peaks obs.	freq.	#
12473	11814	55	143.5640	3	1	
14740	15000	70	13.7959	3	2	
17150	16821	61	29.0892	3	3	
17782	17665	74	2.4998	5	4	
22108	21910	46	18.5274	4	6	
22940	23033	88	1.1169	4	7	
24182	24060	105	1.3500	6	10	
25247	25244	87	0.0012	6	11	
27473	27888	267	2.4159	4	12	
28620	28184	82	28.2713	3	14	
30307	30028	266	1.1001	3	16	
31360	31151	246	0.7218	5	20	
32743	33008	170	2.4299	3	21	
34580	34670	56	2.5829	3	22	
36100	36094	71	0.0071	2	26	
37364	37549	148	1.5625	5	29	
39126	38814	333	0.8779	5	31	
39860	39725	368	0.1346	2	34	
41072	40801	260	1.0864	4	38	
42463	42624	251	0.4114	3	40	
43535	43677	117	1.4730	4	43	
45998	45887	451	0.0606	5	47	
47120	47529	57	51.4869	2	50	
48314	48603	201	2.0673	5	52	
49617	49600	298	0.0033	3	57	

Table 6.1: Comparison of measured ($f^{(obs)}$) and predicted ($f^{(pre)}$) resonant frequencies of shale MSH HTI. $\sigma^{(obs)}$ is the uncertainty in each frequency calculated from repeated measurements, $(\frac{f^{(pre)}-f^{(obs)}}{\sigma^{(obs)}})^2$ is the relative contribution of $f^{(obs)}$ to the total χ^2 , # peaks. obs is the number of measurements that each mode was observed in and freq. # is the number of the identified mode.

Shale MSH HTI					
c_{11}	c_{33}	c_{12}	c_{44}	c_{66}	χ^2
11.4 ± 1.0	14.5 ± 1.0	4.9 ± 0.3	4.3 ± 0.2	2.1 ± 0.1	6.5
V_{P0}	V_{S0}	ϵ	δ	γ	
2590 ± 110	1110 ± 30	0.14 ± 0.1	-0.4 ± 0.1	0.5 ± 0.1	

Table 6.2: Summary of elastic moduli (GPa), seismic velocities (m s^{-1}) Thomsen anisotropy parameters (dimensionless) of Shale MSH HTI. Errors in c_{ij} values are estimated from the inversion and propagated through to Thomsen’s parameters.

possible travel times on the oscilloscope but are not rigorously determined.

Significant frequency dispersion is observed in four of the elastic moduli (we are not able to measure the off diagonal entries in the stiffness matrix using simple time-of-flight techniques). The average decrease in elastic moduli is 1.1 GPa. Comparison with the time-of-flight measurements from Blum et al. (2013) using non-contacting laser methods gives bigger decreases in c_{11} , c_{33} , c_{44} and c_{66} . The P wave anisotropy ϵ is calculated as 14% using RUS compared to 30% as measured with laser-based time-of-flight measurements.

6.2 Vertical Transverse Isotropic (VTI) Sample

Shale MSH (VTI) is 5.88 cm high with a diameter of 3.80 cm and a density of 2.1 g/cm³. 26 resonant modes were measured. The data was acquired between 10 and 70 kHz with a sweep rate of 0.001 Hz. Data had to be acquired over a wider frequency range for the VTI sample than for the HTI sample in order to measure a comparable number of modes. This is because the HTI sample does not have any doublet resonances and so has more observable modes and the VTI shale has a slightly higher length to diameter ratio. Seven measurements were made, three with V101 transducers and four with V151 transducers, and the sample rotated and remounted between sweeps, similar to the data acquisition for the HTI sample. The loading of the sample was 12.7 ± 1.6 g. Table 6.4 compares the measured and predicted frequencies and the relative error contribution of each mode. The variance is dominated by the first mode due to the small error estimation. This mode can be assigned a weight of zero and excluded from the χ^2 calculations (Migliori and Sarro, 1997).

Table 6.3 shows the results of the inversion; the fitted elastic moduli, the degree of misfit χ^2 and Thomsen's parameters. For a VTI model $\chi^2 = 8.6$ which is a significant improvement over an isotropic model which has a χ^2 value of 87. It is interesting to note that the isotropic model is a substantially better, but still poor, fit for the VTI

