NONLINEAR SURFACE ACOUSTIC WAVES IN CUBIC CRYSTALS
6th International Workshop on Nonlinear Elasticity in Materials
by R. E. Kumon and M. F. Hamilton

SLIDE NOTES

Notes on COVER PAGE and OUTLINE

- The objective of this talk is to present and explain of the major research results from my dissertation.
- This talk is prepared for the 6th International Workshop on Nonlinear Elasticity in Materials in Leuven, Belgium during June 18–22, 2001.
- This work is supported by the U. S. Office of Naval Research.
- The talk will be divided into three sections: (1) Background, (2) Results from the (001) plane, and (3) Results from the (111) plane.

Notes on NONLINEAR SURFACE WAVES

- Surface waves are elastic waves which occur at stress-free surface of a semi-infinite solid. They have have the properties that (1) their amplitude decays with an exponential envelope into the solid and (2) they propagate non-dispersively. A schematic diagram is shown in the top figure.
- In order to appreciate the waveform distortion of finite amplitude surface waves seen in the more general crystalline case, it is helpful to know how such waves distort in higher symmetry cases.
- The bottom set of figures shows the kind of nonlinear waveform distortion that occurs for surface waves in isotropic media (Rayleigh waves) or certain planes of mirror symmetry in cubic crystals. The waveforms shown in the plots correspond to an initially sinusoidal wave propagating along the surface in the x direction. The graphs show snapshots of the longitudinal and vertical velocity waveforms in the retarded time frame (moving along with the wave at the linear wave speed) at the various distances shown. Here the distance is scaled such that $X{=}1$ corresponds to a characteristic length scale (e.g., the estimated shock formation distance in cases where shocks form).
- The longitudinal velocity waveform distorts in way that is similar to a fluid with the peaks advancing and troughs receding. However, unlike a fluid, cusps form in the longitudinal velocity waveform while a peak forms in the vertical velocity waveform in the shock front region. This distortion is characteristic of nonlinear surface acoustic waves.
  - The cusping occurs because the generation of higher harmonics causes more of the energy of the wave to be concentrated at the surface. (Recall that the energy of a sinusoidal wave is concentrated within approximately one wavelength of the surface.)

Notes on SURFACE WAVES IN CRYSTALS

- This figure shows the particle motion of a typical surface acoustic wave in an anisotropic medium. Consider the case of a surface acoustic wave with an initially sinusoidal velocity waveform in an isotropic and anisotropic material. Assume that the x axis is in the propagation direction and that the z axis is normal to the surface cut.
- In order to be a surface acoustic wave, the wave must satisfy the stress-free boundary conditions at the surface and decay into the solid with an exponential envelope. The depth dependence of the vertical displacement u_z and horizontal displacement u_x is plotted against the depth in wavelengths for the linear SAW propagating in Si in the $\langle 001\rangle$ direction. The amplitudes oscillate and decay thereby giving rise to alternating regions of retrograde and prograde elliptical motion. As can be seen from the figure, most of the motion is confined to within a wavelength of the surface.
  - Isotropic material: In contrast, the amplitude of a surface acoustic wave in an isotropic material (usually called a Rayleigh wave) decays away purely exponentially into the solid.

- Because crystals are anisotropic, the wave propagation is different depending on how the crystal is cut and the direction that the wave is traveling.
  - The surfaces of cut crystals have traditionally been described using a crystallographic convention called Miller indices. Miller indices are defined by finding three noncollinear atoms on the surface that intersect the crystal axes and then applying the following method:
    1. Find the intercepts of the three basis axes in terms of the lattice constants.
    2. Take the reciprocals of these numbers and reduce to the smallest three integers having the same ratio. The result is enclosed in parentheses (hkl). [from C. Kittel, *Introduction to Solid State Physics*, 2nd ed. (John Wiley & Sons, New York, 1965), p. 34] Note that if the Miller indices are interpreted as a vector components, the resulting vector is normal to the surface of the cut.
  - Directions are specified in a different way:

    The indices of a direction in a crystal are expressed as the set of the smallest integers which have the same ratios as the components of a vector in the desired direction referred to the axis vectors. The integers are written in square brackets, [uvw]. The x axis is the [100] direction; the $-y$ axis is the [$0\bar{1}0$] direction. A full set of equivalent directions is denoted this way: $\langle$uvw$\rangle$. [from C. Kittel, *Introduction to Solid State Physics*, 2nd ed. (John Wiley & Sons, New York, 1965), p. 34]

  This presentation will use both of these notations frequently.
- Because it is surface phenomena that are being studied, it is necessary to specify how the surface is oriented with respect to the crystalline axes and, in addition, the direction in which the wave is travelling. The special case of a mirror plane mirror is the (001) plane, as shown in the bottom left figure. However, this mirror symmetry is eliminated in the (111) plane as shown in the bottom right figure.

