

# 1 Introduction

## 2 Theory of Linear Elasticity

We begin by summarizing the fundamental equations for elastic deformation, which will be used to uncover the elastic wave equation.

In the basic theory covered in chapters 1 and 3 of the book by Landau and Lifshitz [1, 2], the following assumptions apply.

1. Deformations are large in comparison to the distances between atoms in the elastic body. In the case of crystalline structures (discussed in a later section), the deformations are large in comparison to the lattice constant.
2. Elastic deformation occurs over an infinite domain where there are no deformations at infinity.
3. Deformations are small enough such that Hooke's Law applies (stresses depend linearly on strains), the deformations are thermodynamically reversible, and they are also isothermal.
4. The deformed material is isotropic. This is a good assumption to start with because it will lead us to a simple stress tensor which will enable a high-level overview of the elastic wave equation in this first section. Elasticity in a crystalline material will be examined later in the report.
5. Deformations are homogeneous, meaning that every element of the body deforms as the whole does, and the deformations are affine.

Note that the term 'elastic body' refers to a deformable solid, such that the deformations are thermodynamically reversible. That is, no energy is lost in the deformation process and thus, the deformed solid will return to its original undeformed state spontaneously when the force causing the deformation is removed.

### 2.1 The Strain Tensor

Strain refers to the change in distance between two points in a solid after deformation divided by the original distance between the points at equilibrium. The most general form of the strain tensor is nonlinear.

$$u_{ik} = \frac{1}{2} \left( \frac{\partial u_i}{\partial x_k} + \frac{\partial u_k}{\partial x_i} + \frac{\partial u_l}{\partial x_i} \frac{\partial u_l}{\partial x_k} \right). \quad (1)$$

However, because displacements  $u_i$  are always considered small in this discussion, we will neglect the third term and simply regard the strain tensor to be given by

$$u_{ik} = \frac{1}{2} \left( \frac{\partial u_i}{\partial x_k} + \frac{\partial u_k}{\partial x_i} \right). \quad (2)$$

Figure 1 below shows a picture of the strains present in a section of a deformed two-dimensional elastic body.

### 2.2 Force and Equilibrium

The total force on an elastic body is due to the internal stresses integrated over the volume of the body.

$$\mathbf{F}_{net} = \int_V \hat{\mathbf{F}} dV, \quad (3)$$

where  $\hat{\mathbf{F}}$  is the force per unit volume. Now, the force vector  $\hat{\mathbf{F}}$  is the divergence of the rank two stress tensor  $\sigma_{ik}$ . That is, we have the relationship

$$\hat{F}_i = \frac{\partial \sigma_{ik}}{\partial x_k}. \quad (4)$$

Figure 2 is a depiction of the components of the stress tensor.

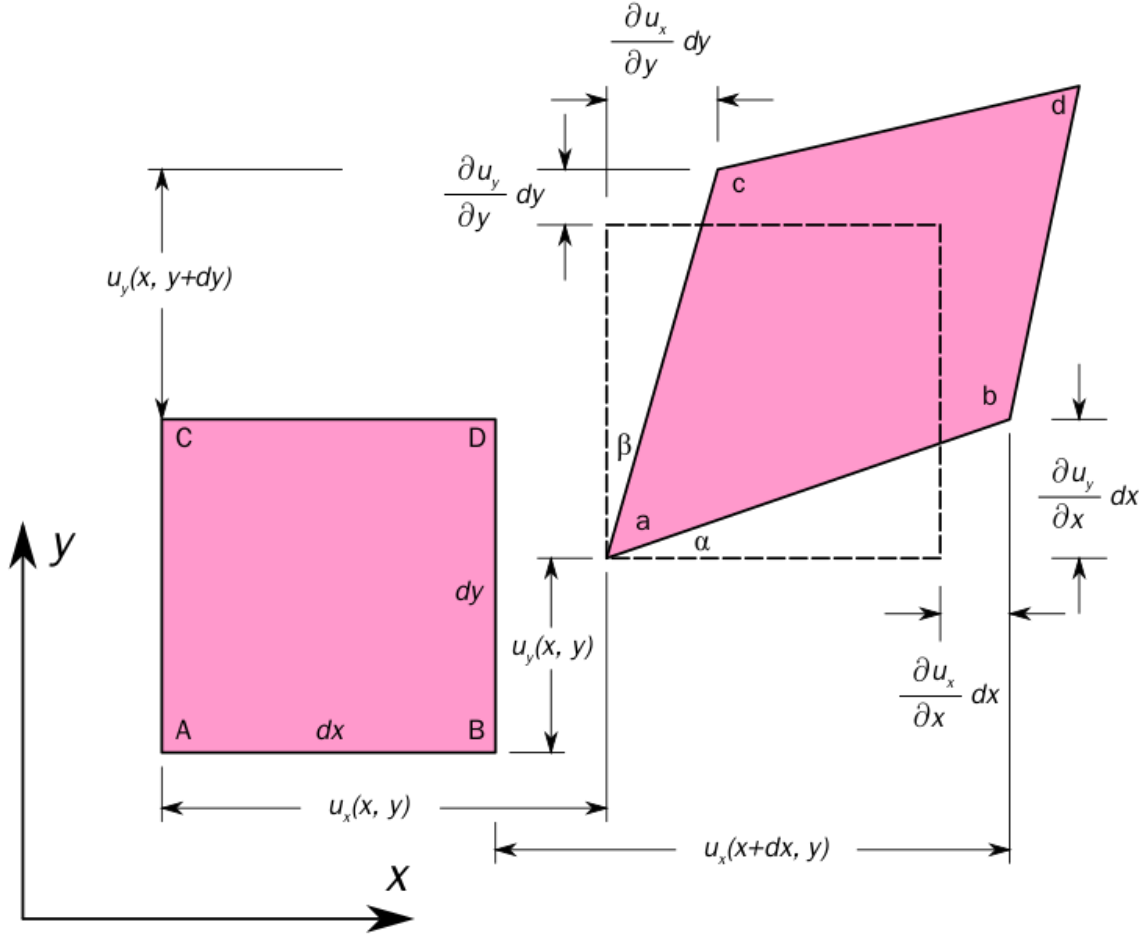


Figure 1: Depiction of section of elastic body being deformed and the appearance of various strains.

Thus, by application of the divergence theorem, we have

$$\int F_i dV = \int \frac{\partial \sigma_{ik}}{\partial x_k} dV = \oint \sigma_{ik} df_k. \quad (5)$$

In equilibrium, all the internal stresses in the body must sum to zero. This can be expressed as

$$\frac{\partial \sigma_{ik}}{\partial x_k} = 0. \quad (6)$$

If we have an external force  $\mathbf{P}$  applied to the surface of the body, the equation for equilibrium on the surface of the body is

$$\sigma_{ik} n_k = p_k, \quad (7)$$

where  $\mathbf{n}$  is the unit outward normal to the surface.

### 2.3 Deformations and Derivation of Elastic Wave Equation

Now, we seek to find an expression for the stress tensor in terms of the strain tensor. From there, we will utilize the equilibrium equation (6), along with Newton's second law, to establish the general elastic wave equation. We start by finding an expression for the work done by the internal stresses in a body undergoing a small deformation. This can be

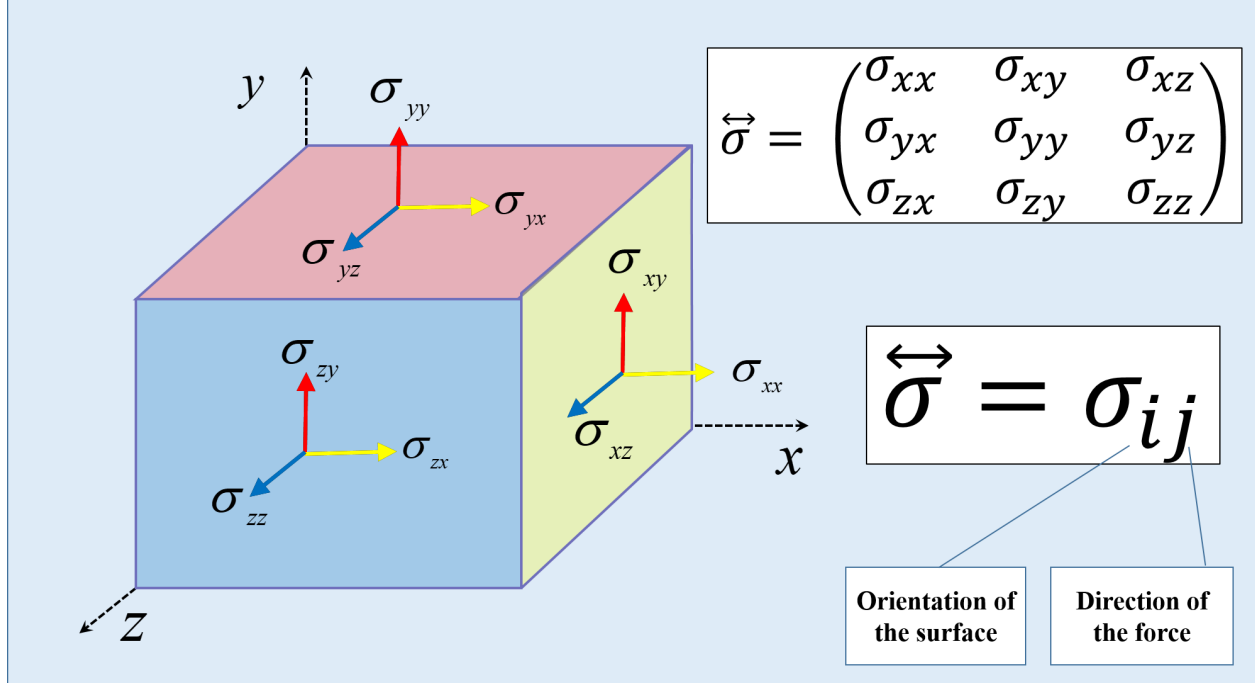


Figure 2: Depiction of the components of the stress tensor.

done by integrating force dotted with displacement  $F_i \delta u_i$  over the volume of the body. Let  $\delta R$  denote the work done by the internal stresses per unit volume. Then, the work is given by

$$W = \int \delta R dV = \int F_i \delta u_i dV = \int \frac{\partial \sigma_{ik}}{\partial x_k} \delta u_i dV. \quad (8)$$

Integration by parts gives

$$W = \oint \sigma_{ik} \delta u_i df_k - \int \sigma_{ik} \frac{\partial u_i}{\partial x_k} dV. \quad (9)$$

From assumption 2, we neglect the first integral and compute

$$\int \delta R dV = -\frac{1}{2} \int \sigma_{ik} \left( \frac{\partial \delta u_i}{\partial x_k} + \frac{\partial \delta u_k}{\partial x_i} \right) dV = -\frac{1}{2} \int \sigma_{ik} \delta \left( \frac{\partial u_i}{\partial x_k} + \frac{\partial u_k}{\partial x_i} \right) dV = - \int \sigma_{ik} \delta u_{ik} dV.$$

The second term in the above equation comes from the fact that work per unit volume is equal to the stress multiplied by the strain. Hence,

$$\delta R = -\sigma_{ik} \delta u_{ik}, \quad (10)$$

where  $u_{ik}$  is the strain tensor, which is given by (2). The change in internal energy for a reversible process (see assumption 3) is given by  $dU$ , where

$$dU = TdS - dR = TdS + \sigma_{ik} du_{ik}. \quad (11)$$

The Helmholtz free energy  $F$  is given by  $F = U - TS$  so that

$$dF = -SdT + \sigma_{ik} du_{ik}. \quad (12)$$

Thus, for a constant temperature deformation, we have the Maxwell relation

$$\sigma_{ik} = \left( \frac{\partial F}{\partial u_{ik}} \right)_T. \quad (13)$$

The subscript ‘ $T$ ’ denotes that deformations occur at constant temperature  $T$ . The Helmholtz free energy is useful for describing a reversible elastic process since (see assumption 3) the elastic medium maintains essentially constant volume (the volume change of the body is negligible). For a deformed isotropic body, we have the following equation for the free energy  $F$ .

$$F = F_0 + \frac{1}{2}\lambda u_{ii}^2 + \mu u_{ik}^2, \quad (14)$$

where  $\lambda$  and  $\mu$  are called the *Lamè coefficients*. This relation (14) is the second-order Taylor expansion of the free energy about zero strain, which corresponds to the equilibrium state of the solid. Note that there is no linear strain terms in (14), which makes sense as we should have zero stress in the material at zero strain. In what follows, we are only interested in the free energy after deformation, so that only the second two terms on the right hand side of (14) are considered.