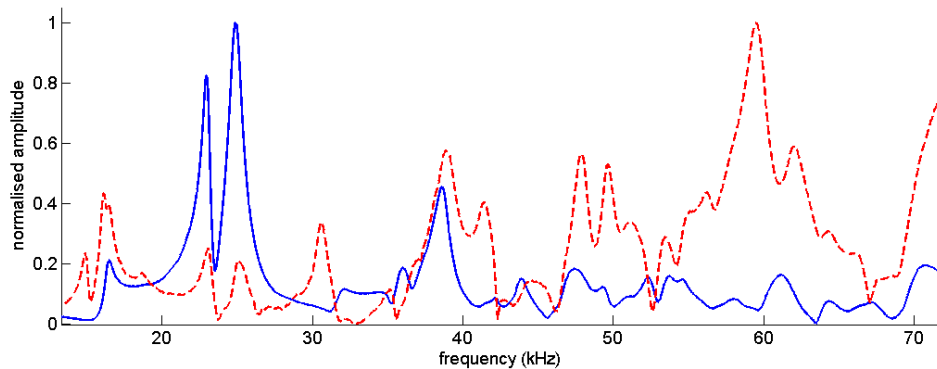


Figure 6.2: Resonant spectrum for shale MSH VTI from 12 to 72 kHz. The blue solid line is measured using V101 transducers and the red dashed line is measured with V151 transducers.

sample than for the HTI. This is likely because both isotropic and VTI symmetries are axisymmetric and have some of the same resonances whereas an HTI sample has significantly different symmetry and hence resonant modes, as discussed in Chapter 3. χ^2 decreases to 3.9 when an average error of 223 Hz is used, calculated from the ten modes measured in five or more sweeps.

The P and S wave velocities parallel to the symmetry axis are $V_{P0} = 2880 \pm 70 \text{ ms}^{-1}$ and $V_{S0} = 1800 \pm 30 \text{ ms}^{-1}$. Perpendicular to the symmetry axis $V_{P90} = 3120 \pm 60 \text{ ms}^{-1}$ and the 'fast' S wave polarisation has a velocity of $1770 \pm 30 \text{ ms}^{-1}$. The anisotropy of the VTI sample is less than the HTI. There appears to be no shear wave anisotropy. The 'fast' S wave polarisation (as predicted by the card model proposed by Thomsen (1986b); Winterstein (1992)) has the same speed, within the margins of error, as the 'slow' polarisation. This is also shown by $\gamma = -0.01 \pm 0.03$. The sign of this is uncertain but it indicates that between the horizontal and vertical shear wave speeds differ by at most 4%. This is significantly different to shale MSH HTI which displays 50% anisotropy in the shear wave in RUS measurements. It is a further indication of the inhomogeneity of shale MSH. Similarly, the large error in δ means the sign is uncertain. It is likely to be positive as the P wave velocity is faster in the horizontal than in the vertical direction. However, this does not exclude local variations in the near-vertical. The P wave anisotropy is between 4% and 14%.

The Q factor of the first peak at 14897 Hz is 24.2, similar to the HTI sample. Despite significant variations in physical properties attenuation may be similar between the samples. Further work needs to be done to determine the Q factor of more resonances for each sample.

Time-of-flight measurements were used to provide initial estimates of the c_{ij} values. The time-of-flight measurements are less complicated than RUS, relying on simple kinematics not Rayleigh-Ritz approximations and inverse theory. Therefore, they provided a useful confirmation that the VTI sample had substantially different physical properties to the HTI sample. For the P and S waves along the length of the cylinder the travel times were $19 \pm 0.5 \mu\text{s}$ and $33 \pm 1.5 \mu\text{s}$ respectively. These times correspond to velocities of $V_{P0} = 3090 \pm 90 \text{ ms}^{-1}$ and $V_{S0} = 1780 \pm 90 \text{ ms}^{-1}$ and elastic moduli of $c_{33} = 20.1 \pm 1.4 \text{ GPa}$ and $c_{44} = 6.6 \pm 0.6 \text{ GPa}$. c_{33} decreases when measured using

Shale MSH VTI					
c_{33}	c_{23}	c_{12}	c_{44}	c_{66}	χ^2
17.4 ± 0.8	4.9 ± 0.6	7.3 ± 0.4	6.8 ± 0.2	6.6 ± 0.2	8.6
V_{P0}	V_{S0}	ϵ	δ	γ	
2880 ± 70	1800 ± 30	0.09 ± 0.05	0.03 ± 0.14	-0.01 ± 0.03	

Table 6.3: Summary of elastic constants (GPa), seismic velocities (m s^{-1}) Thomsen anisotropy parameters (dimensionless) for Shale MSH VTI. Errors in c_{ij} values are estimated from the inversion and propagated through to Thomsen's parameters..

resonance methods at lower frequencies but no change is observed in c_{44} . By measuring travel times across the diameter of the cylinder the velocities $V_{P90} = 3450 \pm 110 \text{ ms}^{-1}$ and $V_{SH90} = 2110 \pm 100 \text{ ms}^{-1}$ are calculated. These correspond to elastic moduli of $c_{11} = 25.0 \pm 1.6 \text{ GPa}$ and $c_{66} = 9.3 \pm 0.9 \text{ GPa}$. For this VTI shale sample there is a clear dependence of elastic moduli on frequency. Three of the elastic moduli decrease by an average of 3.3 GPa. However, c_{44} is unchanged within the error margins.