Notes on **NONLINEAR THEORY**

- Briefly, the approach used here involves calculating the Hamiltonian energy function through cubic order in the wave variables, choosing appropriate generalized coordinates, applying the equations of motion in canonical form, and deriving evolution equations for the slowly varying amplitudes in a suitable retarded time frame. The approach is outlined in M. F. Hamilton, Yu. A. Il'inskii, and E. A. Zabolotskaya, "Nonlinear surface acoustic waves in crystals," J. Acoust. Soc. Am. **105**, 639-651 (1999).
  - Note that computing the Hamiltonian the quadratic order would only give rise to linear terms in the model equations. Thus, the potential energy terms to at least cubic order in the strain must be included to model nonlinear effects.
  - Note also that this method is very general. It is applicable to any elastic material for which the second- and third-order elastic constants are known and to any cut and direction in such a material.
  - Assumptions:
    1. It is assumed that the nonlinear solution is close to the linear solution; in particular the depth dependence of each frequency is the same as in the linear solution.
    2. It is assumed that the wave fronts are planar.
    3. It is assumed that the wave is progressive, i.e., travels only in one direction. (It should be possible to extend the theory to include compound waves; only the results will be more complicated.)
- The components of the velocity in the solid are assumed to take the form shown in the slide. Here v_j is the jth component of velocity, k is the characteristic wavenumber, and ω is the characteristic angular frequency of the signal. Because surface acoustic waves are nondispersive, i.e., their wave speed is not frequency dependent, $\omega/k = c$ where c is the SAW speed in the direction of propagation.
  - The coordinate system for the solution is always chosen such that the the z-axis is perpendicular to the surface of the solid and the x-axis is in the direction of the propagation of the wave. Because the elastic constants are typically given with respect to the crystalline axes, the elastic constants must always first be transformed into the aforementioned coordinate system before substitution into the model equations described in the slide.

- The functions u_{nj} describe the depth dependence of the nth harmonic of the jth component. The values of $l_3^{(s)}$ and $q_j^{(s)}$ that determine these functions are found by solving the linear problem. This is the result of Assumption 1 above.
- Note that on the surface the expressions for the waveforms simplify to

$$v_j(x,z,t) = \sum_{n=-\infty}^{\infty} v_n(x) \sum_{s=1}^{3} \beta_j^{(s)} e^{in\tau} \qquad [v_n^* = v_{-n}]$$

where $\tau = kx - \omega t$ is the retarded time and the $\beta_j^{(s)}$ are constants determined from the linear problem.

- The coupled, nonlinear spectral evolution equations that result from this approach are shown above. Here v_n is the complex amplitude of the nth harmonic, α_n is the attenuation coefficient for the nth harmonic, ω is the characteristic angular frequency, ρ is the density of the material, c is the SAW speed for the direction of propagation, and S_{lm} is the nonlinearity matrix.
  - In practice, these equations are first converted to a nondimensional form before they are solved. Let v_0 be the characteristic velocity amplitude of the signal. If $V = v/v_0$ and $X = x/x_0$ where

$$x_0 = \frac{\rho c^4}{4|S_{11}|\omega v_0} ,$$

then the evolution equations take the form

$$\frac{dV_n}{dX} + A_n V_n = \frac{n^2}{8|S_{11}|} \sum_{l+m=n} \frac{lm}{|lm|} S_{lm} v_l v_m$$