Ignoring the term  $F_0$ , we may rewrite  $F$  as

$$F = \mu(u_{ik} - \frac{1}{3}\delta_{ik}u_{ll})^2 + \frac{1}{2}Ku_{ll}^2, \quad (15)$$

where  $K$  is the bulk modulus, and  $\mu$  is the shear modulus. The first term on the right hand side of (15) is the free energy due to pure shear, and the second term is the free energy due to hydrostatic compression. Pure shear is any deformation which alters only the shape of the volume element onto which the shear is applied, while hydrostatic compression is any deformation that changes only the volume of the element and not its shape. Pictures to illustrate are shown below in Figures 3,4.

Taking temperature to be constant, we compute

$$dF = Ku_{ll}du_{ll} + 2\mu(u_{ik} - \frac{1}{3}u_{ll}\delta_{ik})d(u_{ik} - \frac{1}{3}u_{ll}\delta_{ik}) = [Ku_{ll}\delta_{ik} + 2\mu(u_{ik} - \frac{1}{3}u_{ll}\delta_{ik})]du_{ik}.$$

Hence, we find that the stress tensor is given by

$$\sigma_{ik} = Ku_{ll}\delta_{ik} + 2\mu(u_{ik} - \frac{1}{3}u_{ll}\delta_{ik}). \quad (16)$$

The subscript  $l$  in this notation represents an index that is summed over. For example, if  $i \neq k$ , then

$$\sigma_{ik} = 2\mu u_{ik}.$$

But if  $i = k$ , then

$$\begin{aligned} \sigma_{kk} &= K(u_{11} + u_{22} + u_{33}) + 2\mu(u_{kk} - \frac{1}{3}(u_{11} + u_{22} + u_{33})) = (K - \frac{2}{3}\mu)(u_{11} + u_{22} + u_{33}) + 2\mu u_{kk} \\ &= \lambda(u_{11} + u_{22} + u_{33}) + 2\mu u_{kk}. \end{aligned}$$

For isotropic materials, we can write the free energy  $F$  in terms of the bulk material properties  $E$  (modulus of elasticity) and  $\nu$  (Poisson’s ratio). First, the Lamé coefficients may be given in terms of  $E$  and  $\nu$  by

$$\lambda = \frac{E\nu}{(1+\nu)(1-2\nu)}, \mu = \frac{E}{2(1+\nu)}, K = \frac{E}{3(1-2\nu)}. \quad (17)$$

Poisson’s ratio is given by

$$\nu = -\frac{u_{xx}}{u_{zz}} = \frac{1}{2} \frac{3K - 2\mu}{3K + \mu}, \quad (18)$$

the ratio of transverse compression to longitudinal extension. Poisson’s ratio is best understood in terms of a rod, which, under longitudinal extension, will narrow in its transverse dimension (transverse compression). However,  $\nu$  is purely a material property and does appear in the general elastic wave equation for isotropic materials, regardless of the geometry of the material. We can then express the free energy  $F$  in terms of  $E$  and  $\nu$  as

$$F = \frac{E}{2(1+\nu)} \left( u_{ik}^2 + \frac{\nu}{1-2\nu} u_{ll}^2 \right). \quad (19)$$

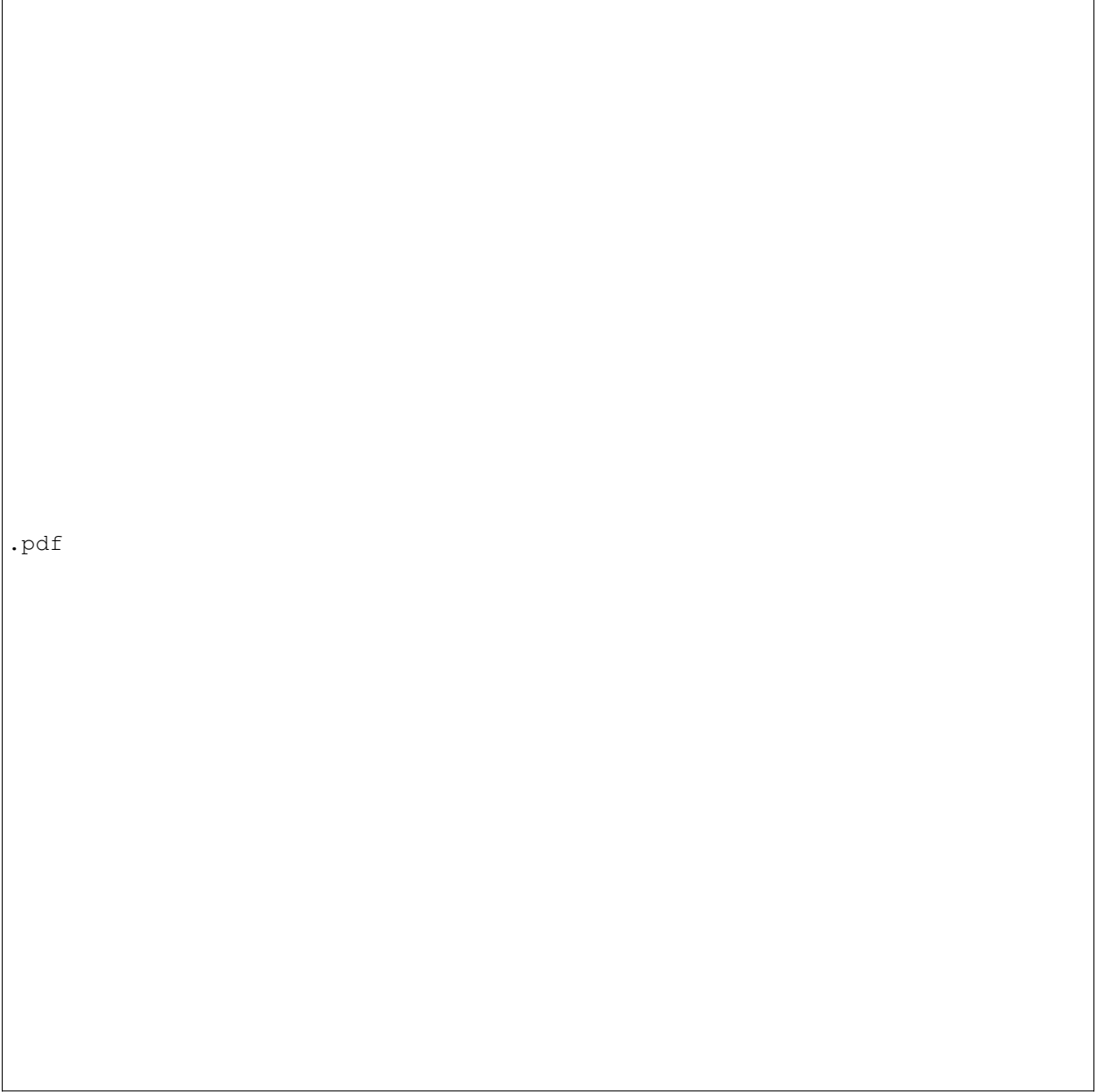


Figure 3: Depiction of pure shear.

The stress tensor is given by

$$\sigma_{ik} = \frac{E}{1+\nu} \left( u_{ik} + \frac{\nu}{1-2\nu} u_{ll} \delta_{ik} \right). \quad (20)$$

By substituting (20) into the simple equilibrium equation (6), we have

$$\frac{\partial \sigma_{ik}}{\partial x_k} = \frac{E\nu}{(1+\nu)(1-2\nu)} \frac{\partial u_{ll}}{\partial x_i} + \frac{E}{1+\nu} \frac{\partial u_{ik}}{\partial x_k}. \quad (21)$$

Substituting the expression for the strain tensor (2), we arrive at

$$\frac{E}{2(1+\nu)} \frac{\partial^2 u_i}{\partial x_k^2} + \frac{E}{2(1+\nu)(1-2\nu)} \frac{\partial^2 u_l}{\partial x_i \partial x_l} = 0. \quad (22)$$

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Figure 4: Depiction of pure shear.

In vector notation, this becomes

$$\frac{E}{2(1+\nu)}\Delta\mathbf{u} + \frac{E}{2(1+\nu)(1-2\nu)}\nabla(\nabla\cdot\mathbf{u}) = 0. \quad (23)$$

This equation (23) applied only if the deformation is caused exclusively by surface forces. If the deformation is effected by body forces  $\mathbf{f}$  (per unit volume) as well, then the above equation becomes

$$\frac{E}{2(1+\nu)}\Delta\mathbf{u} + \frac{E}{2(1+\nu)(1-2\nu)}\nabla(\nabla\cdot\mathbf{u}) + \mathbf{f} = 0. \quad (24)$$

The internal forces acting to deform an elastic body will cause acceleration of the body according to

$$\rho u_i'' = \frac{\partial \sigma_{ik}}{\partial x_k} + f_i, \quad (25)$$

which is nothing more than a statement of Newton's second law. This leads to the **elastic wave equation**

$$\rho \mathbf{u}'' = \frac{E}{2(1+\nu)} \Delta \mathbf{u} + \frac{E}{2(1+\nu)(1-2\nu)} \nabla (\nabla \cdot \mathbf{u}) + \mathbf{f}. \quad (26)$$

## 2.4 Solution for Elastic Waves in an Infinite Elastic Medium

For a non-forced plane elastic wave in an infinite elastic and isotropic medium, (26) reduces to the equations

$$\frac{\partial^2 u_x}{\partial x^2} - \frac{1}{c_l^2} \frac{\partial^2 u_x}{\partial t^2} = 0, \quad \frac{\partial^2 u_y}{\partial x^2} - \frac{1}{c_t^2} \frac{\partial^2 u_y}{\partial t^2} = 0, \quad (27)$$

where

$$c_l = \sqrt{\frac{E(1-\nu)}{\rho(1+\nu)(1-2\nu)}}, \quad c_t = \sqrt{\frac{E}{2\rho(1+\nu)}} \quad (28)$$

are the wave speeds of the longitudinal and transverse waves, respectively. The motion of the longitudinal waves are along the direction of wave propagation, while the motion of the transverse waves are orthogonal to the direction of wave propagation. Figure 5 below is a depiction of a plane wave in a plane material of finite thickness.