The anisotropy estimates are different in the different frequency ranges. Time-of-flight measurements give the S wave anisotropy γ as 20% while RUS indicates no S wave anisotropy. For the P waves the anisotropy is 12% by time-of-flight compared to 9% calculated by resonance methods.

Shale MSH VTI					
$f^{(obs)}$ (Hz)	$f^{(pre)}$ (Hz)	$\sigma^{(obs)}$ (Hz)	$(\frac{f^{(pre)}-f^{(obs)}}{\sigma^{(obs)}})^2$	# peak obs.	freq. #
14897	15335	22	396.3719	4	1
16334	16131	136	2.2280	7	2
22977	22961	82	0.0381	6	3
24810	25860	259	16.4354	7	4
30587	30671	13	41.7515	4	5
35310	35060	118	4.4887	4	8
36550	37542	234	17.9718	5	9
38589	39018	104	17.0156	4	11
41706	41813	199	0.2891	7	12
42513	42638	225	0.3086	5	13
43800	43703	142	0.4666	3	15
46720	46006	85	70.5600	3	17
48027	48408	212	3.2298	2	18
49488	49581	59	2.4846	3	21
51342	50758	144	16.4475	6	22
52343	52339	240	0.0003	4	23
53490	53702	160	1.7556	3	24
54537	54803	253	1.1054	6	27
56273	55941	112	8.7870	4	28
59854	60285	380	1.2864	3	30
61740	61005	471	2.4352	6	34
64193	64164	194	0.0223	5	37
66320	65875	246	3.2723	3	40
67193	66743	247	3.3192	2	41
68042	68046	112	0.0013	3	42
69950	70062	154	0.5289	4	44

Table 6.4: Comparison of measured ($f^{(obs)}$) and predicted ($f^{(pre)}$) resonant frequencies of shale MSH VTI. $\sigma^{(obs)}$ is the uncertainty in each frequency calculated from repeated measurements, $(\frac{f^{(pre)}-f^{(obs)}}{\sigma^{(obs)}})^2$ is the relative contribution of $f^{(obs)}$ to the total χ^2 , # peaks. obs is the number of measurements that each mode was observed in and freq. # is the number of the identified mode. Note that doublets are only counted as one mode.

Chapter 7

Conclusion

Resonant ultrasound spectroscopy is shown to be a useful technique for determining the physical properties of rocks. It can be used to determine the complete elastic tensor of a sample as well as to provide attenuation information.

There are several experimental issues which are the main focus of this dissertation. Sample geometry, transducer position, loading and rate of sweep must all be examined when making RUS measurements. The symmetry of the sample is a major consideration for geological samples, which are often hexagonally symmetric. VTI and HTI symmetry have significant differences and need to be treated separately.

The relationship between the elastic moduli and the measured resonant frequencies is complicated with the forward problem solved using a variational approximation. Inverse procedures pose numerous challenges even for a simple forward model. These challenges are amplified by a complicated forward model and can create confusion and misinterpretation of results.

RUS fills an experimental gap between low frequency stress-strain methods and high frequency time-of-flight measurements. The elastic moduli are calculated by resonance methods and compared with the time-of-flight results. Frequency dispersion is observed with the elastic moduli decreasing with frequency.

7.1 Future Work

There are several areas in which future work should focus.

- Measuring VTI and HTI cores of the same rock should enable better results by providing complementary information. To test this theory additional shale samples with less lateral inhomogeneity should be measured.
- Doublets are observed in isotropic and VTI but not in HTI cylinders. It is hypothesised that this is because an HTI cylinder is not axisymmetric. However, further work is needed to determine if this is the cause or not.
- Preliminary results indicate that the relationship between the loading and the resonant frequencies of an HTI sample may be more complicated than for axisymmetric samples. For shale MSH HTI the resonant frequencies decreased by ~ 20 Hz for a ~ 30 g increase the amount of loading. Further work is required to investigate this, such as measuring the effect of loading of different types of normal modes.
- The work with the jackets should be extended to the shale samples. This would be a further step towards making RUS measurements under pressure.

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Appendices

Appendix A

RUS Methodology

Resonant ultrasound spectroscopy is a useful technique for determining the elastic properties of rock samples and quantifying anisotropy. However, the resonant frequencies are not coupled to the sample's elastic properties in a simple way. Therefore, the technique can lead to confusion and misinterpretation (Zadler et al., 2004). We provide a guide to making RUS measurements and discuss experimental and processing issues not covered in the main text.

A.1 Experimental Setup

In order to perform RUS measurements several pieces of equipment are required:

- **Transducers:** a source and receiver transducer pair for applying the driving force to the sample and measuring the response.
- **Function Generator:** for generating the driving force that is sent to the source and transducer and to the lock-in amplifier as a reference signal.
- **Amplifier:** for amplifying and filtering the response.