where $A_n = \alpha_n x_0$.
  - The *ad hoc* attenuation term $\alpha_n = n^2\alpha_1$ is added to the left-hand side for purposes of numerical stability when solving the equations. It assumes that the attenuation coefficient for any frequency component is proportional to the square of that frequency as has been observed in quartz [E. Salzmann, T. Plieninger, and K. Dransfeld, "Attenuation of elastic surface waves in quartz at frequencies of 316 MHz and 1047 MHz," Appl. Phys. Lett. **13**, 14–15 (1968)]. For all the cases shown here the dimensionless value of A_1 = 0.025. This attenuation is sufficiently weak that its main effect is to stabilize the portion of the waveform in the neighborhood of the shock without significantly the remainder of the waveform. Note that the dimensionless value of A_1 here is the analog of the Goldberg number Γ for nonlinear acoustic waves in fluids.
  - Physically, the nonlinearity coefficients S_{lm} represent the strength of the coupling between different harmonics in the wave. They are given by a complicated analytical expression which can be determined completely by knowing the second- and third-order elastic constants of the material.
  - For the case of isotropic materials, these equations can be shown to reduce to the evolution equations previously derived by Zabolotskaya [E. A. Zabolotskaya, "Nonlinear propagation of plane and circular waves in isotropic solids," *J. Acoust. Soc. Am.* **91**, 2569–2575 (1992)].
  - While Hamilton's equations describe the evolution of a system in time, the evolution equations listed in the slide evolve in space, not time. Informally speaking, the transformation between the two is done by moving into retarded time frame and thereby replacing $\partial/\partial t$ with $c\,\partial/\partial x$. It is possible to demonstrate formally that this is the proper transformation and that it is not an approximation [E. Yu. Knight, M. F. Hamilton, Yu. A. Il'inskii, and E. A. Zabolotskaya, "General theory for the spectral evolution of nonlinear Rayleigh waves," *J. Acoust. Soc. Am.*, **102**, 1402-1417 (1997)].

- These equations may be solved as follows. By first solving the linear problem for the eigenvalues, eigenvectors, and small-signal wave speed, the nonlinearity matrix can be constructed. Once the nonlinearity matrix is determined, the model equations can be integrated. The spectral evolution equations were solved numerically using the spectral "source" condition corresponding to an initially sinusoidal wave. A fourth-order Runge-Kutta routine was used to integrate the system. The waveform expansions used had 200 harmonics. Note that the multiple sum on the right side of the spectral evolution equations implies that the number of computational steps is proportional to the square of the number of harmonics. Hence performing the full integration is generally a computationally intensive activity.

- In theory, there are an infinite number of equations to integrate. For purposes of computation, the velocity waveform expansions were truncated such that only terms with $n = -200$ to $n = 200$ were included in the sum. However, because the velocity waveforms must be real-valued, $v_{-n} = v_n^*$. Therefore only 200 spectral amplitudes must be determined and, correspondingly, only 200 equations must be integrated.
- To minimize numerical aliasing effects, only the first 150 harmonics were used to reconstruct the waveforms shown later in the talk.

- It turns out that in higher symmetry cases (e.g., isotropic media or planes of mirror symmetry in cubic crystals) the matrix elements are real-valued [e.g., (001) plane]. However, in the more general lower symmetry cases, the matrix elements are complex-valued [e.g., (111) plane].

Notes on NONLINEARITY MATRIX FOR SI (001)

- The nonlinearity matrix elements are a complicated function of many quantities. The expression for the dimensionless elements $\widehat{S}_{lm}$ is shown in the slide. Here the values of $\lambda_3^{(s)}$ and $x_j^{(s)}$ are parameters of the depth dependence functions u_{nj} derived by solving the linear problem while the d'_{ijklmn} values are derived from the second-order elastic constants c_{ijkl} and third-order elastic constants d_{ijklmn}.
  - Note that the elastic constants c_{ijkl} and d_{ijklmn} are the elastic constants in a coordinate system in which the x-axis is parallel to the direction of the wave propagation.
  - In general the nonlinearity matrix elements are complex. However, due to the symmetry of this particular case all of the matrix elements are real.
  - The matrix elements are scaled by c_{44} to make them dimensionless. The negative sign is introduced to make the sign of the matrix elements consistent with matrix elements used previously to describe SAWs in isotropic media.

- Physically, the nonlinearity matrix elements describe the strength of the energy coupling between various harmonics of the wave. In particular, the $\widehat{S}_{lm}$ matrix element describes how energy is transferred from the lth and mth harmonics to the $(l+m)$th harmonic.

- The figure shows the matrix elements $\widehat{S}_{11}$, $\widehat{S}_{12}$, and $\widehat{S}_{13}$ plotted as a function of angle from the $\langle 100 \rangle$ direction for SAWs in Si on the (001) plane. Other matrix elements follow a similar pattern including approximately (but not exactly) the same location of zero crossings.