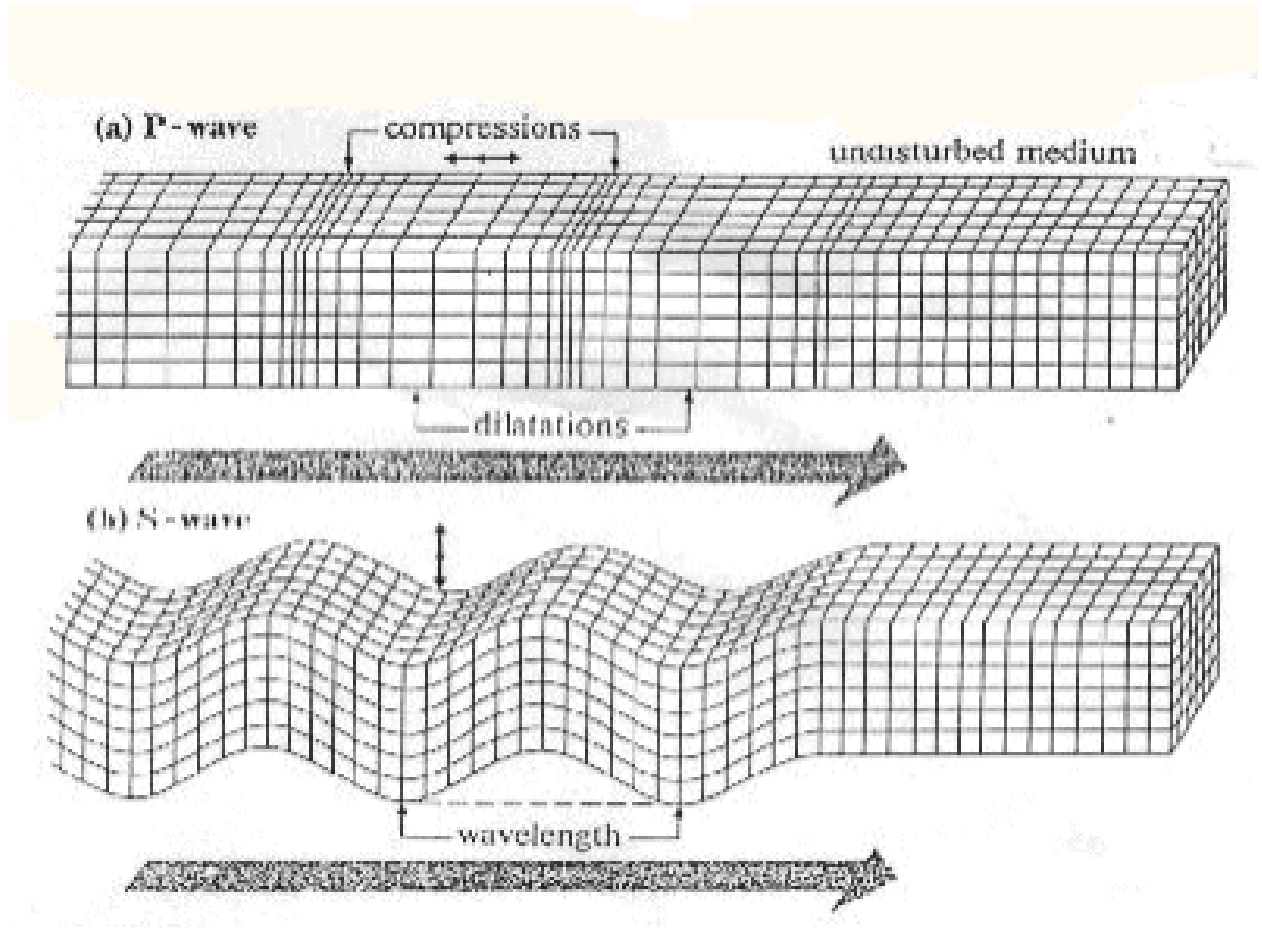


Figure 5: Depiction of plane waves in plane material of finite thickness. The P-waves are longitudinal, and the S-waves are transverse, or shear waves.

More generally, for an infinite elastic medium that need not be a plane, we can work directly with (26) (with  $\mathbf{f} = \mathbf{0}$ ) in terms of  $c_t$  and  $c_l$  defined above.

$$\mathbf{u}'' = c_t^2 \Delta \mathbf{u} + (c_l^2 - c_t^2) \nabla (\nabla \cdot \mathbf{u}) \quad (29)$$

Longitudinal waves ( $\mathbf{u}_l$ ) correspond to changes in volume of regions in the elastic body, while transverse waves ( $\mathbf{u}_t$ ) are not caused by changes in volume. We thus require that

$$\nabla \cdot \mathbf{u}_t = 0, \quad \nabla \times \mathbf{u}_l = 0.$$

We can decompose  $\mathbf{u}$  into the sum  $\mathbf{u}_l + \mathbf{u}_t$ . Substitution of this sum gives

$$\mathbf{u}_l'' + \mathbf{u}_t'' = c_t^2 \Delta(\mathbf{u}_l + \mathbf{u}_t) + (c_l^2 - c_t^2) \nabla(\nabla \cdot \mathbf{u}_l). \quad (30)$$

Taking the divergence of both sides gives

$$\nabla \cdot \mathbf{u}_l'' = c_t^2 \Delta(\nabla \cdot \mathbf{u}_l) + (c_l^2 - c_t^2) \Delta(\nabla \cdot \mathbf{u}_l),$$

implying that

$$\nabla \cdot (\mathbf{u}_l'' - c_l^2 \Delta \mathbf{u}_l) = 0.$$

By a similar argument with the curl operator, we also have that

$$\nabla \times (\mathbf{u}_t'' - c_t^2 \Delta \mathbf{u}_t) = 0.$$

If both the curl and divergence of a vector field are zero, this implies that the vector field is identically zero. Thus, the above equations imply that

$$\frac{\partial^2 \mathbf{u}_l}{\partial t^2} - c_l^2 \Delta \mathbf{u}_l = 0, \quad \frac{\partial^2 \mathbf{u}_t}{\partial t^2} - c_t^2 \Delta \mathbf{u}_t = 0. \quad (31)$$

To summarize, by applying the assumptions on the first page, we can determine a nice linear vector PDE for elastic waves. Moreover, we can break the wave solution into independent transverse and longitudinal waves.

## 2.5 Rayleigh Waves

I will summarize the fundamental concepts of Rayleigh waves, which are surface waves with amplitudes that decay exponentially with depth into a material. The following derivation of the solution is taken from [1]. We take as an ansatz

$$u = f(x_2) e^{i(k_1 x_1 - \omega t)}. \quad (32)$$

Here,  $x_1$  and  $x_2$  are the plane wave propagation directions along the material and into the material, respectively. Note that in the material,  $x_2$  decreases with depth and is always less than zero. The relevant coordinate system is shown below in Figure 6. Note that  $x_2 = 0$  at the surface of the material. The positive  $x_3$  axis points into the figure. This is in agreement with the right-hand rule.

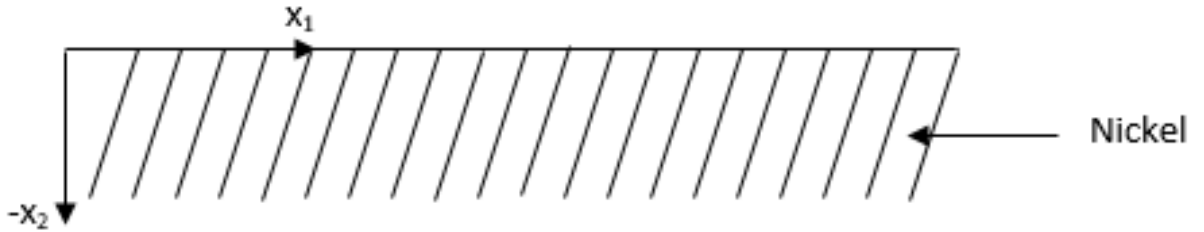


Figure 6: Coordinate system for Rayleigh wave analysis.

Substitution of (32) into the wave equation

$$\frac{\partial^2 u}{\partial t^2} - c^2 \Delta u = 0,$$



where  $u$  is any component of either  $\mathbf{u}_l$  or  $\mathbf{u}_t$ , and  $c$  represents either  $c_l$  or  $c_t$ , gives the ODE

$$\frac{d^2 f}{dx_2^2} = \left( k_1^2 - \frac{\omega^2}{c^2} \right) f. \quad (33)$$

If  $k_1^2 - \omega^2/c^2 < 0$ , we have an ordinary plane wave whose amplitude does not decay within the body. Thus, to ensure the existence of Rayleigh waves, we require that  $k_1^2 - \omega^2/c^2 > 0$ . This gives the solutions for  $f$ :

$$f(x_2) = C \exp \left( \pm \sqrt{k_1^2 - \frac{\omega^2}{c^2}} x_2 \right).$$

In the context of [1], we want the solution to decay with decreasing  $x_2$  (into the material). This gives (since  $x_2 < 0$ ),

$$u = C e^{i(k_1 x_1 - \omega t)} e^{\kappa x_2}, \quad (34)$$

where

$$\kappa = \sqrt{k_1^2 - \omega^2/c^2}. \quad (35)$$

To determine the displacement vector  $\mathbf{u}$ , which is a specific linear combination of  $\mathbf{u}_l$  and  $\mathbf{u}_t$ , we need to incorporate boundary conditions. At the free surface ( $x_2 = 0$ ), we have the stress free condition

$$\sigma_{ik} n_k = 0.$$

Because we are considering an isotropic material in this derivation, the stress tensor  $\sigma_{ik}$  has the same definition ((16))

$$\sigma_{ik} = K u_{ll} \delta_{ik} + 2\mu (u_{ik} - \frac{1}{3} u_{ll} \delta_{ik}).$$

Thus,

$$\sigma_{x_1 x_2} = \sigma_{x_3 x_2} = \sigma_{x_2 x_2} = 0.$$

Referring to the stress-strain relation for isotropic materials, the above implies that

$$u_{x_1 x_2} = 0, \quad u_{x_3 x_2} = 0, \quad \lambda(u_{x_1 x_1} + u_{x_3, x_3}) + (\lambda + 2\mu) u_{x_2 x_2} = 0.$$

Applying the definitions of  $\lambda$  and  $\mu$ , the third condition above is equivalent to

$$\nu(u_{x_1 x_1} + u_{x_3, x_3}) + (1 - \nu) u_{x_2 x_2} = 0.$$

Because all quantities are independent of the variable  $x_3$ , the second of the above conditions gives

$$u_{x_3, x_2} = \frac{1}{2} \left( \frac{\partial u_{x_3}}{\partial u_{x_2}} + \frac{\partial u_{x_2}}{\partial u_{x_3}} \right) = \frac{1}{2} \frac{\partial u_{x_3}}{\partial x_2} = 0.$$

Using (34), this gives  $u_{x_3} = 0$ , which means that the wave does not vary in the direction perpendicular to the propagation directions  $x_1$  and  $x_2$ . The transverse part of the wave must satisfy  $\nabla \cdot \mathbf{u}_t = 0$ :

$$\frac{\partial u_{tx_1}}{\partial x_1} + \frac{\partial u_{tx_2}}{\partial x_2} = 0.$$

Note that the subscripts  $tx_1$  and  $tx_2$  do not represent partial derivatives, but rather the components of  $\mathbf{u}_t$  in the  $x_1$  and  $x_2$  directions. This gives us the equation

$$ik_1 u_{tx_1} + \kappa_t u_{tx_2} = 0. \quad (36)$$

This gives use the equations

$$u_{tx_1} = \kappa_t a e^{ik_1 x_1 + \kappa_t x_2 - i\omega t}, \quad u_{tx_2} = -ik_1 a e^{ik_1 x_1 + \kappa_t x_2 - i\omega t}, \quad (37)$$

where  $a$  is a constant. The longitudinal part  $\mathbf{u}_l$  satisfies  $\nabla \times \mathbf{u}_l = 0$ :

$$\frac{\partial u_{lx_1}}{\partial x_2} - \frac{\partial u_{lx_2}}{\partial x_1} = 0.$$