The equipment used was:

- V101-RM and V151-RB Olympus Panametric ultrasonic transducers with a frequency of 0.5 MHz. The V101 and V151 transducers produce longitudinal and

shear waves respectively.

- SRS DS345 Function Generator
- SRS SR850 Lock-in Amplifier

A lock-in amplifier is preferable to a pre-amplifier as it is able to measure at the exact frequency of the driving force enhancing the signal to noise ratio. Additionally, measuring the magnitude of the response as opposed to the sinusoidal oscillations of the signal eliminates the need to perform a Fourier transform. This removes the issue of aliasing and allows for a reduced sampling rate, allowing for significantly smaller acquisition files, decreased computation time and increased efficiency. Data was fed to a PC through a PCI oscilloscope card and acquisition was done in AlazarDSO. See Figure A.1 for an overview of the experimental setup.

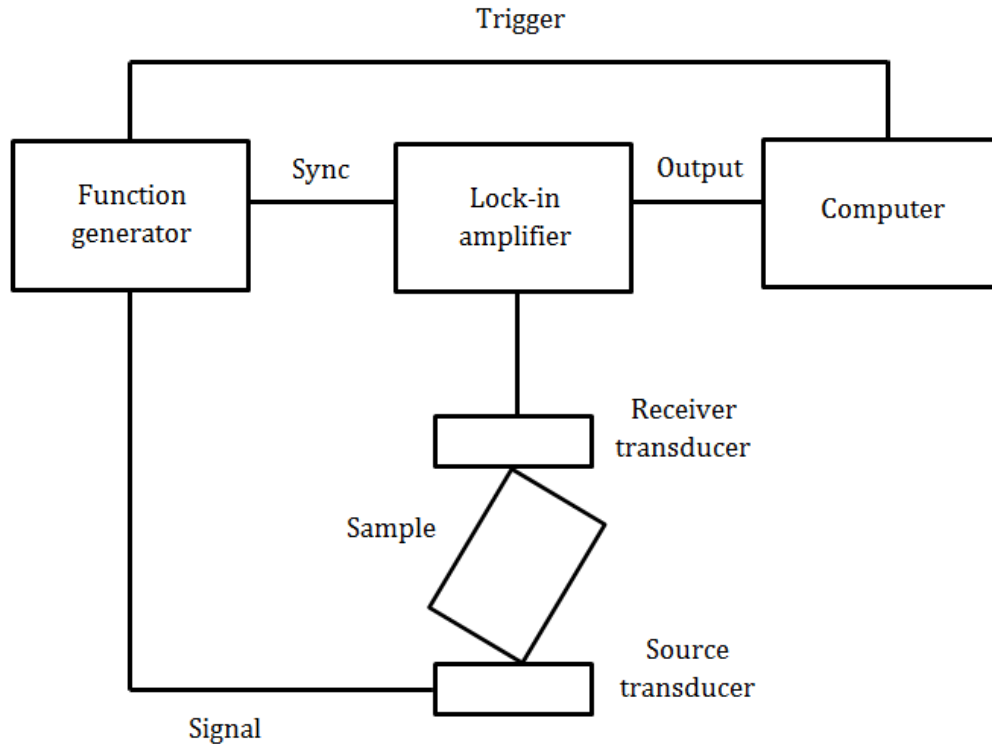


Figure A.1: Schematic diagram of experimental setup

The function generator produces three signals; a 10 V peak-to-peak sinusoidal signal to the source transducer which vibrates the sample of interest, a trigger signal to the PC which initiates recording, and a sync signal (a square wave with the same frequency as the signal sent to the transducer) which is passed to the reference-in channel of the lock-in amplifier. The sync signal allows the lock-in to phase-lock to the frequency of interest eliminating other signals enabling a high signal-to-noise ratio.

The sensitivity/gain of the lock-in must be adjusted depending on the sample and the coupling in order to get a measurable reading. If the output appears as random noise an incorrect gain setting is the most likely culprit. For shale MSH (HTI) the sensitivity was 100 mV f.s. with an associated gain of 40 dB.

A.2 Experimental Considerations

A.2.1 Sample Geometry

Sample geometry is a significant consideration and can strongly influence the quality of results that are achievable from a RUS experiment. Most geological samples are cylindrical and cylindrical samples are the focus of this report. However, resonant methods can be used to measure the properties of arbitrary geometries (Visscher et al., 1991). In addition to cylinders *formod-aniso* and *RUS-inverse* are capable of dealing with spheres and parallelepipeds.

