MODELING OF HARMONIC GENERATION AND SHOCK FORMATION IN NONLINEAR SURFACE ACOUSTIC WAVES IN SEVERAL REAL CRYSTALS

R. E. Kumon and M. F. Hamilton
Department of Mechanical Engineering
The University of Texas at Austin

Yu. A. Il'inskii and E. A. Zabolotskaya
MacroSonix Corporation
Richmond, Virginia

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OUTLINE

- Anisotropy and Cubic Crystals
- Theory
- Wave Speed Variation for Various Cuts and Crystals
- Waveform Distortion for Various Crystals
- Waveform Distortion for Various Directions
- Atypical Energy Trapping
- Conclusion & Future Work

ANISOTROPY AND CUBIC CRYSTALS

Stress-strain relation:

$$\sigma_{ij} = c_{ijkl}e_{kl} + d_{ijklmn}e_{kl}e_{mn}$$

c_{ijkl} $\rightarrow$ Second Order Elastic (SOE) constants

d_{ijklmn} $\rightarrow$ Third Order Elastic (TOE) constants

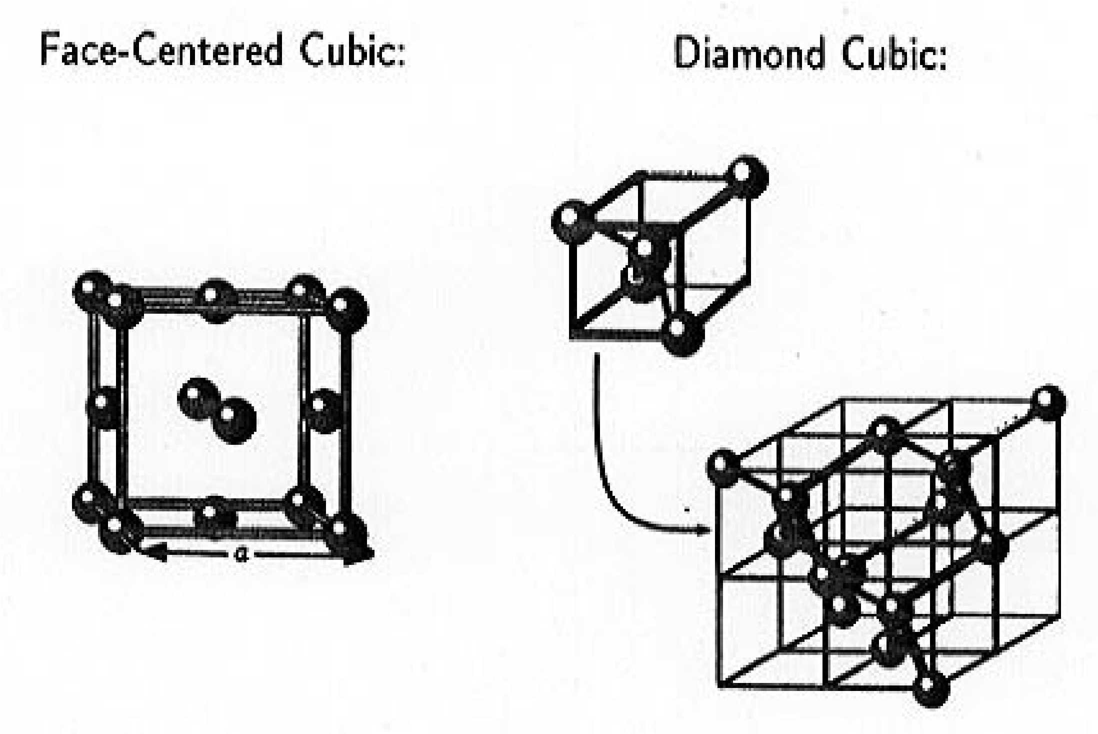
Cubic crystals:

Parameters	Cubic Crystal	Isotropic
SOE	3 independent	2 independent
TOE	6 independent	3 independent
Anisotropy Ratio	$\eta = \dfrac{2c_{2323}}{(c_{1111} - c_{1122})}$	$\eta = 1$

Specific Examples:

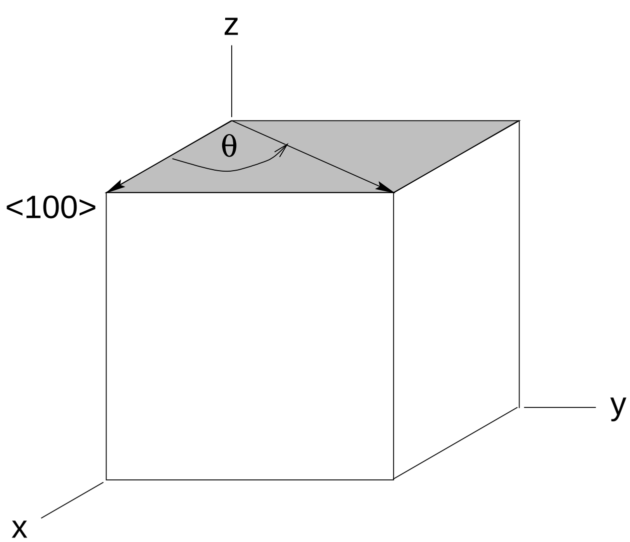
Crystal	Type	Anisotropy Ratio η
KCl	Face-centered cubic	0.375
Ni	Face-centered cubic	2.38
Si	Diamond cubic	1.57