This leads to the equation

$$ik_1 u_{lx_2} - \kappa_l u_{lx_1} = 0. \quad (38)$$

This gives use the equations

$$u_{lx_1} = k_1 b e^{ik_1 x_1 + \kappa_l x_2 - i\omega t}, \quad u_{lx_2} = -i\kappa_l b e^{ik_1 x_1 + \kappa_l x_2 - i\omega t}, \quad (39)$$

where  $b$  is a constant. We arrive at the system of equations

$$\frac{\partial u_{x_1}}{\partial x_2} + \frac{\partial u_{x_2}}{\partial x_1} = 0, \quad (40)$$

$$c_l^2 \frac{\partial u_{x_2}}{\partial x_2} + (c_l^2 - c_t^2) \frac{\partial u_{x_1}}{\partial x_1} = 0. \quad (41)$$

Substituting  $u_{x_1} = u_{lx_1} + u_{tx_1}$  and  $u_{x_2} = u_{lx_2} + u_{tx_2}$ , the result is the system

$$a(k_1^2 + \kappa_t^2) + 2bk_1\kappa_l = 0, \quad (42)$$

$$2ac_t^2\kappa_t k_1 + b[c_l^2(\kappa_l^2 - k_1^2) + 2c_t^2 k_1^2] = 0. \quad (43)$$

Dividing the second equation by  $c_t^2$  and substituting

$$\kappa_l^2 - k_1^2 = -\omega^2/c_l^2 = -(k_1^2 - \kappa_t^2)c_t^2/c_l^2,$$

we get

$$2a\kappa_t k_1 + b(k_1^2 + \kappa_t^2) = 0 \quad (44)$$

For the first of (42) and (44) to be compatible, we require that

$$(k_1^2 + \kappa_t^2)^2 = 4k_1^2\kappa_t\kappa_l.$$

Squaring and substituting the values of  $\kappa_t^2$  and  $\kappa_l^2$ , we arrive at the dispersion relation

$$\left(2k_1^2 - \frac{\omega^2}{c_t^2}\right)^4 = 16k_1^4 \left(k_1^2 - \frac{\omega^2}{c_t^2}\right) \left(k_1^2 - \frac{\omega^2}{c_l^2}\right). \quad (45)$$

Now, substituting  $\omega = c_t k_1 \xi$ , we obtain the polynomial equation

$$\xi^6 - 8\xi^4 + 8\xi^2 \left(3 - 2\frac{c_t^2}{c_l^2}\right) - 16 \left(1 - \frac{c_t^2}{c_l^2}\right) = 0.$$

I solved this equation in Mathematica, and the result is that there is one real root  $\xi \approx 0.9325$ . The single dispersion relation is

$$\omega(k_1) = c_t \xi k_1.$$

A plot of this single linear dispersion is shown in Figure 7.

## 2.6 Elastic Waves in crystals

Solutions to the elastic wave equation will differ based on the geometry of the problem, and the imposed boundary and initial conditions. Due to the second partial time derivative, the posed problem must have prescribed initial data for  $\mathbf{u}$  and  $\mathbf{u}_t$ . Problems considered in this report involve plane wave propagation in one or more material layers. The material layers may vary in thickness and material type. But the same boundary conditions apply. We require that at the interface between different materials, shear and longitudinal stresses and displacements match. This is really ensuring continuity of the wave solutions between layers. A particular case is the plane interface between vacuum and material, in which we require that the stresses are zero. We will also require that the frequency  $\omega$  and wavenumber  $k_1$  (indicating waves per distance in the  $x_1$  direction) are constant between layers. This condition is Snell's Law, and basically states that the momentum of the elastic waves parallel to the material interface must be conserved.

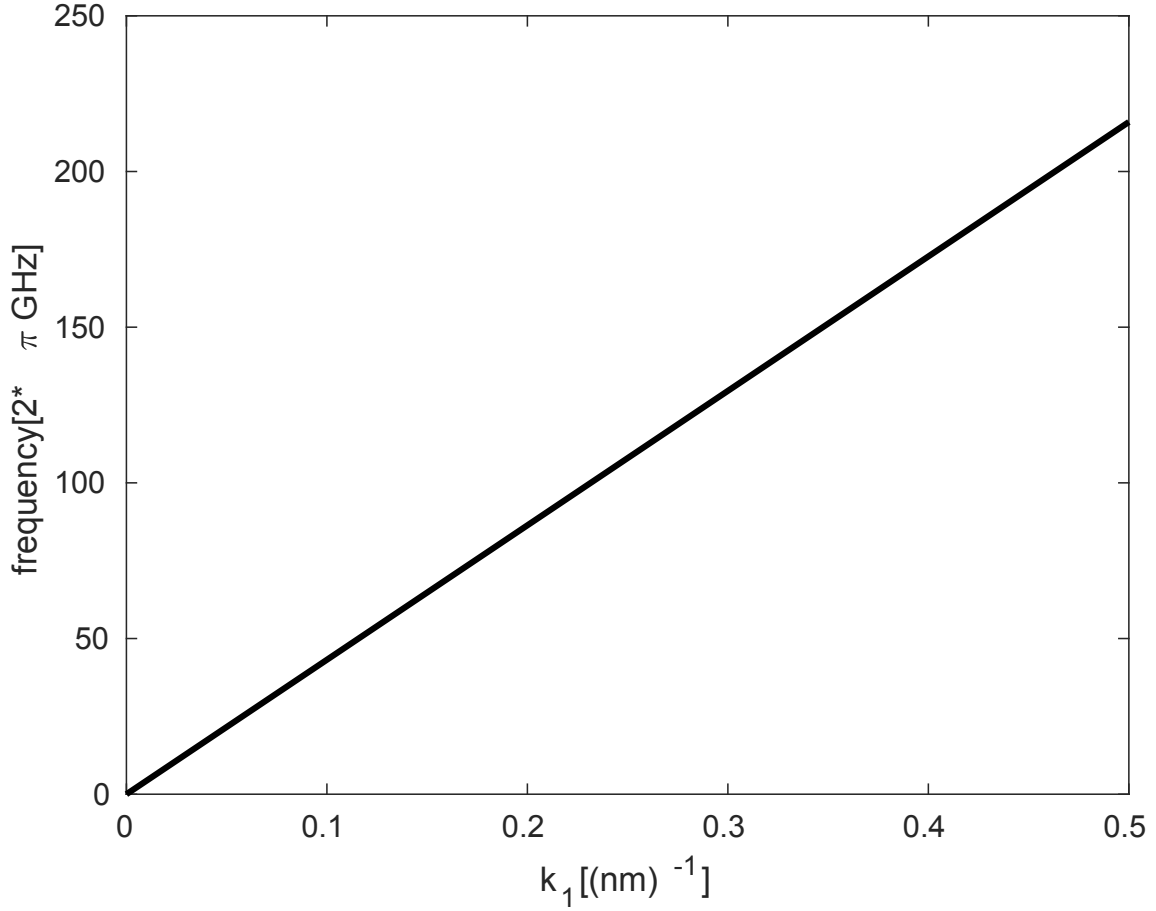


Figure 7: Rayleigh dispersion curve for nickel.

Surface waves are elastic waves that propagate near the surface of a body. In particular, Rayleigh waves are surface waves which decay exponentially in amplitude with depth into the material and are examined in [1] (pp. 94-97).

For crystalline materials, the equation of motion is given by

$$\rho u_i'' = \lambda_{iklm} \frac{\partial u_i}{\partial x_k \partial x_l}, \quad (46)$$

where the stress tensor is given by

$$\sigma_{ik} = \lambda_{iklm} u_{lm}.$$

This is summation notation, and is equivalent to the expanded form

$$\sigma_{ik} = \sum_{lm} \lambda_{iklm} u_{lm}.$$

We can also illustrate with the following matrix equation, relating stress and strain.

$$\begin{bmatrix} \sigma_{xx} \\ \sigma_{yy} \\ \sigma_{zz} \\ \sigma_{yz} \\ \sigma_{zx} \\ \sigma_{xy} \end{bmatrix} = \begin{bmatrix} \lambda_{xxxx} & \lambda_{xxyy} & \lambda_{xxzz} & \lambda_{xxyz} & \lambda_{xxzx} & \lambda_{xxxy} \\ \lambda_{yyxx} & \lambda_{yyyy} & \lambda_{yyzz} & \lambda_{yyyz} & \lambda_{yyzx} & \lambda_{yyxy} \\ \lambda_{zzxx} & \lambda_{zzyy} & \lambda_{zzzz} & \lambda_{zzyz} & \lambda_{zzzx} & \lambda_{zzxy} \\ \lambda_{yzxx} & \lambda_{yzyy} & \lambda_{yzzz} & \lambda_{yzyz} & \lambda_{yzzx} & \lambda_{yzxy} \\ \lambda_{zxxx} & \lambda_{zxyy} & \lambda_{zxxx} & \lambda_{zxyz} & \lambda_{zxzx} & \lambda_{zxxy} \\ \lambda_{xyxx} & \lambda_{xyyy} & \lambda_{xyyz} & \lambda_{xyyz} & \lambda_{xyzx} & \lambda_{xyxy} \end{bmatrix} \cdot \begin{bmatrix} u_{xx} \\ u_{yy} \\ u_{zz} \\ u_{yz} \\ u_{zx} \\ u_{xy} \end{bmatrix}.$$

For an isotropic material, using the equation (16), we obtain the simplified matrix relation between stress and strain.

$$\begin{bmatrix} \sigma_{xx} \\ \sigma_{yy} \\ \sigma_{zz} \\ \sigma_{yz} \\ \sigma_{zx} \\ \sigma_{xy} \end{bmatrix} = \begin{bmatrix} \lambda + 2\mu & \lambda & \lambda & 0 & 0 & 0 \\ \lambda & \lambda + 2\mu & \lambda & 0 & 0 & 0 \\ \lambda & \lambda & \lambda + 2\mu & 0 & 0 & 0 \\ 0 & 0 & 0 & 2\mu & 0 & 0 \\ 0 & 0 & 0 & 0 & 2\mu & 0 \\ 0 & 0 & 0 & 0 & 0 & 2\mu \end{bmatrix} \cdot \begin{bmatrix} u_{xx} \\ u_{yy} \\ u_{zz} \\ u_{yz} \\ u_{zx} \\ u_{xy} \end{bmatrix}.$$

with  $\lambda$  and  $\mu$  defined in (17). If we assume that the solution takes the form

$$\mathbf{u} = \mathbf{u}_0 e^{i(\mathbf{k} \cdot \mathbf{x} - \omega t)},$$

substitution into the equation (46) will lead to a dispersion relation (relationship between the wave frequency  $\omega$  and the wave vector  $\mathbf{k}$ ). This will give the directions of polarization of the wave. More details are given in [1] (pp. 92-93).

### 3 Problem of Interest: Plane Waves in Multi-layered Media

#### 3.1 Problem Description

The specific elastic problem of interest involves elastic wave propagation in a 50 nm thick Ni (nickel) layer atop a 100 nm thick Si3N4 (silicon nitride) layer with vacuum half-spaces on either side of the material. A paper by Michael Lowe [3] addresses several numerical methods (Transfer Matrix and Global Matrix) of solving the dispersion relation for this problem. The basic idea is to pose the solution formulas for the longitudinal and shear wave displacements and incorporate boundary conditions between layers and boundary conditions on the exterior surfaces of the material. This leads to a matrix equation that relates the displacements and stresses in one layer to another layer. The global matrix method in particular leads to a singular matrix equation that can be solved to find the dispersion relation between wave frequency and wave number. Later in this report, the global matrix method (GMM) is explained and applied first for a single material layer between two vacuum half-spaces. Then, the problem of interest, in which we have two material layers in contact between two vacuum half-spaces, is explained.