Consider an elongated bar compared to a squat sample with a low length to diameter ratio. The elongated bar will have a simpler spectra than the squat sample (Figure 4.2). While mode identification and comparison between repeated measurements will be easier there will be fewer normal modes within a given frequency range (Zadler et al., 2004). Therefore, in order measure the same number of modes, acquisition must be extended to higher frequencies. Additionally, the first mode which is sensitive to V_P is at a much higher frequency in an elongated bar than in a short squat cylinder (Zadler et al., 2004) and to determine the elastic moduli associated with the P wave speed higher frequency modes must be measured. Hence, for an elongated cylindrical sample acquisition must be performed to higher frequencies. This is an issue if the experimental apparatus has an upper limit on the frequency. This was the case with

our setup as the lock-in amplifier was unable to function above 102 kHz.

A squat sample will have more modes within a given frequency range and resonances which are sensitive to V_P at lower frequencies. However, the spectra will be more complicated making mode identification and comparison between repeated measurements a challenge. Sample geometry is a compromise between the two extremes; requiring acquisition to high frequencies or challenging mode identification.

For samples with hexagonal symmetry there is another important consideration. Hexagonal samples can be divided into two special cases; VTI and HTI symmetry. A VTI cylinder is axisymmetric and will have doublets or degenerate modes which are multiple normal modes with the same frequency. A cylindrical HTI sample does not have degenerate modes. However, within a given frequency range there are the same number of modes for both symmetries and hence for HTI there are more observable resonances within a given frequency range providing more data for the inverse procedure. However, the spectra is more complicated than for a VTI sample.

Resonance methods were first used to measure the elastic properties of elongated rods, with length to diameter ratios of ten or more, because those were the only geometries where the forward resonance problem could be practically solved (Zadler et al., 2004). In general, approximation procedures must be used to solve the generalized symmetric eigenvalue problem that arises from the resonance calculations in the forward problem (Holland, 1968). The Rayleigh-Ritz method can be used, and the success of this method often depends on the choice of basis functions. Holland (1968) and Demarest (1969), amongst others, developed basis functions that enabled the forward problem to be solved for a limited variety of geometries such as isotropic spheres and parallelepipeds. The *xyz* algorithm discovered by Visscher et al. (1991) enabled the forward problem to be solved for arbitrary geometries, including the squat cylinders we investigate.

A.2.2 Transducer Location

Our measurements were made with contacting transducers and transducer coupling influences the excitation of normal modes. The sample was pinned edge on between the transducer to excite the maximum number of modes (Zadler et al., 2004), as discussed

in Chapter 4. The location of the transducer on the sample controls which modes are excited. Rotating the sample between measurements can result in different resonances being excited and observed. In order to excite all possible resonances and to ensure repeatability between experiments the sample must be rotated and remeasured multiple times. The resonant frequencies are determined from the sum of the measured spectra.

The effect of rotation is most significant for HTI samples. For VTI samples when the sample is rotated the transducers stay on the same isotropic layer. There is little variation in the observed resonances (Figure A.2). For HTI symmetry rotating the sample can cause the transducers to align parallel to the planes of isotropy, or orthogonal, or at an arbitrary angle to them. This causes significant changes in the measured spectra (Figure A.3).

Figures A.4 and A.5 show the power spectra of two large earthquakes; the 1994 Bolivian earthquake $M_w = 8.2$ and the 2011 Tohoku event in Japan $M_w = 9.0$. An earthquake can be considered analogous to the source transducer and the whole Earth as the sample of interest. The two spectra are significantly different despite the resonant modes of the Earth being the same. This shows that the location of the source (transducer or earthquake) determines which modes are excited and can be measured. In global seismology the spectra from earthquakes all over the world are summed together in order to determine the resonant frequencies of the Earth. This is analogous to our approach where the location of the source and receiver are varied by rotation.

A.2.3 Loading

The derivation of the forward problem assumes a stress-free boundary condition on the surface of the sample (Zadler et al., 2004). However, the sample is pinned between two contacting transducers and the top transducer must exert a downwards force on the sample to hold it in place. This applies pressure to the sample and can cause cracks and micro-fractures in the rock to close, increasing the stiffness and hence the seismic velocities of the sample. The effect of this is to increase the resonant frequencies of the sample. Therefore, under in-situ pressure the resonant frequencies are expected to be higher and hence, the elastic moduli will be different to those we have measured at atmospheric pressure.

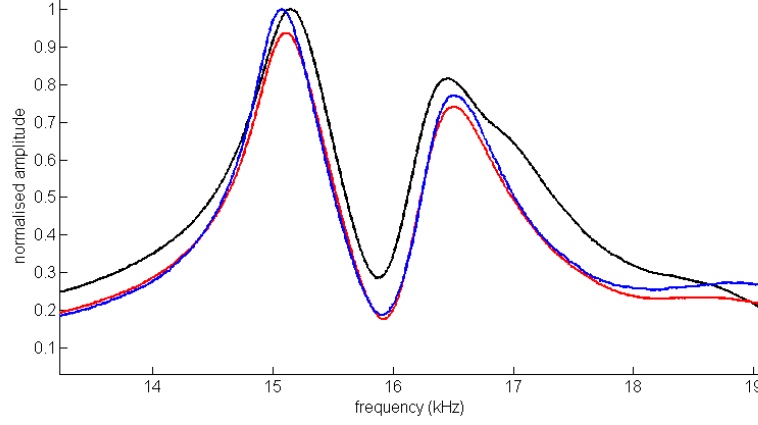


Figure A.2: Effect of transducer location on a VTI sample. Three sweeps are made with the sample rotated approximately 120° each time. There is little variation in the frequency of the two resonances between sweeps and all modes are excited equally in all sweeps. Transducer location is not as important for VTI samples as it is for HTI.