ANISOTROPY AND CUBIC CRYSTALS (continued)

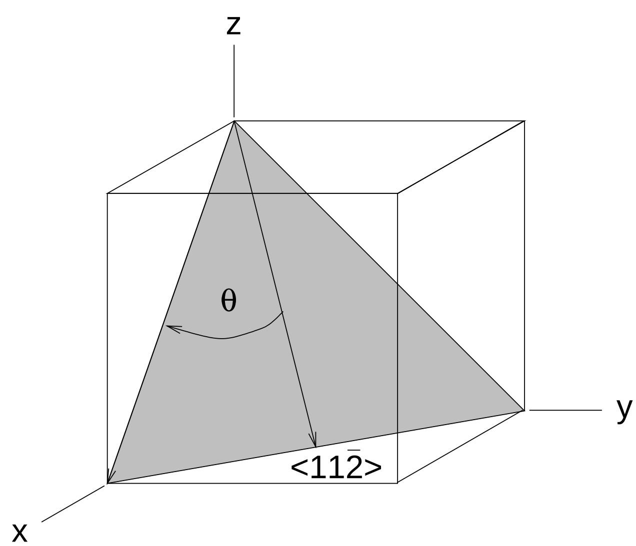


Typical Planes for Crystal Cuts:

(001) plane



(111) plane



THEORY

Approach:

Hamiltonian formalism (Hamilton, Il'inskii, Zabolotskaya, 1996)

Velocity waveforms in solid:

$$\begin{aligned} v_i(x,z,t) &= \sum_{n=-\infty}^{\infty} v_n(x) u_{ni}(z) e^{in(k_0 x - \omega_0 t)} \\ u_{ni}(z) &= \sum_{s=1}^{3} \beta_i^{(s)} e^{ink_0 l_3^{(s)} z} \end{aligned}$$

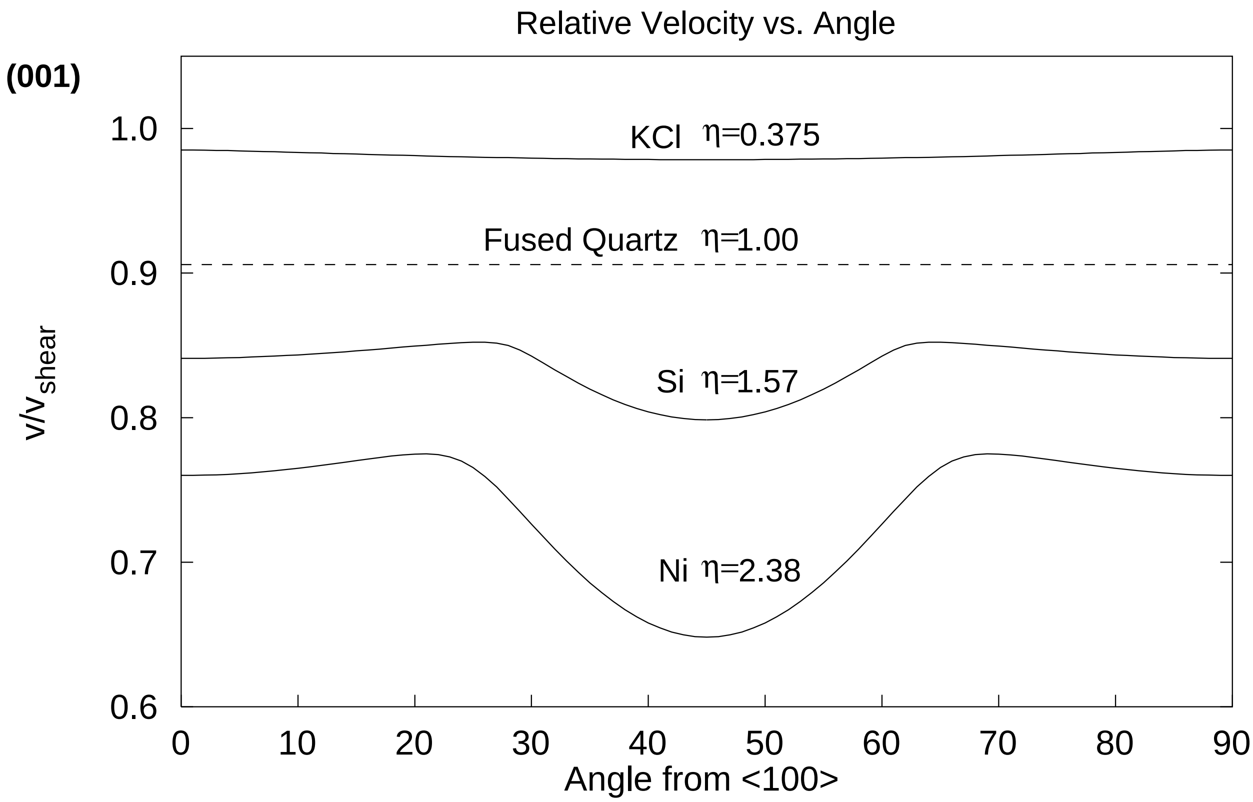
Coupled spectral evolution equations:

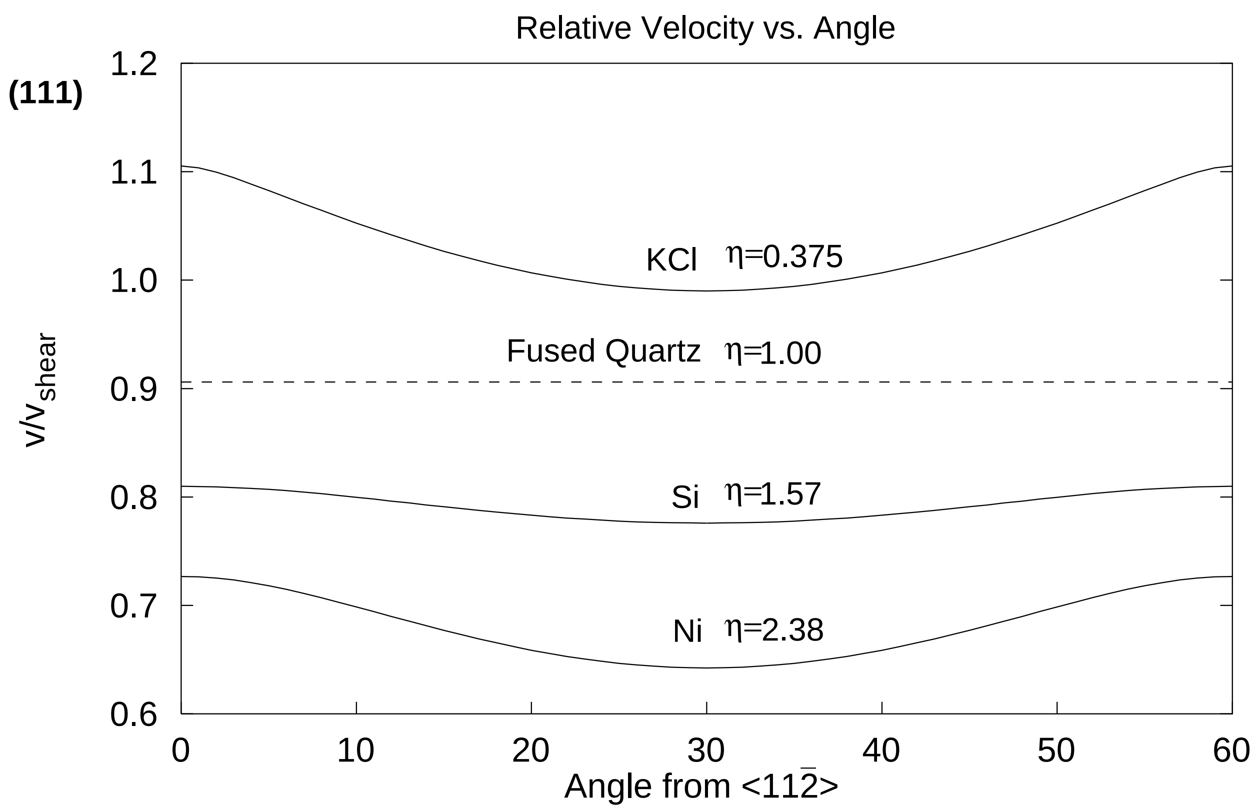
$$\frac{dv_n}{dx} + \alpha_n v_n = \frac{\omega_0 n^2}{2\rho c^4}\left(2\sum_{m=n+1}^{\infty} R^*_{m-n,n} v_m v^*_{m-n} - \sum_{m=1}^{n-1} R_{m,n-m} v_m v_{n-m}\right)$$

Solution Procedure:

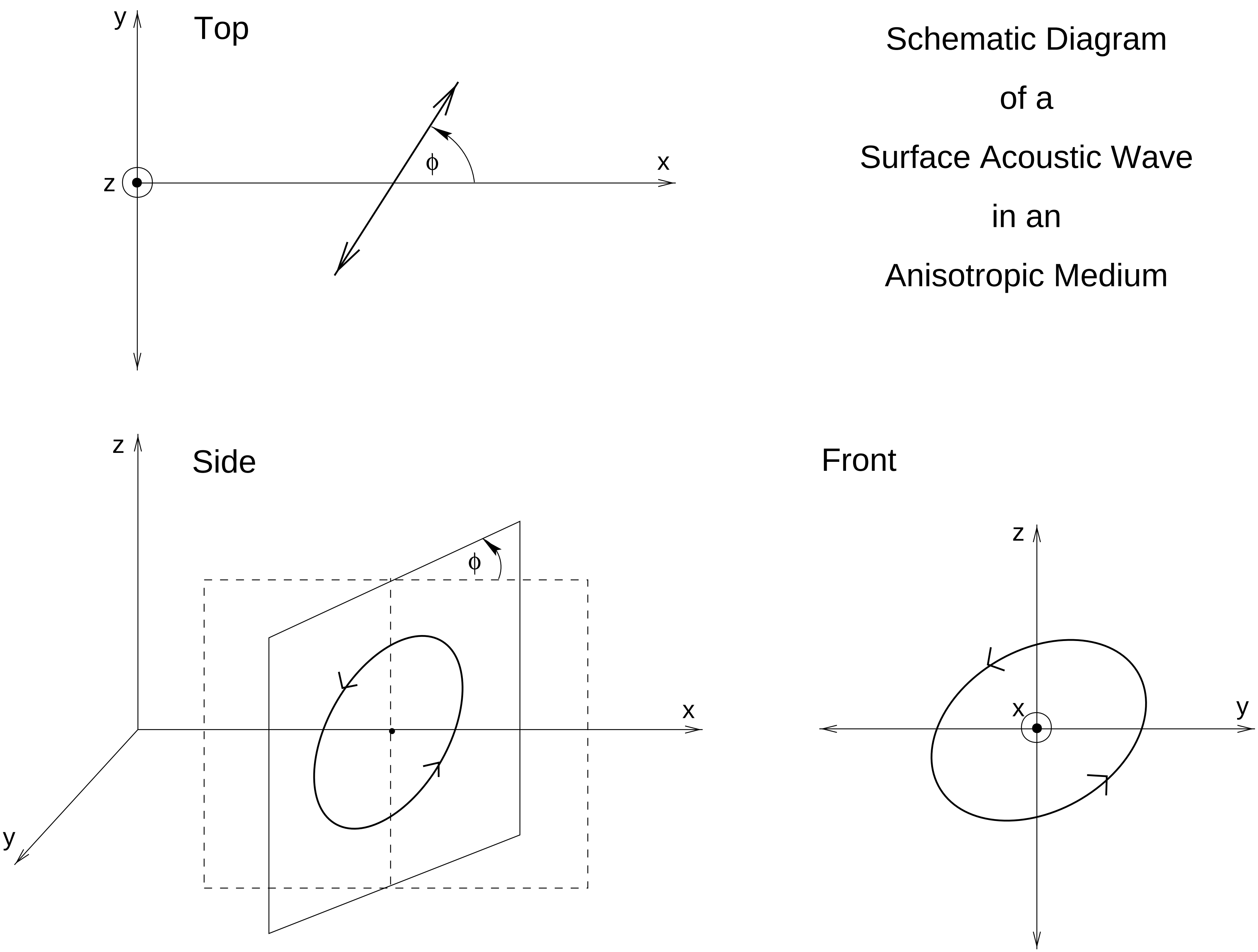
1. Numerically solve linear problem for eigenvalues, eigenvectors, and small-signal wave speed c.
2. Construct nonlinearity matrix R_{mn}.
3. Numerically integrate spectral evolution equations using a 4th order Runge-Kutta routine (∼200 harmonics).