The relevant properties of the materials for this problem are listed as follows.

- Young's modulus for nickel: 197 giga-pascals
- Density of Nickel: 8908 kg-m<sup>3</sup>
- Shear modulus for nickel: 142 gig-pascals
- Young's modulus for silicon nitride: 171 giga-pascals
- Density of silicon nitride: 3124 kg-m<sup>3</sup>
- Shear modulus for silicon nitride: 127 giga-pascals

We calculate Poisson's ratio  $\nu$  for both materials as follows.

$$\nu = \text{Abs} \left( \frac{E}{2\mu} - 1 \right),$$

where  $E$  and  $\mu$  are the elastic modulus and shear modulus, respectively. For nickel,  $\nu_{\text{nickel}} \approx 87/284$ , and for silicon nitride,  $\nu_{\text{silicon nitride}} \approx 83/254$ . These values are used in the global matrix method calculation (see report for June 10 under the heading "Global Matrix Method").

### 3.2 Global Matrix Method

I want to summarize the main points of the paper by Lowe [3]. Of particular interest is the Global Matrix Method, and how it can be applied to solve the multilayer plane elastic wave problem. The paper begins with the basic elastic wave equation in an isotropic medium

$$\rho \frac{\partial^2 \mathbf{u}}{\partial t^2} = (\lambda + \mu) \nabla (\nabla \cdot \mathbf{u}) + \mu \Delta \mathbf{u} \quad (47)$$

Lowe's derivation is given in his equations (1)-(4). The wave solutions  $\mathbf{u}$  are constructed by separately considering longitudinal waves  $\mathbf{u}_L$  and shear waves  $\mathbf{u}_S$ . The longitudinal wave solution is given by

$$\mathbf{u}_L = \nabla \phi, \quad (48)$$

where  $\phi$  is given by

$$\phi = A_L e^{i(\mathbf{k} \cdot \mathbf{x} - \omega t)} = A_L e^{i(k_1 x_1 + k_2 x_2 + k_3 x_3 - \omega t)}. \quad (49)$$

The shear wave solution is given by

$$\mathbf{u}_S = \nabla \times \psi, \quad (50)$$

where

$$|\psi| = A_S e^{i(\mathbf{k} \cdot \mathbf{x} - \omega t)} = A_S e^{i(k_1 x_1 + k_2 x_2 + k_3 x_3 - \omega t)}. \quad (51)$$

The vector  $\mathbf{k}$  is the wave number and gives the direction of wave propagation (both longitudinal and shear waves). The direction of  $\psi$  is normal to both the direction of wave propagation and particle motion. The value  $\omega$  is the angular frequency. One can check in the general derivation in the first weekly report that these wave solutions satisfy

$$\nabla \times \mathbf{u}_L = 0, \quad \nabla \cdot \mathbf{u}_S = 0.$$

That is, the longitudinal wave solution are irrotational, and the shear wave solution is divergence free. The problem considered in the paper [3] is a multilayer material where the coordinate  $x_1$  is the direction of wave propagation along the material, and  $x_2$  is the direction of wave propagation into the material (material depth). The relevant depiction is figure 2 in the paper. The assumption is that no quantity (stress, displacement, strain, etc) varies in the  $x_3$  direction. This is the concept of the plane wave. The longitudinal and shear wave solutions may be written out as

$$\mathbf{u}_L = A_L e^{i(\mathbf{k} \cdot \mathbf{x} - \omega t)} (k_1 \hat{x}_1 + k_2 \hat{x}_2) \quad (52)$$

$$\mathbf{u}_S = A_S e^{i(\mathbf{k} \cdot \mathbf{x} - \omega t)} (k_1 \hat{x}_1 - k_2 \hat{x}_2), \quad (53)$$

where  $\hat{x}_1$  and  $\hat{x}_2$  are the unit vectors in the  $x_1$  and  $x_2$  directions, respectively. In figure 2 of the paper, there are seen to be four waves in each layer. A similar figure is given in Figure 8 below. Each labeled arrow represents longitudinal and shear waves propagating within a layer originating from above that layer (+) or from below that layer (-). For example, layer 2 is between interfaces  $i1$  and  $i2$  and is seen to have four waves (two for (+) and two for (-)).

The boundary condition between layers is Snell's Law, which requires that all waves interacting at a layer interface must share the same  $k_1$  and  $\omega$ . The wave speed of either the shear or longitudinal waves is given by  $c = \frac{\omega}{|\mathbf{k}|}$ . If we denote the longitudinal wave speed by  $\alpha$ , then we have that

$$\alpha^2 = \frac{\omega^2}{k_1^2 + k_2^2}$$

which implies that

$$k_{2,(L\pm)} = \pm(\omega^2/\alpha^2 - k_1^2)^{1/2} \quad (54)$$

Similarly, if we denote the shear wave speed by  $\beta$ , then

$$k_{2,(S\pm)} = \pm(\omega^2/\beta^2 - k_1^2)^{1/2}. \quad (55)$$

The positive sign denotes a wave traveling downward (into the material, increasing in the  $x_2$  direction), and the negative sign denotes a wave traveling upward.

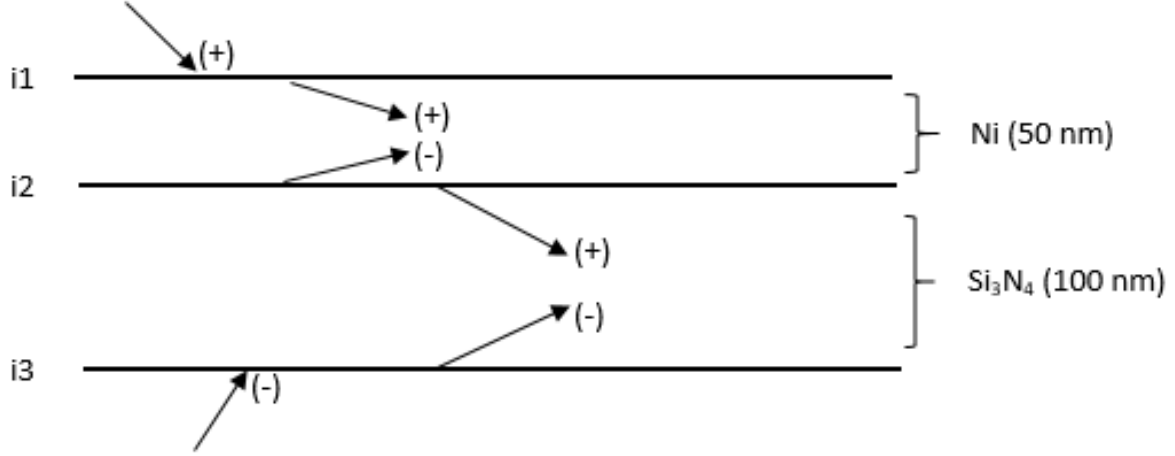


Figure 8: Depiction of waves in multilayered material.

Because another assumption in the paper is isotropic layers (each layer has its own homogeneous properties), the longitudinal and shear wave speeds in each layer may be written as

$$\alpha = \left( \frac{E(1-\nu)}{\rho(1+\nu)(1-2\nu)} \right)^{1/2} \quad (56)$$

$$\beta = \left( \frac{E}{2\rho(1+\nu)} \right)^{1/2}, \quad (57)$$

where  $E$  is the modulus of elasticity,  $\rho$  is the density, and  $\nu$  is Poisson's ratio for that particular layer.

We have the following formulas for the longitudinal and bulk waves in a given layer. The subscript 1 indicates the component of the wave; 1 indicating the  $x_1$ -direction, and  $x_2$  indicating the  $x_2$ -direction. The subscript  $L$  denotes a longitudinal wave, and the subscript  $S$  denotes a shear wave.

$$u_{1,L} = A_{(L\pm)} k_1 F e^{\pm i(\omega^2/\alpha^2 - k_1^2)^{1/2} x_2} \quad (58)$$

$$u_{2,L} = \pm (\omega^2/\alpha^2 - k_1^2)^{1/2} A_{(L\pm)} F e^{\pm i(\omega^2/\alpha^2 - k_1^2)^{1/2} x_2} \quad (59)$$

$$u_{1,S} = \pm (\omega^2/\beta^2 - k_1^2)^{1/2} A_{(S\pm)} F e^{\pm i(\omega^2/\beta^2 - k_1^2)^{1/2} x_2} \quad (60)$$

$$u_{2,S} = -A_{(S\pm)} k_1 F e^{\pm i(\omega^2/\beta^2 - k_1^2)^{1/2} x_2}, \quad (61)$$

where  $F$  is an 'invariant' of the system given by

$$F = e^{i(k_1 x_1 - \omega t)}. \quad (62)$$

Figure 9 should be helpful in illustrating the equations (58).

The stresses  $\sigma_{ij}$  may be calculated from the equations (58) based on the following formulas.

$$\sigma_{11} = \lambda(u_{11} + u_{22} + u_{33}) + 2\mu u_{11} \quad (63)$$

$$\sigma_{22} = \lambda(u_{11} + u_{22} + u_{33}) + 2\mu u_{22} \quad (64)$$

$$\sigma_{33} = \lambda(u_{11} + u_{22} + u_{33}) + 2\mu u_{33} \quad (65)$$

$$\sigma_{12} = \mu u_{12}, \quad \sigma_{23} = \mu u_{23}, \quad \sigma_{13} = \mu u_{13} \quad (66)$$

$$u_{11} = \frac{\partial u_1}{\partial x_1}, \quad u_{22} = \frac{\partial u_2}{\partial x_1}, \quad u_{33} = \frac{\partial u_3}{\partial x_1}, \quad (67)$$

$$u_{12} = \frac{\partial u_1}{\partial x_2} + \frac{\partial u_2}{\partial x_1}, \quad u_{23} = \frac{\partial u_2}{\partial x_3} + \frac{\partial u_3}{\partial x_2}, \quad u_{13} = \frac{\partial u_1}{\partial x_3} + \frac{\partial u_3}{\partial x_1}. \quad (68)$$

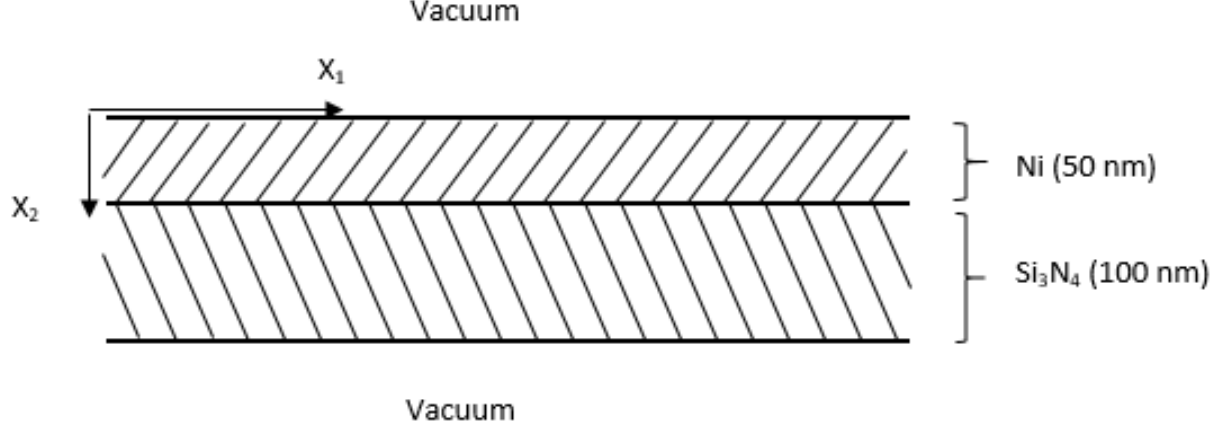


Figure 9: Coordinate system for multilayer plane wave analysis.