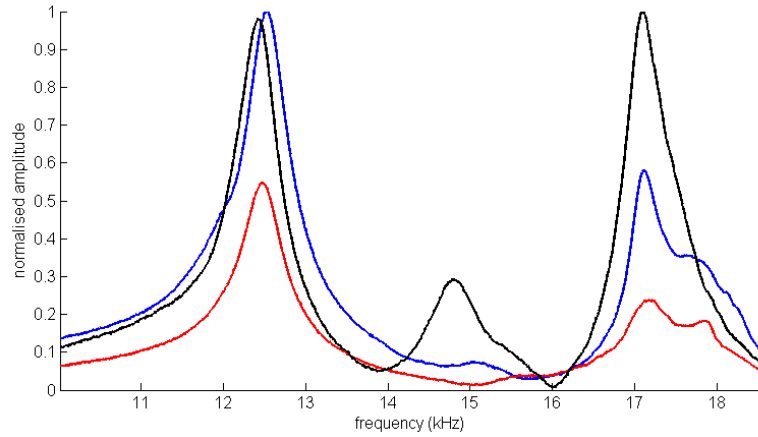


Figure A.3: Effect of transducer location on a HTI sample. Three sweeps are made with the sample rotated approximately 120° each time. At 15 kHz there is a substantial peak that is only excited in one of the sweeps. This shows that transducer location is important for HTI samples. Different transducer locations excite different resonances. In order to excite the maximum number of resonances multiple sweeps must be recorded with the sample rotated between measurements. Resonances are then determined from all sweeps.

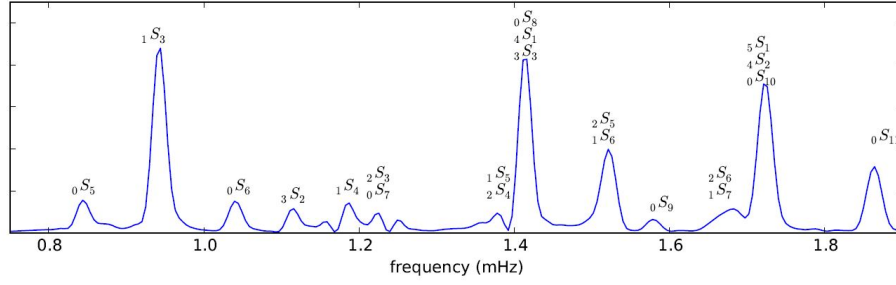


Figure A.4: Power spectra from 1994 Bolivian earthquake $M_w = 8.2$

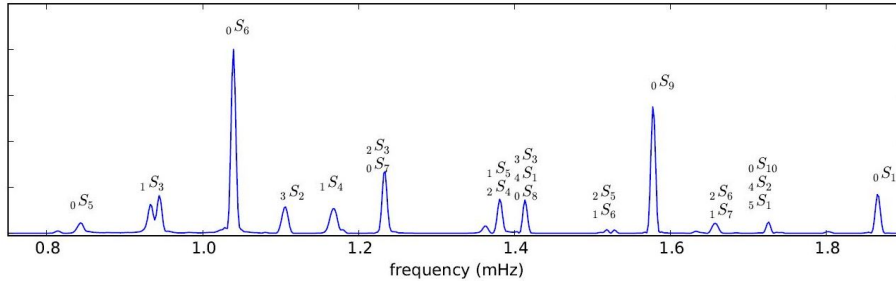


Figure A.5: Power spectra from 2011 Tohoku earthquake $M_w = 9.0$

A scale is located underneath the sample in order to measure the loading. If the experimental apparatus allows for variable loading measurements should be made for different loading values so that the frequencies can be extrapolated to the expected value at zero loading.