WAVE SPEED VARIATION

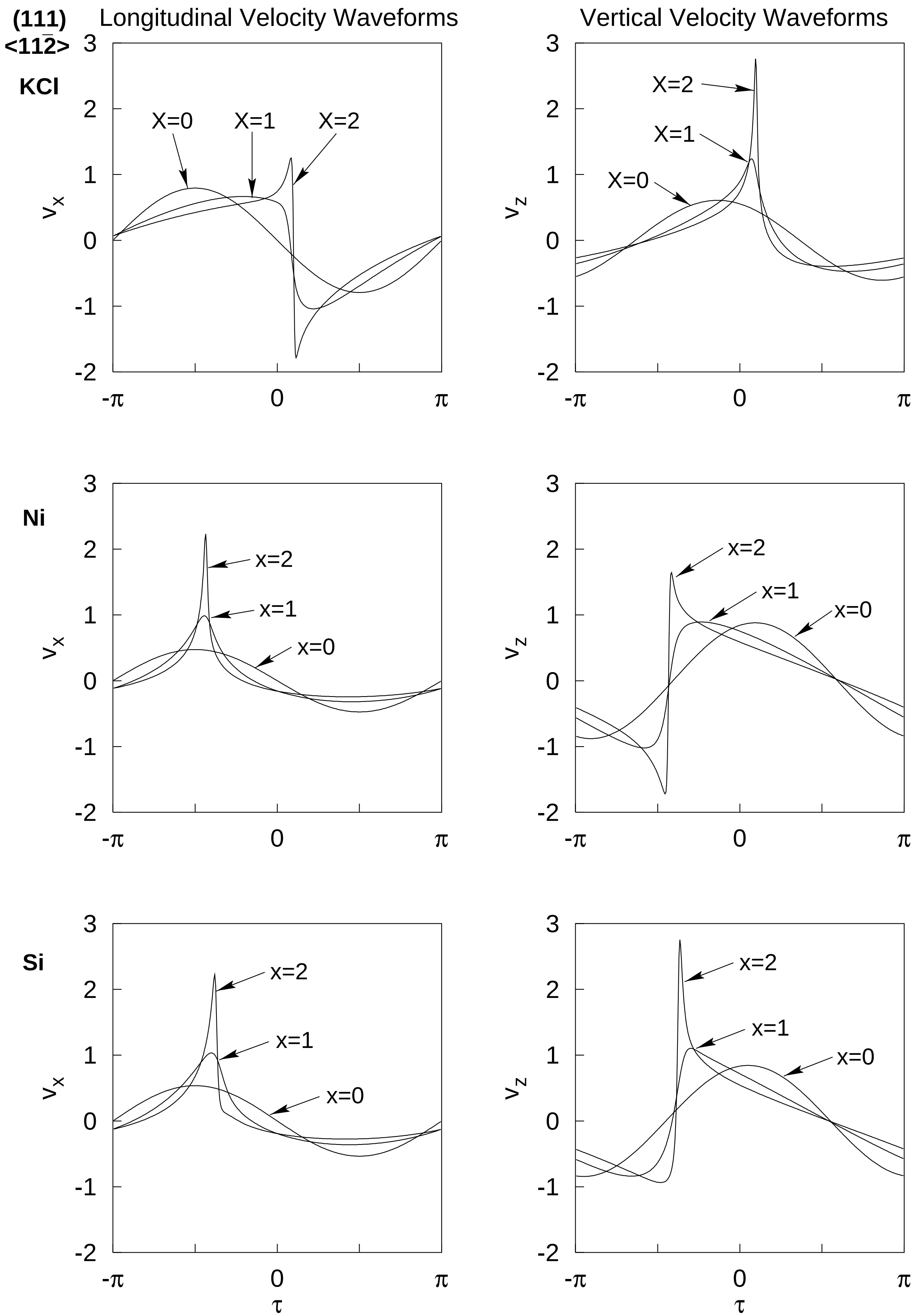




Schematic Diagram of a Surface Acoustic Wave in an Anisotropic Medium

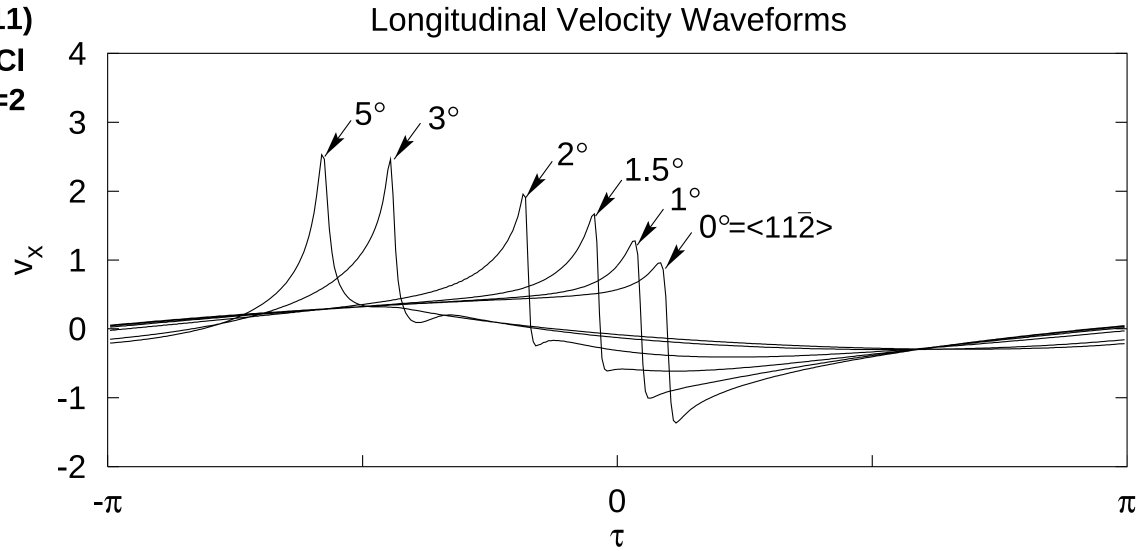


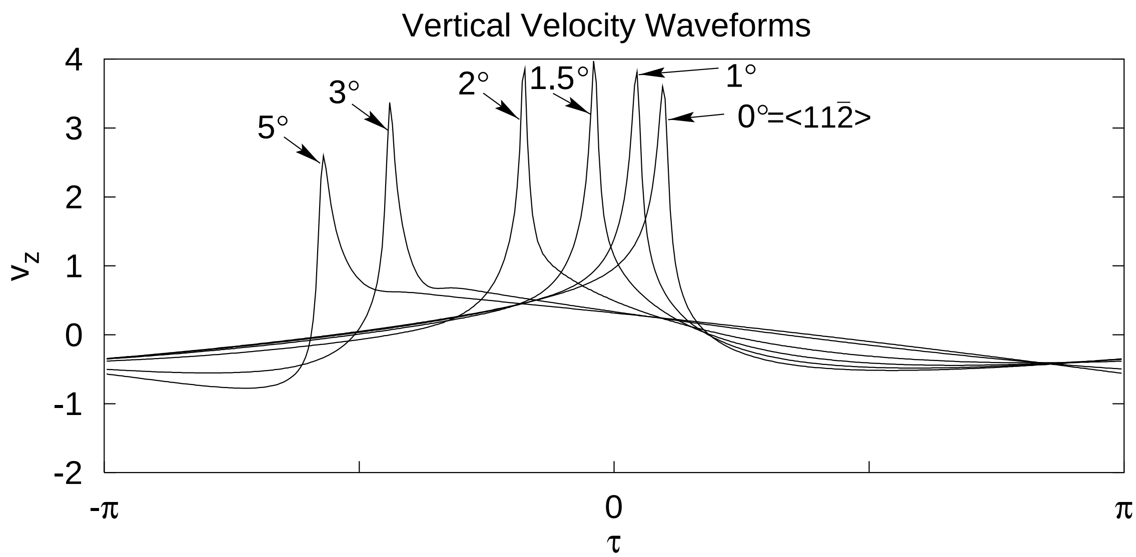
WAVEFORM DISTORTION: CRYSTALS

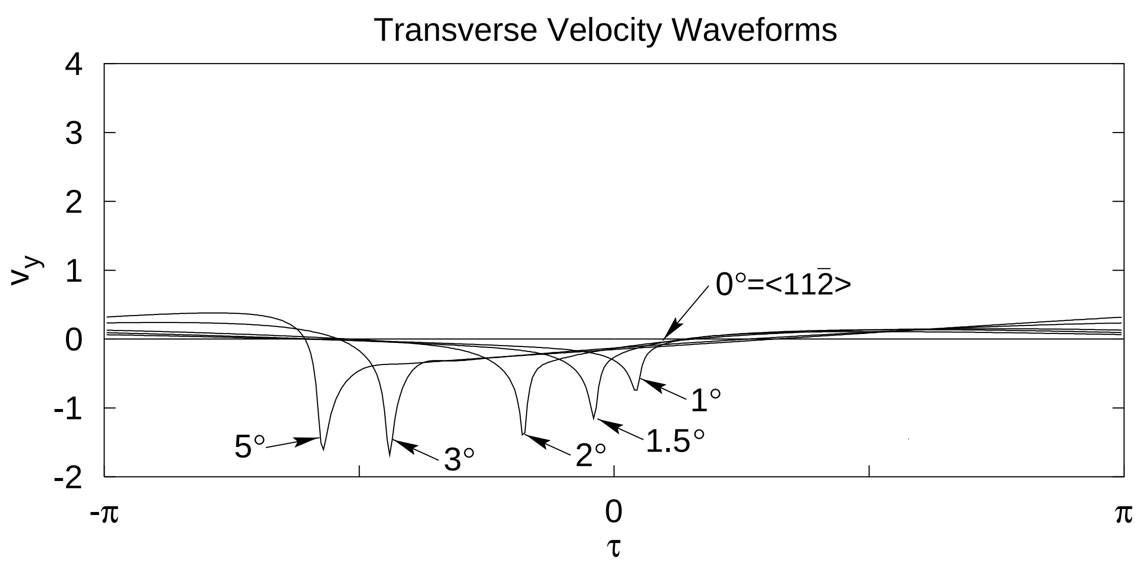