Thus, the formulas for the stresses may be calculated to yield, for the longitudinal waves

$$\sigma_{11} = i(\omega^2 - 2\beta^2\omega^2/\alpha^2 + 2\beta^2k_1^2)\rho A_{L(\pm)} F e^{\pm i(\omega^2/\alpha^2 - k_1^2)^{1/2}x_2} \quad (69)$$

$$\sigma_{22} = i(\omega^2 - 2\beta^2k_1^2)\rho A_{L(\pm)} F e^{\pm i(\omega^2/\alpha^2 - k_1^2)^{1/2}x_2} \quad (70)$$

$$\sigma_{33} = i(1 - 2\beta^2/\alpha^2)\omega^2\rho F e^{\pm i(\omega^2/\alpha^2 - k_1^2)^{1/2}x_2} \quad (71)$$

$$\sigma_{12} = \pm i2\beta^2k_1(\omega^2/\alpha^2 - k_1^2)^{1/2}\rho F e^{\pm i(\omega^2/\alpha^2 - k_1^2)^{1/2}x_2} \quad (72)$$

$$\sigma_{13} = \sigma_{23} = 0. \quad (73)$$

and for the shear waves

$$\sigma_{11} = \pm i2\beta^2k_1(\omega^2/\beta^2 - k_1^2)^{1/2}\rho A_{(S\pm)} F e^{\pm i(\omega^2/\beta^2 - k_1^2)^{1/2}x_2} \quad (74)$$

$$\sigma_{22} = -\sigma_{11} \quad (75)$$

$$\sigma_{12} = i(\omega^2 - 2\beta^2k_1^2)\rho A_{(S\pm)} F e^{\pm i(\omega^2/\beta^2 - k_1^2)^{1/2}x_2} \quad (76)$$

$$\sigma_{33} = \sigma_{13} = \sigma_{23} = 0. \quad (77)$$

At any interface between layers, we require that the displacement components  $u_1, u_2$  and the normal stress  $\sigma_{22}$ , and the shear stress  $\sigma_{12}$  be continuous. The displacements and stresses at any location  $x_2$  in a layer are found by summing the contributions from the four waves in the layer. To write the equations efficiently, the author defines the following quantities

$$C_\alpha = (\omega^2/\alpha^2 - k_1^2)^{1/2}, \quad C_\beta = (\omega^2/\beta^2 - k_1^2)^{1/2}, \quad g_\alpha = e^{i(\omega^2/\alpha^2 - k_1^2)^{1/2}x_2}, \quad g_\beta = e^{i(\omega^2/\beta^2 - k_1^2)^{1/2}x_2} \quad (78)$$

$$B = \omega^2 - 2\beta^2k_1^2. \quad (79)$$

If we omit the invariant  $F$ , we obtain the following system of equations for a given layer.

$$\begin{bmatrix} u_1 \\ u_2 \\ \sigma_{22} \\ \sigma_{12} \end{bmatrix} = \begin{bmatrix} k_1g_\alpha & \frac{k_1}{g_\alpha} & C_\beta g_\beta & -\frac{C_\beta}{g_\beta} \\ C_\alpha g_\alpha & -\frac{C_\alpha}{g_\alpha} & -k_1g_\beta & -\frac{k_1}{g_\beta} \\ i\rho B g_\alpha & \frac{i\rho B}{g_\alpha} & -2i\rho k_1\beta^2 C_\beta g_\beta & \frac{2i\rho k_1\beta^2 C_\beta}{g_\beta} \\ 2i\rho k_1\beta^2 C_\alpha g_\alpha & -\frac{2i\rho k_1\beta^2 C_\alpha}{g_\alpha} & i\rho B g_\beta & \frac{i\rho B}{g_\beta} \end{bmatrix} \begin{bmatrix} A_{(L+)} \\ A_{(L-)} \\ A_{(S+)} \\ A_{(S-)} \end{bmatrix}$$

This is what the author refers to as the ‘field matrix’  $[D]$ .

The author proceeds to discuss the Transfer Matrix Method and the Global Matrix Method. I will summarize the Global Matrix Method. The goal of either method is to establish the dispersion relation (relationship between  $\omega$  and

$k_1$ ) for each wave. The Global Matrix Method is based on the observation that in order to ensure continuity between layers, we need for the following equation to hold

$$[D]_{ln,bottom} \begin{bmatrix} A_{(L+)} \\ A_{(L-)} \\ A_{(S+)} \\ A_{(S-)} \end{bmatrix}_{ln} = [D]_{l(n+1),top} \begin{bmatrix} A_{(L+)} \\ A_{(L-)} \\ A_{(S+)} \\ A_{(S-)} \end{bmatrix}_{l(n+1)}$$

at layer  $n$ , where  $[D]$  is the matrix in the above equation. This may be expressed in the single matrix equation

$$\begin{bmatrix} [D_{2b}] & \mathbf{0} \\ \mathbf{0} & [D_{3t}] \end{bmatrix} \begin{bmatrix} A_{(L+)}n \\ A_{(L-)}n \\ A_{(S+)}n \\ A_{(S-)}n \\ A_{(L+)}(n+1) \\ A_{(L-)}(n+1) \\ A_{(S+)}(n+1) \\ A_{(S-)}(n+1) \end{bmatrix} = \{0\},$$

where the  $b$  and  $t$  denote the 'bottom' and 'top' layers, respectively.

The author extends the formulation of this equation to 5 layers, using the matrix definitions

$$[D_t] = \begin{bmatrix} k_1 & k_1 g_\alpha & C_\beta & -C_\beta g_\beta \\ C_\alpha & -C_\alpha g_\alpha & -k_1 & -k_1 g_\beta \\ i\rho B & i\rho B g_\alpha & -2i\rho k_1 \beta^2 C_\beta & 2i\rho k_1 \beta^2 C_\beta g_\beta \\ 2i\rho k_1 \beta^2 C_\alpha & -2i\rho k_1 \beta^2 C_\alpha g_\alpha & i\rho B & i\rho B g_\beta \end{bmatrix}$$

$$[D_b] = \begin{bmatrix} k_1 g_\alpha & k_1 & C_\beta g_\beta & -C_\beta \\ C_\alpha g_\alpha & -C_\alpha & -k_1 g_\beta & -k_1 \\ i\rho B g_\alpha & i\rho B & -2i\rho k_1 \beta^2 C_\beta g_\beta & 2i\rho k_1 \beta^2 C_\beta \\ 2i\rho k_1 \beta^2 C_\alpha g_\alpha & -2i\rho k_1 \beta^2 C_\alpha & i\rho B g_\beta & i\rho B \end{bmatrix}.$$

Note that the definitions of  $[D_t]$  and  $[D_b]$  are different than for the matrix  $[D]$ . This is because the author changes his convention for the origin of each wave in each layer (from his convention for applying the Transfer Matrix Method). Specifically, he defines the origin of downward travelling waves ( $L+$ ,  $S+$ ) to be the top of the layer and the origin of upward travelling waves ( $L-$ ,  $S-$ ) to be the bottom of the layer. A list is provided below for the four layer problem to showcase what values of depth ( $x_2$ ) are chosen for each  $[D]$  matrix. The author proceeds to display the problem with for five layers (two vacuum half-spaces and three material layers) with the matrix equation

$$\begin{bmatrix} [D_{1b}] & [-D_{2t}] & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & [D_{2b}] & [-D_{3t}] & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & [D_{3b}] & [-D_{4t}] & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & [D_{4b}] & [-D_{5t}] \end{bmatrix} \cdot \begin{bmatrix} \{A_1\} \\ \{A_2\} \\ \{A_3\} \\ \{A_4\} \\ \{A_5\} \end{bmatrix} = \{0\},$$

which is a 12 by 12 matrix. In general, for  $n$  layers, the above system is  $4(n-1)$  equations in  $4n$  unknowns. Thus, we must specify four of the wave amplitudes in the above equations must be known and moved to the right hand side. If we specify the four amplitudes in the half-spaces ( $A_{(L+)}1$ ,  $A_{(S+)}1$ ,  $A_{(L-)}5$ ,  $A_{(S-)}5$ ), then we have

$$\begin{bmatrix} [D_{1b}^-] & [-D_{2t}] & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & [D_{2b}] & [-D_{3t}] & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & [D_{3b}] & [-D_{4t}] & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & [D_{4b}] & [-D_{5t}^+] \end{bmatrix} \cdot \begin{bmatrix} \{A_1^-\} \\ \{A_2\} \\ \{A_3\} \\ \{A_4\} \\ \{A_5^+\} \end{bmatrix} = \begin{bmatrix} [-D_{1b}^+] & \mathbf{0} \\ \mathbf{0} & [D_{5t}^-] \end{bmatrix} \begin{bmatrix} \{A_1^+\} \\ \{0\} \\ \{0\} \\ \{0\} \\ \{A_5^-\} \end{bmatrix}$$

The  $+$ ,  $-$  vectors and matrices are given by

$$\{A^+\} = \begin{bmatrix} A_{(L+)} \\ A_{(S+)} \end{bmatrix}$$



$$\{A^-\} = \begin{bmatrix} A_{(L-)} \\ A_{(S-)} \end{bmatrix}$$

$$[D^+] = \begin{bmatrix} D_{11} & D_{13} \\ D_{21} & D_{23} \\ D_{31} & D_{33} \\ D_{41} & D_{43} \end{bmatrix}$$

$$[D^-] = \begin{bmatrix} D_{12} & D_{14} \\ D_{22} & D_{24} \\ D_{32} & D_{34} \\ D_{42} & D_{44} \end{bmatrix}$$

The author points out on page 539 of the paper that for vacuum half spaces, we can set densities to zero and  $\alpha$  and  $\beta$  to arbitrary nonzero values for the  $[D^+]$  and  $[D^-]$  matrices appearing in the above system. This makes sense because the vacuum has zero density. Finally, by setting the determinant of the matrix on the left hand side equal to zero, we obtain the characteristic relationship between  $\omega$  and  $k_1$ . This is the dispersion relation and the mathematical approach that Tom used.

### 3.3 Solution for Single Material Layer

We can apply the numerical approach in [3] to find the dispersion relationships for the single layer of nickel in the two vacuum half-spaces. This is a three-layer problem (two vacuum layers plus one material layer). I expect only two major acoustic dispersion lines (corresponding to the transverse and longitudinal waves). The setup is

$$\begin{bmatrix} [D_{1b}^-] & [-D_{2t}] & \mathbf{0} \\ \mathbf{0} & [D_{2b}] & [-D_{3t}^+] \end{bmatrix} \cdot \begin{bmatrix} \{A_1\} \\ \{A_2\} \\ \{A_3\} \end{bmatrix} = \{0\},$$

with the  $[D]$  matrices having the same definitions as previously. It is instructive to explain what values of  $x_2$  to use for each part of the matrices  $[D_t]$  and  $[D_b]$ . This is shown in the list below.