For an axisymmetric cylinder the resonant modes observed will be either axisymmetric (torsional or extensional) where the energy travels purely up or down the cylinder, or non-axisymmetric or flexural where the energy travels along paths tilted with respect to the cylindrical axis. Flexural modes occur in pairs with the same resonant frequency called doublets or degenerate modes. For axisymmetric modes loading causes the peak to be shifted in frequency. For non-axisymmetric modes loading can influence the two modes in a doublet differently causing different shifts. The two members of a doublet that would appear as a single peak in an unloaded sample can become spread into two distinct peaks in the loaded sample (Zadler et al., 2004; Zadler, 2005). The same phenomenon can occur as a result of a poorly manufactured sample with a crack in one side or sub-parallel faces. For parallelepiped samples a 1% chip out of the corner of

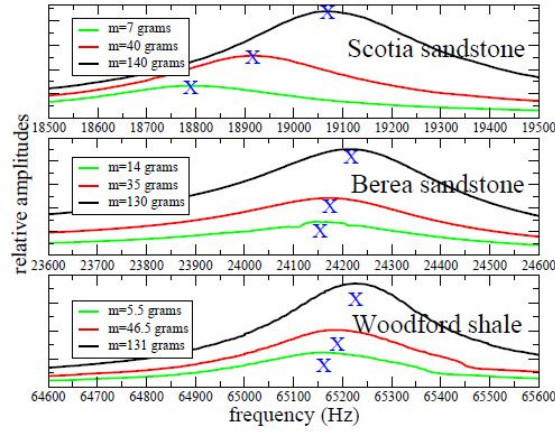


Figure A.6: Resonant modes can be shifted up in frequency when additional loading is applied to the sample. The porosity could be correlated to the magnitude of the change. From Zadler (2005).

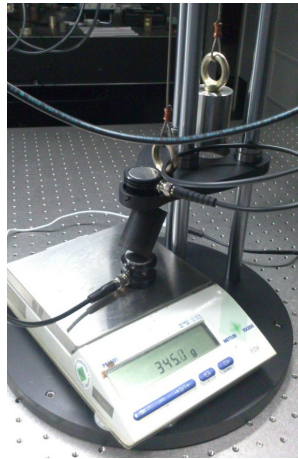


Figure A.7: Showing the experimental apparatus. The top transducer is balanced with a counterweight and is able to be adjusted accurately in order to minimize the loading force that the sample experiences. The scale under the bottom transducer measures the total mass of the system allowing us to calculate the external loading and to keep the loading constant between successive measurements.

a sample can produce a 1% change in the frequency of resonant modes (Ulrich et al., 2002).

A.2.4 Rate of Sweep

Another important consideration is the rate of sweep. If the rate of sweep is too fast the resonant modes will be shifted up in frequency. The correct rate can be chosen by sweeping up and down in frequency. If the resulting spectra do not overlap exactly then the rate of sweep is too fast (Zadler, 2005). Figure A.8 shows the spectra for shale MSH from 10 to 20 kHz sweeping up and down in frequency at three different rates of sweep, 0.05, 0.01 and 0.001 Hz. The difference in frequency of the resonant modes between the up and down sweeps are 190, 55 and 7 Hz respectively. An error of 190 Hz due to rate of sweep would significantly increase the uncertainty in the frequencies. Therefore, the rate of sweep should be as slow as possible so that the difference between up and down sweeps is minimised. However, there may be a practical lower limit of the possible rate of sweep due to time considerations or equipment restrictions.

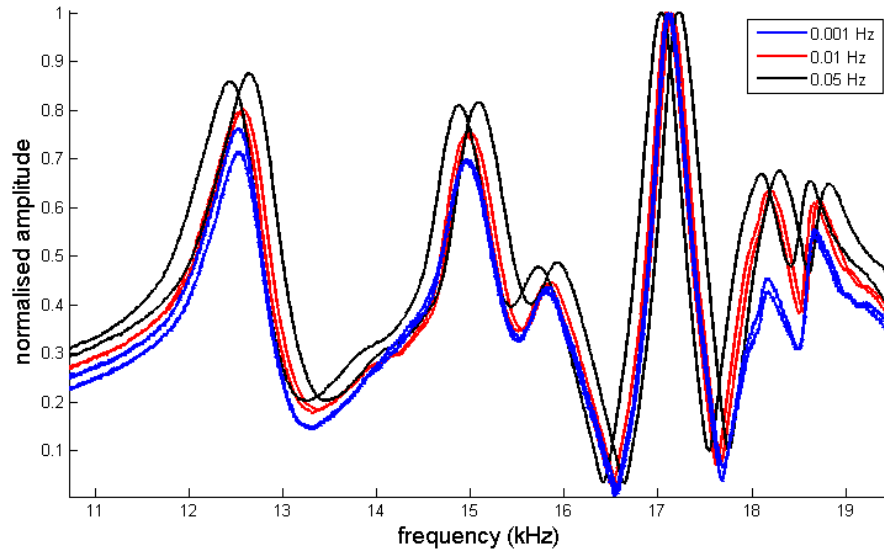


Figure A.8: The rate of sweep is important. If the sweep is too fast the peaks will be shifted upwards in frequency. Therefore, the correct rate of sweep is chosen by measuring sweeps up and down in frequency and confirming that the two spectra match exactly.