- As will be shown in subsequent slides, the nonlinear evolution of the wave can be classified into three regions as indicated in the figure. The nonlinearity matrix elements start negative in Region I, pass through zero, become positive in Region II, pass through zero again, and then become negative once again in Region III. The strongest nonlinearity occurs in the $0^\circ \leq \theta \leq 5^\circ$ and $25^\circ \leq \theta \leq 30^\circ$ regions. On the other extreme, the waveform evolution is predicted to be linear (to third order in the wave variables) around $\theta \approx 21^\circ$ and $\theta \approx 32^\circ$.
  - While the matrix elements go to zero near $\theta = 45^\circ$, the wave also degenerates into an exceptional bulk shear wave (also known as a surface skimming bulk wave) in that direction and the assumptions of the theory (namely that the amplitude of the wave decays away exponentially into the solid) are no longer satisfied.
  - As can be seen in the graph, the nonlinearity matrix elements not only change sign twice over the interval $0^\circ < \theta < 45^\circ$ but the magnitude changes substantially, nearly tripling in Region II. It can be shown that the proportional change of the nonlinearity matrix elements as a function of direction is much larger than the change of the SAW speed over the same range.

Notes on SIMULATIONS WITH SINUSOIDS FOR SI (001)

- The nature of the waveform distortion can be characterized by looking at the nonlinearity matrix elements. In the center of the figure is a reproduction of the plot of the $\widehat{S}_{11}$ matrix element as a function of propagation direction. Waveforms are examined for two directions, $\theta = 0^\circ$ and $\theta = 26^\circ$ degrees, that exhibit distortion characteristic of propagation in their respective regions.

- First look at the $\theta = 26^\circ$ direction in Region II. The waveforms shown in the top two graphs correspond to an initially sinusoidal wave propagating along the surface in this direction. The graphs show snapshots of the longitudinal and vertical velocity waveforms in the retarded time frame (moving along with the wave at the linear wave speed) at the various distances shown.
- For both cases shown, there is a small transverse component. However it is just related to the other components by a transformation described by linear theory.
- Note that $\widehat{S}_{11}$ is positive. Hence the coefficient of nonlinearity will also be positive and the waveform should distort like a fluid does with the peaks advancing and the troughs receding.
- However, unlike a fluid, cusps form in the longitudinal velocity waveform while a peak forms in the vertical velocity waveform in the shock front region. This distortion is characteristic of nonlinear surface acoustic waves even in isotropic media. This occurs because the generation of higher harmonics causes more of the energy of the wave to be concentrated at the surface. Recall that the energy of a sinusoidal wave is concentrated within approximately one wavelength of the surface (see Notes on NONLINEAR SURFACE WAVES).
- Now look at the $\theta = 0^\circ$ direction in Region I. Here $\widehat{S}_{11}$ is lower in magnitude and negative. Because $\widehat{S}_{11}$ is negative, the coefficient of nonlinearity is also negative and the waveform will distort in a fashion opposite of that of a fluid with the peaks receding and the troughs advancing. This is clearly seen in the waveforms shown.
- The waveforms in Region III distort in a way similar to those in Region I. However, there the nonlinearity is much weaker. This is due to the fact that in this region the wave is gradually degenerating into a bulk wave as the $\theta = 45^\circ$ direction is approached. As this occurs, the energy of the wave penetrates deeper and deeper into the solid and is correspondingly weaker at the surface. This reduced surface amplitude then makes the nonlinear effects weaker.

Notes on EXPERIMENT

- The approach used here generates SAW via a pressure shock induced by laser excitation. This method was described previously by Lomonosov and Hess [A. Lomonosov and P. Hess, "Laser excitation and propagation of nonlinear surface acoustic wave pulses," *Nonlinear Acoustics in Perspective*, R. J. Wei, ed., (Nanjing University Press, Nanjing, China, 1996), pp. 106–111].
- The basic setup is shown in the diagram. The SAW pulse was generated by a Nd:YAG laser that was focused with a cylindrical lens into a thin strip 6 mm by 50 μm on the surface of crystal. To detect the resulting SAW pulse, optical probe beams were employed. This can be done because probe beam deflection is proportional to the vertical velocity component v_z at the surface. The probe beam deflections were detected by split photodiodes with a bandwidth of 500 MHz. The probe beams irradiated spots approximately 4 μm in diameter on the surface at distances approximately 5 mm and 20 mm from the excitation region.
  - Experimental details: The Nd:YAG laser that generated the surface waves had a wavelength of 1064 nm (infrared), pulse duration 7 ns, and energy up to 50 mJ. A strongly absorbing carbon layer in the form of an aqueous suspension was placed on the surface of the Si in the excitation region to facilitate energy transfer to the surface and prevent cracking. The transient SAW waveforms were then measured absolutely with a calibrated probe-beam deflection setup using stabilized cw Nd:YAG laser probe beams with a wavelength of 532 nm (green visible) and power of 40 mW.
  - Diffraction effects: Diffraction effects were negligible in this experiment. The Rayleigh distance was computed to be 300 mm, more than an order of magnitude greater than the shock formation distance of 21 mm.
- Surface wave pulses in these experiments had durations of 20–40 ns and peak strains between 0.005 and 0.010. As will be shown, pulses of this magnitude exhibit nonlinear behavior that give rise to waveform distortion and shock formation.
  - For example, a previous experiment (described in the Lomonosov and Hess reference above) generated SAW in Si with particle velocities of over 40 m/s. Because the surface acoustic wave speed for silicon in this direction is 4730 m/s, the Mach number equals 0.0085. The same experiment generated peak-to-peak particle displacements of over 700 nm. Because the lattice constant for Si is only 0.543 nm, this means that the displacement is nearly 1300 times the size of the atoms in the crystal.