- No  $x_2$  appears for submatrices  $[D_{1b}^-]$  and  $[D_{4t}^+]$
- $i1$ :
  - $[D_{2t}]$ :  $x_{(2+)} = 0 \text{ nm}$ ,  $x_{(2-)} = -50 \text{ nm}$
- $i2$ :
  - $[D_{2b}]$ :  $x_{(2+)} = 50 \text{ nm}$ ,  $x_{(2-)} = 0 \text{ nm}$

For our particular problem, we have four layers (two vacuum half-spaces and two material layers). So, the matrix problem we are interested in is

$$\begin{bmatrix} [D_{1b}^-] & [-D_{2t}] & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & [D_{2b}] & [-D_{3t}] & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & [D_{3b}] & [-D_{4t}^+] \end{bmatrix} \cdot \begin{bmatrix} \{A_1\} \\ \{A_2\} \\ \{A_3\} \\ \{A_4\} \end{bmatrix} = \{0\}.$$

Again, the values of  $x_2$  to use for each part of the matrices  $[D_t]$  and  $[D_b]$  are shown in the list below.

- No  $x_2$  appears for submatrices  $[D_{1b}^-]$  and  $[D_{4t}^+]$
- $i1$ :
  - $[D_{2t}]$ :  $x_{(2+)} = 0 \text{ nm}$ ,  $x_{(2-)} = -50 \text{ nm}$
- $i2$ :

- $[D_{2b}]$ :  $x_{(2+)} = 50 \text{ nm}$ ,  $x_{(2-)} = 0 \text{ nm}$
- $[D_{2t}]$ :  $x_{(2+)} = 0 \text{ nm}$ ,  $x_{(2-)} = -100 \text{ nm}$
- $i3$ :
- $[D_{3b}]$ :  $x_{(2+)} = 100 \text{ nm}$ ,  $x_{(2-)} = 0 \text{ nm}$

### 3.4 Nondimensionalization

It is helpful to nondimensionalize the plane elastic wave problem for isotropic materials covered in [3]. For one, this will aid in finding the roots of the characteristic equation, as it will reduce the values of the characteristic function near its roots. Furthermore, nondimensionalization will aid in accurate matrix inversion when calculating the eigenfunctions from the dispersion relations. I will first explain the nondimensionalization, and then provide plots of the calculated dispersion results for both the single layer and the 4-layer problems, as was done for the raw method, keeping all units.

We begin by writing the elastic wave equation ((47)).

$$\rho \frac{\partial^2 \mathbf{u}}{\partial t^2} = (\lambda + \mu) \nabla (\nabla \cdot \mathbf{u}) + \mu \Delta \mathbf{u}.$$

Now, apply the scalings

$$x = x_c \bar{x}, \quad t = t_c \bar{t}.$$

Substituting into the above pde gives

$$\frac{\partial^2 \mathbf{u}}{\partial \bar{t}^2} = \frac{E}{\rho(1+\nu)} \frac{t_c^2}{x_c^2} \left[ \frac{1}{1-2\nu} \bar{\nabla} (\bar{\nabla} \cdot \mathbf{u}) + \frac{1}{2} \bar{\Delta} \mathbf{u} \right]. \quad (80)$$

This suggests that we want the rescaling of space and time to satisfy

$$\frac{t_c}{x_c} = \sqrt{\frac{\rho(1+\nu)}{E}}.$$

This will result in the scaled problem

$$\frac{\partial^2 \mathbf{u}}{\partial \bar{t}^2} = \frac{1}{1-2\nu} \bar{\nabla} (\bar{\nabla} \cdot \mathbf{u}) + \frac{1}{2} \bar{\Delta} \mathbf{u}.$$

In order for the new variables  $\bar{x}, \bar{t}$  to be dimensionless, we need  $x_c [=] 1/m$  and  $t_c [=] 1/t$ . Also, we want to choose  $t_c$  small enough so that all quantities in the problem are at most order one. This can be achieved by defining the scalings as follows

$$x_c = t_c \sqrt{\frac{E}{\rho(1+\nu)}}, \quad t_c = 10^{-12} \quad (81)$$

since  $\sqrt{E/(\rho(1+\nu))}$  has units of  $s/m$ . The next step is to calculate all quantities needed in the  $[D]$  matrices in nondimensional terms (in terms of the above rescaling). Because for the four-layer problem, we are dealing with two materials, we must choose the rescaling using properties of one material and adjusting for the second material. Specifically we chose the nickel properties (subscript 2).

$$x_c = t_c \sqrt{\frac{E_2}{\rho_2(1+\nu_2)}}, \quad t_c = 10^{-12}.$$

Then, we can immediately calculate

$$\begin{aligned}
\bar{k}_1 &= x_c k_1 \\
\bar{\omega} &= t_c \omega \\
\bar{\alpha}_2 &= \sqrt{\frac{3 - 2\nu_2}{2(1 - 2\nu_2)}}, \quad \bar{\beta}_2 = \frac{1}{\sqrt{2}} \\
\bar{C}_{\alpha 2} &= \sqrt{\frac{\bar{\omega}^2}{\bar{\alpha}_2^2} - \bar{k}_1^2}, \quad \bar{C}_{\beta 2} = \sqrt{\frac{\bar{\omega}^2}{\bar{\beta}_2^2} - \bar{k}_1^2} \\
\bar{B}_2 &= \bar{\omega}^2 - 2(\bar{\beta}_2 \bar{k}_1)^2 \\
g_{\alpha 2} &= \exp\left(i \bar{C}_{\alpha 2} \frac{x_2}{x_c}\right), \quad g_{\beta 2} = \exp\left(i \bar{C}_{\beta 2} \frac{x_2}{x_c}\right).
\end{aligned} \tag{82}$$

Now, we find the remaining necessary nondimensional quantities by correcting for the second material (subscript 3).

$$\begin{aligned}
\bar{\alpha}_3 &= \sqrt{\frac{E_3(1 - \nu_3)}{\rho_3(1 + \nu_3)(1 - 2\nu_3)}} \frac{t_c}{x_c}, \quad \bar{\beta}_3 = \sqrt{\frac{E_3}{\rho_3(1 + \nu_3)}} / \sqrt{\frac{E_2}{\rho_2(1 + \nu_2)}} \\
\bar{C}_{\alpha 3} &= \sqrt{\frac{\bar{\omega}^2}{\bar{\alpha}_3^2} - \bar{k}_1^2}, \quad \bar{C}_{\beta 3} = \sqrt{\frac{\bar{\omega}^2}{\bar{\beta}_3^2} - \bar{k}_1^2} \\
\bar{B}_3 &= \bar{\omega}^2 - 2(\bar{\beta}_3 \bar{k}_1)^2 \\
g_{\alpha 3} &= \exp\left(i \bar{C}_{\alpha 3} \frac{x_2}{x_c}\right), \quad g_{\beta 3} = \exp\left(i \bar{C}_{\beta 3} \frac{x_2}{x_c}\right).
\end{aligned} \tag{83}$$

Finally,

$$\bar{\rho}_2 = 1, \quad \bar{\rho}_3 = \rho_3 / \rho_2.$$

Figures 12, 13, ?? and ?? below show the calculated dispersion results for the one layer nickel problem and the four-layer nickel-silicon nitride problem, the first two being the results computed without nondimensionalization, and the second two the results computed with nondimensionalization. The black line in each plot represents the dispersion relation for nickel, shown in Figure 7. To create these dispersion plots, a numerical approach was employed in Matlab. A code is employed which loops through a range of wave numbers  $k_1$ . For each value of  $k_1$ , the quantity  $1/|\det(S)|$  is calculated at a grid of frequencies  $\omega$ . Matlab then extracts the local maxima of  $1/|\det(S)|$ , which, for  $k_1$  fixed, is a function of  $\omega$ . These points are effectively the roots of the characteristic equation  $\det(S) = 0$  at fixed  $k_1$ . The points  $(k_1, \omega)$  are saved and plotted to produce the desired figures.

There are several comments to be made on the dispersion plots. Firstly, there are more curves in the plots without nondimensionalization. This suggests that the nondimensionalization causes us to lose some information. On the other hand, the nondimensionalization may be necessary if we want to find the roots to high accuracy via a numerical solver (the numerical solver in Matlab does not work with the basic GMM without nondimensionalization). There are also more dispersion relations seen for the multilayer problem and there are several curves in common between the multilayer and single layer problems (as it should be since nickel is common to both). Finally, note that the lowest linear dispersion seen in Figures ?? and ?? seems to agree with the Rayleigh wave calculation for Nickel, seen in Figure 7. It is important to keep in mind that the colored points in these plots are the estimated roots of the characteristic equation. These correspond to the approximate local minima of the characteristic function. We need to determine which of these points indicate true roots. We can do this by applying bisection to both the real and imaginary parts of characteristic function near each of these estimated roots. The tolerance chosen is  $10^{-3}$  in frequency, so that the algorithm terminates when the bisection window in frequency is smaller than this tolerance. This weeds out the true roots from the pool of estimated roots. These points are plotted atop the pool of estimated roots as the black and red circles. For the four-layer problem, the circles seem to agree with many of the estimated roots. However, for the single layer problem, the circles appear to be too few in number. The single-variable bisection may not be sufficient and it may be more effective in the future to utilize a secant method to hone in on roots in  $k_1$  and  $\omega$  simultaneously.

Questions going forward:

1. How can we be sure that we are finding all roots?

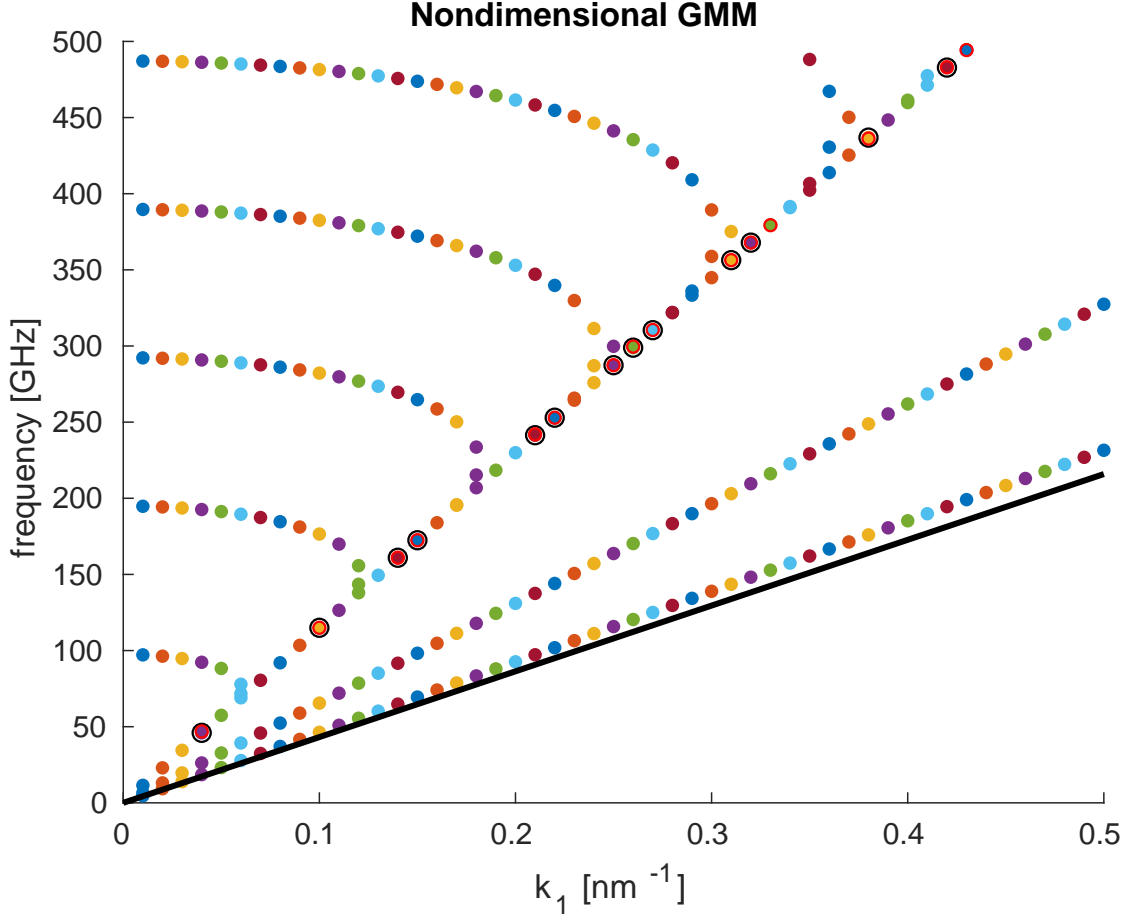


Figure 10: Calculated dispersion data for single nickel layer in vacuum using nondimensional GMM.