A.3 Data Acquisition

In order to make a RUS measurement the frequency bounds and rate of sweep must be chosen carefully. It is important to measure the first resonant frequency otherwise all modes will be incorrectly identified and the inversion can give a grossly inaccurate answer. In many samples (isotropic and VTI) the frequency of the fundamental mode is given by the reciprocal of the two-way travel-time of the slowest S wave (for HTI samples the situation is more complicated. However, the reciprocal of the two-way travel-time of the slow S wave will give a ball-park estimation of the frequency of the fundamental mode). For centimetre sized samples subtracting ~ 5 kHz from the estimated fundamental frequency provides an appropriate lower frequency bound on the measurements. The upper frequency bound depends on how many resonant peaks are required for the inversion and the geometry of the sample. There may be a limit on the maximum frequency due to equipment constraints or because the consistent identification of peaks between repeated measurements is compromised as the modes become more closely spaced at higher frequencies.

Once the frequency bounds have been determined the next step is to sweep up and down in frequency, either over the whole frequency band or smaller subintervals. If the peaks differ between the up and down frequency sweeps then the rate of sweep should be reduced until they agree. This ensures that the frequencies are not perturbed by the sampling rate.

A measurement can now be performed sweeping between the chosen frequency bounds at a determined rate. The sample should be remounted, rotated and remeasured as many times as possible to excite the maximum number of modes and to enable uncertainties in the resonant frequencies to be calculated. Different transducers (V101 and V151) can be used to excite different modes (P and S wave modes respectively).

A.4 Inversion

Once the resonant modes have been measured the frequencies are passed to the inversion by a text file *freq_data* which contains two columns, the measured resonant frequencies in MHz and the associated weighting of each observed mode. The weighting is generally

one for observed modes and zero for peaks guessed at by the forward code. Intermediate values can be used for observed but uncertain peaks. The overall structure of the inverse procedure is to start with a few frequencies and slowly add more, updating c_{ij} values and increasing the order of the fit as more modes are added. There are several tricks to the inversion procedure which are outlined below.

- To begin the inversion start with the same number of frequencies as c_{ij} 's that are being inverting for. This eliminates problems that occur in the inversion when there are more unknowns than data.
- Add frequencies to the inversion one or two at a time. If a peak is missed there are three options:
 1. Let the forward code guess at the frequency of the missing mode. Insert this frequency with a weight of zero. It will act as a placeholder and not contribute to the final χ^2 value.
 2. Review the recorded data. The missing peak may be small or poorly defined and have been overlooked. Insert this frequency with a weighting that reflects the confidence with which the peak is identified.
 3. Remeasure and rotate the sample. The missing peak may not have been excited. By changing the transducer location the mode may become observable.
- Periodically update *param_data* with the revised c_{ij} values.
- Maintain the upper frequency bound as ~ 10 kHz above the highest frequency used in the inversion.
- As more frequencies are added increase the degree of the polynomial fit to achieve more accurate results.

A curious property of RUS measurements is that independent of experimental apparatus, sample geometry or other considerations the first one or two modes do not fit

well (Migliori and Sarro, 1997). This is indicated by a large relative error contribution $(\frac{f^{\text{pre}} - f^{\text{obs}}}{\sigma^{\text{obs}}})^2$. Therefore, the first one or two modes are often given a weighting of zero.

Limited analysis on the aluminum and shale samples has indicated that the c_{ij} 's have a greater radius of convergence below the true value than above. Therefore, it is better to underestimate the elastic moduli than to overestimate. For additional details on the inversion procedure refer to the Installation and Help Guide by Zadler and Le Rousseau (2005) available at <http://physics.mines.edu/about/downloads/software/mpl/manual.pdf>.

Appendix B

Recommendations

Two forward models are used in the computations. *formod-aniso* contains one copy of the forward model that is called by a script file *mod-shell* to compute the resonant frequencies based on sample geometry and given elastic moduli. *RUS-inverse* holds another copy of the forward model. It is this copy that is used to determine the predicted frequencies in the inversion process. Having two identical copies of the forward model in different places can lead to confusion and introduce errors when one code is changed but not the other. Therefore, it is recommended that only one copy of the forward model is used and that the other is removed from the computational methods. The preferred method would be to remove the forward model from *RUS-inverse* and make the inversion call *formod-aniso* each time the resonant frequencies need to be computed.

For RUS experiments it is recommended that mutually perpendicular cores are cut to produce HTI and VTI symmetries of the same rock. The two cores can be used to provide complementary information. For example, HTI samples have more observable resonances within a given frequency range which can provide more information for the inversion. In VTI samples the first resonance is often determined by the two-way travel-time of the slow S wave. Therefore, only a single peak needs to be measured to determine c_{44} . This technique will only work if there is not significant lateral heterogeneities in the rock. It does not work for shale MSH as there are significant physical differences between the two samples despite being cut only a few centimetres apart.