- In fact, the strains are so large that in some cases the pulses generated caused the Si crystal to fracture. In part, the optical absorptive liquid placed on the surface (described above) helps to prevent this from occurring.

Notes on EXPERIMENT FOR SI (001)

- This slide shows experimental data taken for nonlinear SAWs propagating in the (001) plane in the directions $\theta = 0^\circ$ and $\theta = 26^\circ$ from $\langle 100 \rangle$. The experimental setup is essentially the same as that described previously (see Notes on EXPERIMENT). This means that the propagation is in Regions I and II, respectively (see Notes on NONLINEARITY MATRIX FOR SI (001)). [This data was first reported in R. E. Kumon, M. F. Hamilton, Yu. A. Il'inskii, E. A. Zabolotskaya, P. Hess, A. Lomonosov, and V. G. Mikhalevich, "Pulsed nonlinear surface acoustic waves in crystals," in *Proceedings of the 16th International Congress on Acoustics and 135th Meeting of the Acoustical Society of America*, edited by P. K. Kuhl and L. A. Crum (Acoustical Society of America, Woodbury, New York, 1998), Vol. 3, pp. 1557–1558.]

- The top set of figures shows the horizontal velocity waveforms for the measurement location closest to the source. In the experiment, the vertical velocity waveform is directly measured, and these horizontal velocity waveforms are computed from linear theory. The left plot shows the data in the $\theta = 0^\circ$ direction with negative nonlinearity, while the right plot shows the data in the $\theta = 26^\circ$ direction with positive nonlinearity.
  - Due to the symmetry of the $\theta = 0^\circ$ direction, there is no transverse velocity component and the particle displacement is contained to the sagittal plane (the plane defined by the normal to the surface and the direction of propagation). In contrast, the particle motion in the $\theta = 26^\circ$ is tilted out of the sagittal plane by about 13°. The resulting transverse velocity v_y component is small, however, and is omitted.
  - The vertical velocity waveforms are significant, but are omitted on this slide.

- The bottom set of figures shows the velocity waveforms for the remote measurement location, 14.6 mm from the close location. The solid lines are the experimental data and the dashed lines are the theoretical predictions.

- First, examine the evolution of the pulse in the $\theta = 0^\circ$ direction. In this region, the coefficient of nonlinearity is negative. Hence in the longitudinal velocity v_x the peaks should travel slower than the SAW speed and troughs should travel faster. This behavior can be seen in the bottom left plot where the trough becomes shallower as it advances and the peak recedes.

- Next, examine the evolution of the pulse in the $\theta = 26^\circ$ direction. In this region, the coefficient of nonlinearity is positive. Hence in the longitudinal velocity v_x the peaks should travel faster than the SAW speed and troughs should travel slower. This behavior can be seen in the bottom right plot where the trough advances.

- Other notes:
  - The pulse at the "close" location was assumed to repeat periodically every 200 ns thereby giving a fundamental Fourier frequency of 5 MHz. The computations were performed with N =1200 harmonics (i.e., $1 \leq n \leq N$, with $v_{-n} = v_n^*$). However, only the first 120 harmonics (600 MHz bandwidth) were used to reconstruct the waveforms to make a fairer comparison with the experiment (500 MHz bandwidth).
  - The absorption coefficient was chosen by assuming classical absorption due to viscosity and heat conduction, for which the quadratic frequency dependence $\alpha_n = n^2 \alpha_1$ is obtained. The harmonic of peak amplitude occurred at 30 MHz, corresponding to the harmonic number n =6. The absorption coefficient α_1 was selected by making $1/\alpha_6 = 100\overline{x}_0$ where $\overline{x}_0 = 50$ mm is the characteristic shock formation distance. By choosing the absorption length to be much longer than the shock formation distance and the total propagation distance, absorption was taken to be weak with respect to the nonlinearity.