#### Future goals:

1. Solidify the methodology for calculating the dispersion relations for isotropic layered materials, and extend this to anisotropic materials.
2. Couple elasticity and magnetism and calculate dispersion relations for elastomeagnetic waves.

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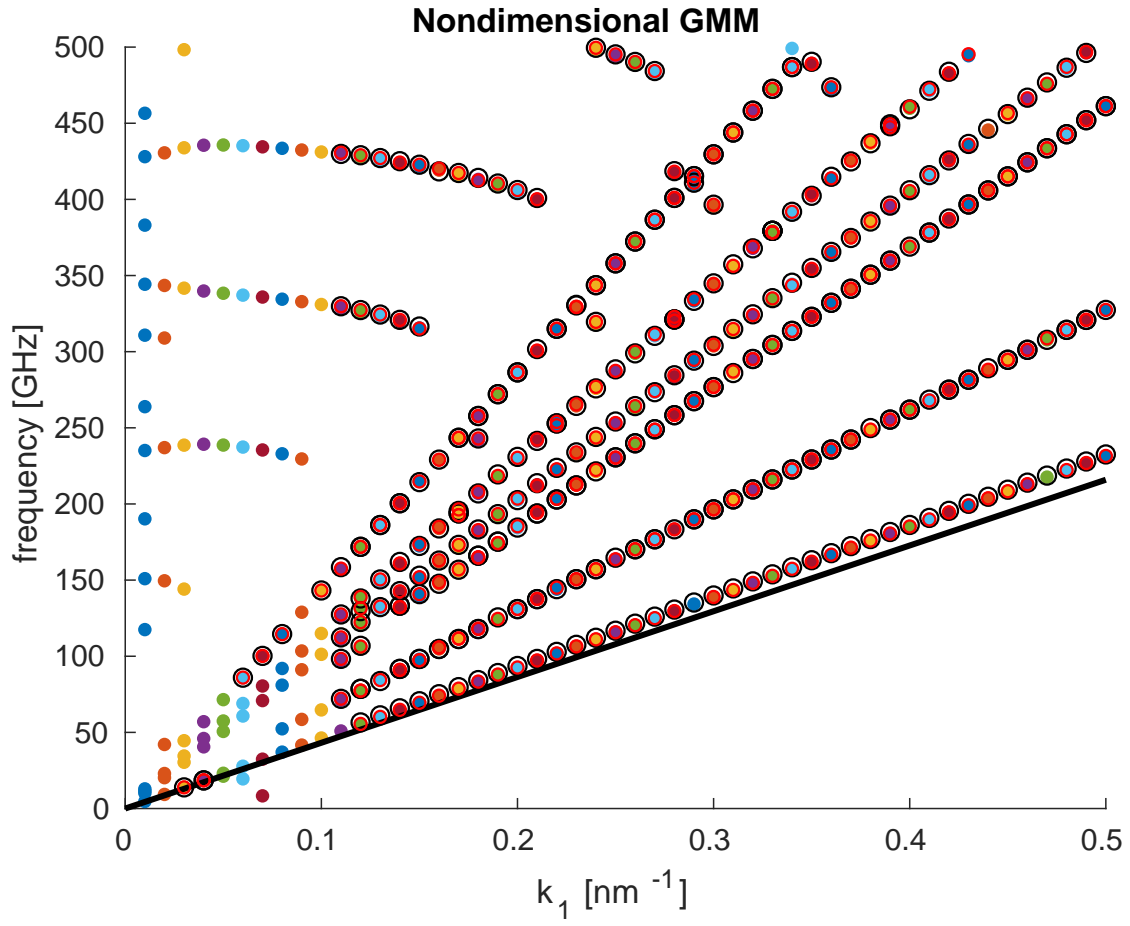


Figure 11: Calculated dispersion data for nickel-silicon nitride bilayer in vacuum using nondimensional GMM.

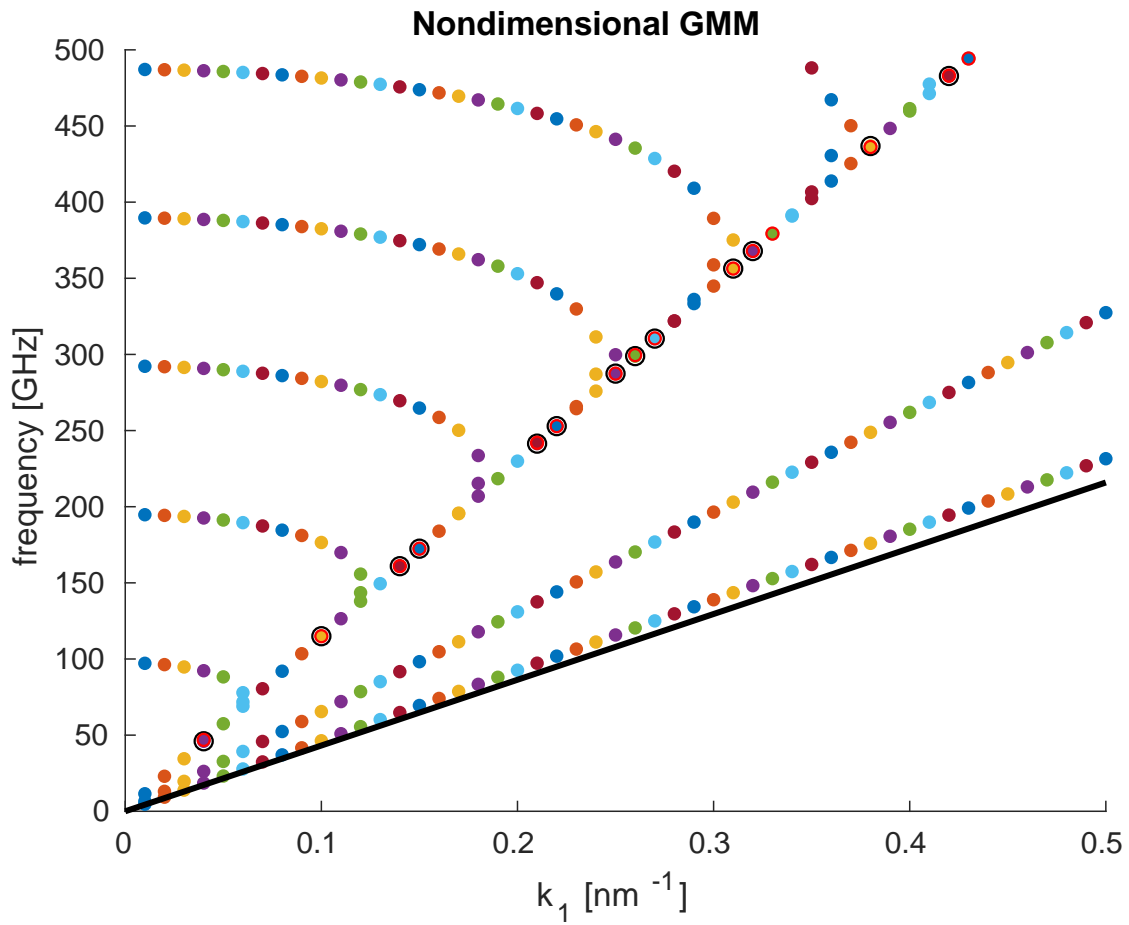


Figure 12: Calculated dispersion data for single nickel layer in vacuum using nondimensional GMM. Black data indicated roots solved for with Matlab function fsolve.

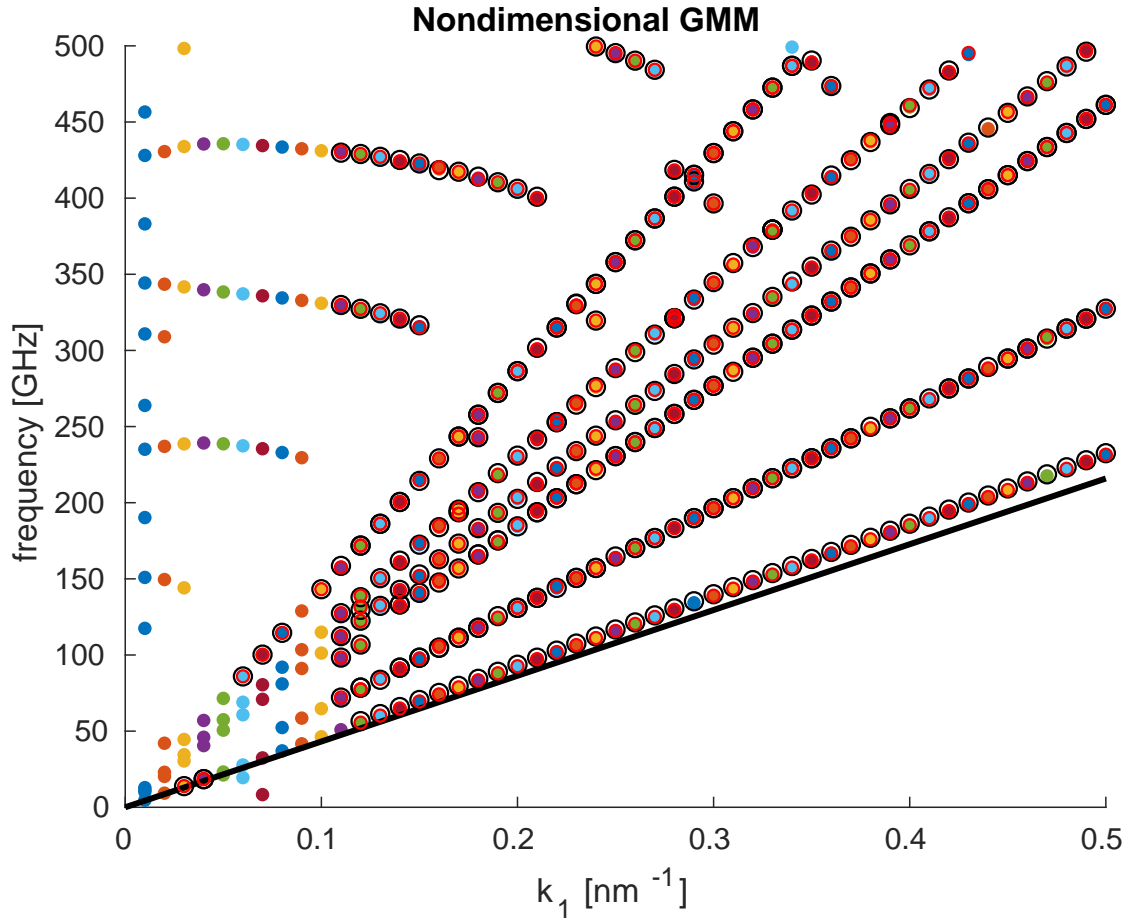


Figure 13: Calculated dispersion data for nickel-silicon nitride bilayer in vacuum using nondimensional GMM. Black data indicated roots solved for with trisection.