WAVEFORM DISTORTION: DIRECTIONS

(111)
KCl
X=2

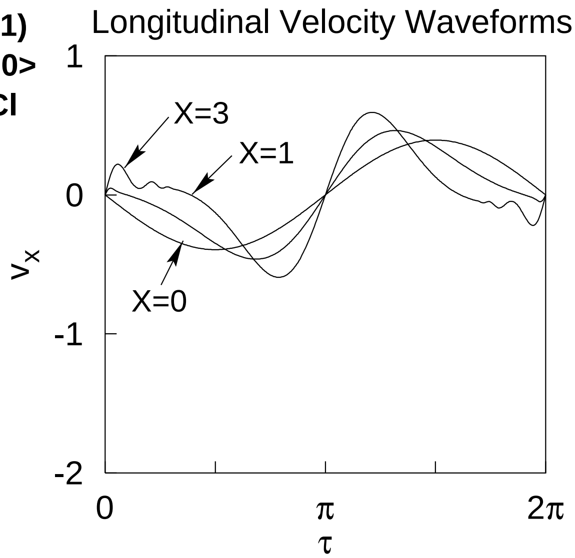


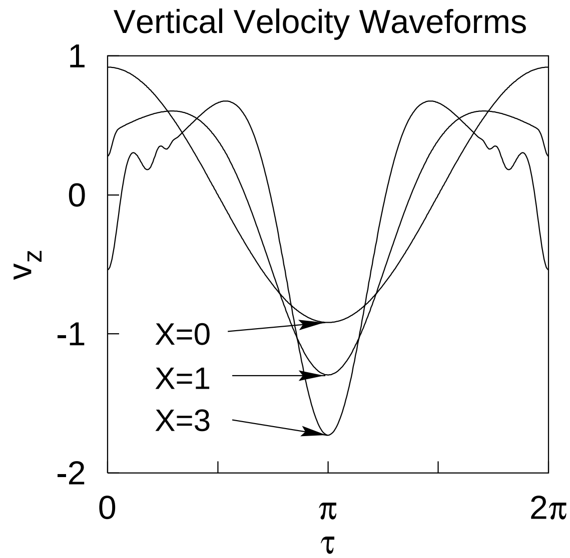




ATYPICAL ENERGY TRAPPING

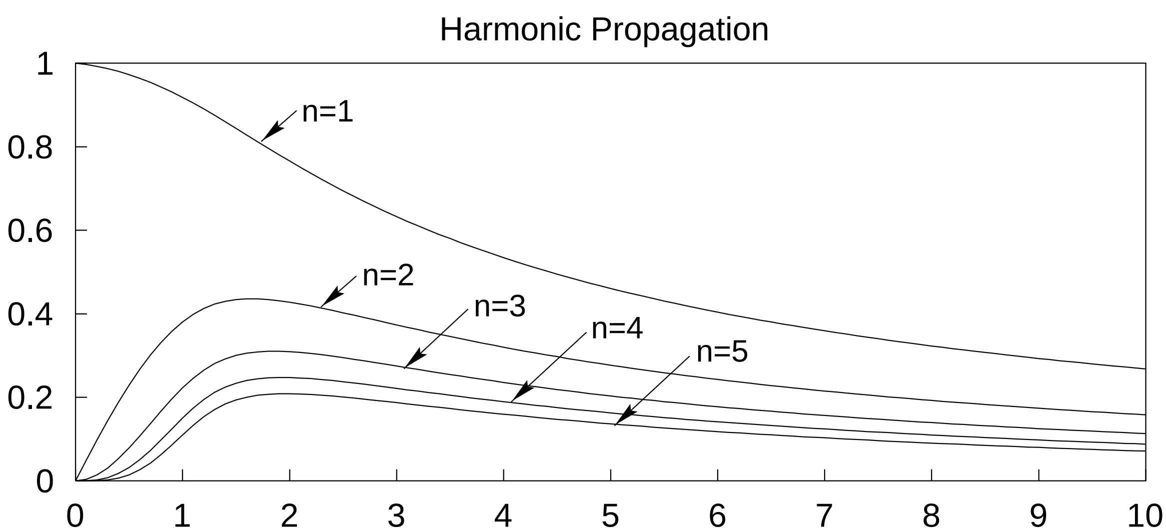
(001)
<100>
KCl



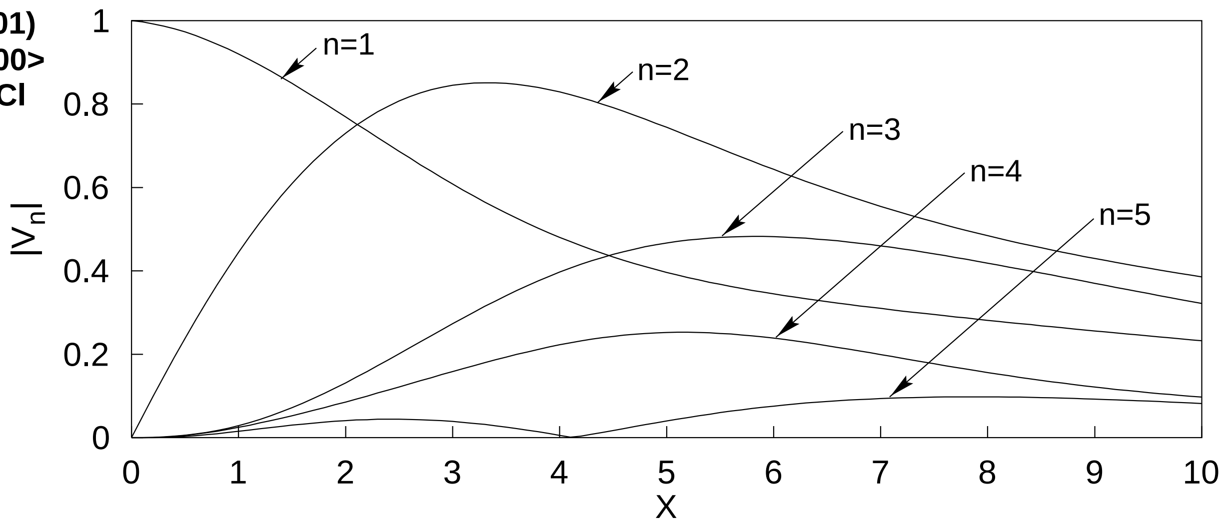


COMPARISON

(111)
<11$\bar{2}$>
KCl



(001)
<100>
KCl



ATYPICAL ENERGY TRAPPING (continued)

Truncated system of evolution equations (no dissipation):

$$\frac{dv_1}{dx} = \frac{\omega_0}{\rho c^4} R_{11}^* v_2 v_1^* \ , \quad \frac{dv_2}{dx} = -\frac{2\omega_0}{\rho c^4} R_{11} v_1^2$$

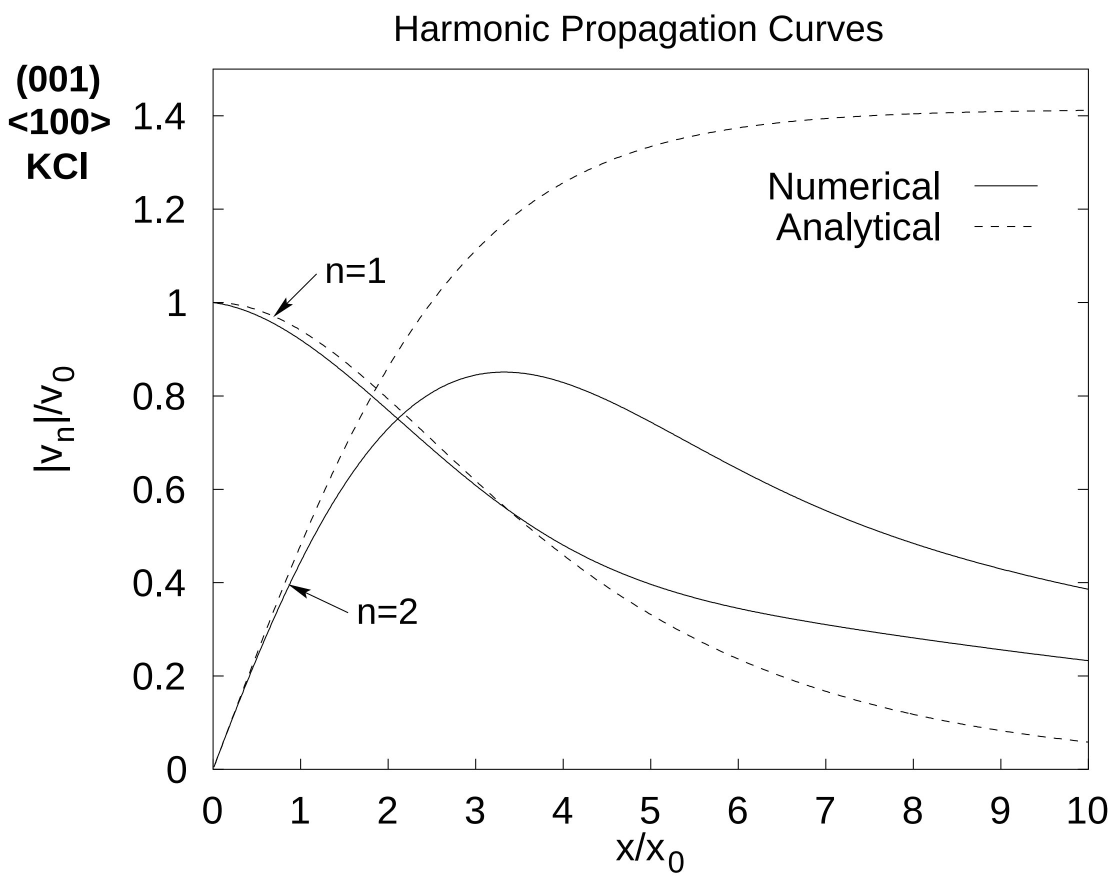
Boundary conditions:

$$v_1 = v_0 \ , \quad v_2 = 0 \quad \text{at} \quad x = 0$$

Analytical solution:

$$\frac{|v_1|}{v_0} = \operatorname{sech}\left(\frac{1}{2\sqrt{2}}\frac{x}{x_0}\right) \ , \quad \frac{|v_2|}{v_0} = \sqrt{2}\tanh\left(\frac{1}{2\sqrt{2}}\frac{x}{x_0}\right)$$

Graphical Comparison of Numerical & Analytical Results:



CONCLUSION & FUTURE WORK

Results:

- Cubic crystal waveforms exhibit:
  - Asymmetric distortion
  - Shocks with cusped spikes
  - Phase shift of waveforms as function of direction
- Prediction of atypical energy trapping in lowest harmonics in a nondispersive medium:
  - KCl for (001) plane in $\langle 100 \rangle$ direction
  - Approximate analytical solution close to source

Future work:

- Relationship between nonlinearity matrix and waveforms
- Analytical expression for shock formation distance
- Pulsed waveform modeling and experimental data comparison
- Investigation of other crystals besides cubic

NONLINEARITY MATRIX & LINEAR THEORY

The nonlinearity matrix is given by

$$R_{n_1 n_2} = - \sum_{s_1,s_2,s_3=1}^{3} \frac{d'_{iklmpq} \beta_i^{(s_1)} \beta_l^{(s_2)} \beta_i^{(s_3)*} l_k^{(s_1)} l_m^{(s_2)} l_q^{(s_3)*}}{2[n_1 l_3^{(s_1)} + n_2 l_3^{(s_2)} + (n_1 + n_2) l_3^{(s_3)*}]}$$

where $\beta_i^{(s)} = C_s \alpha_i^{(s)}$ and

$$d'_{iklmpq} = d_{iklmpq} + c_{ikmq}\delta_{lp} + c_{lmkq}\delta_{ip} + c_{pqkm}\delta_{il} \ .$$

To compute this expression, the linear problem must first be solved.

Start with linearized wave equation

$$\rho \frac{\partial^2 u_i}{\partial t^2} = \frac{\partial \sigma_{ij}}{\partial x_j} = c_{ijkl} \frac{\partial^2 u_k}{\partial x_j \partial x_l} \ . \tag{1}$$

Next assume SAW solution of form

$$u_i = \sum_{s=1}^{3} C_s \alpha_i^{(s)} e^{ik(\mathbf{l_s} \cdot \mathbf{r} - \omega t)} \tag{2}$$

where $l_s = \{1, 0, z\}$. Substitute Eq. (2) into Eq. (1) to yield

$$\rho c^2 \alpha_i = \tilde{c}_{ijkl} l_j l_l \alpha_k \ . \tag{3}$$

Solve Eq. (3) subject to the stress-free surface boundary condition

$$\sigma_{i3} \left|_{x_3=0} = 0 \ . \right. \tag{4}$$

Substituting Eq. (2) into Eq. (4) yields

$$ik \tilde{c}_{i3kl} \sum_{s=1}^{3} C_s \alpha_k^{(s)}(c) l_l^{(s)} = 0 \ . \tag{5}$$

This equation can be solved numerically.