Notes on NONLINEARITY MATRICES IN (001) PLANE

- This slide shows the matrix elements $\widehat{S}_{11}$, $\widehat{S}_{12}$, and $\widehat{S}_{13}$ as a function of direction for Si, Ge, KCl, and NaCl.

- While time does not permit a detailed discussion of each case, it is clear that the materials exhibit a wide variety of behaviors.
- Subsequent slides will focus on describing some of the common features seen in plots shown in this slide. Focus will be placed on Si and KCl.

Notes on OTHER EFFECTS IN (001) PLANE

- Now consider propagation in the direction $\theta \approx 21^\circ$ from $\langle 100 \rangle$ in the (001) plane of silicon. In this direction, $\widehat{S}_{11}$ is close to zero (on the order of 10^{-6}) and three orders of magnitude smaller than its "neigboring" matrix elements $\widehat{S}_{12}$ and $\widehat{S}_{13}$.
- As a result, the interaction of the fundamental with itself to produce a second harmonic is greatly suppressed. Because all the energy of the wave is initially in the fundamental, this suppression implies that essentially all the energy stays there.
- The waveforms for propagation in the direction $\theta \approx 21^\circ$ from $\langle 100 \rangle$ show no distortion. The only change is a decrease in amplitude due to the absorption.
- Next consider propagation in the direction $\theta \approx 3^\circ$ from $\langle 100 \rangle$ in the (001) plane of KCl. In this direction, $\widehat{S}_{12}$ is close to zero (on the order of 10^{-6}) and three orders of magnitude smaller than its "neigboring" matrix elements $\widehat{S}_{11}$ and $\widehat{S}_{13}$. As a result, the interaction of the fundamental with the second harmonic to produce the third harmonic is suppressed.
- The corresponding waveforms do not exhibit shock formation, even at distances farther than those shown in the slide. Instead low frequecy oscillations occur in the waveforms corresponding to the relatively larger amplitudes of the second and third harmonics.
- Finally, consider propagation in the direction $\theta = 10^\circ$ from $\langle 100 \rangle$ in the (001) plane of KCl. In this direction, $\widehat{S}_{11}$ is lower in magnitude than $\widehat{S}_{12}$ and $\widehat{S}_{13}$.
- As a result, energy is transferred to third and higher harmonics at a rate that is more rapid than the transfer to the second harmonic.
- In terms of waveform distortion, this effect results in shock formation occur more rapidly than would otherwise normally be expected.

Notes on NONLINEARITY MATRICES IN (111) PLANE

- This slide shows the matrix elements $\widehat{S}_{11}$, $\widehat{S}_{12}$, and $\widehat{S}_{13}$ as a function of direction for Si, Ge, KCl, and NaCl. Because the matrix elements generally cannot be written in a real-valued form, both the magnitude and phase are shown.
- While time does not permit a detailed discussion of each case, it is clear that the materials exhibit a wide variety of behaviors especially with respect to the phase of the matrix elements.
- Subsequent slides will focus on showing how the phase of the nonlinearity matrix elements can be related to the waveform distortion. Focus will be placed on Si and KCl.
- (Added note: The magnitudes are periodic every $\Delta\theta = 60^\circ$, but the phases are only periodic every $\Delta\theta = 120^\circ$. The same relationships hold true for the lower half-plane roots of the secular equations.)

Notes on SIMULATIONS WITH SINUSOIDS FOR SI (111)

- Next, look at waveform distortion in the (111) plane. Unlike the (001) plane, this plane is not a plane of mirror symmetry, and significantly different distortion occurs. In particular, this slide show simulations performed for silicon in the (111) plane.
- The top left plot shows the longitudinal velocity waveform in the direction $\theta = 0^\circ$ from $\langle 11\bar{2} \rangle$. If the wave were to distort with the "positive" or "negatively" nonlinearity seen previously, then a shock would be expected to form at the zero crossing of the wave. Instead, an asymmetric peak forms around $\omega\tau = 3\pi/2$ in a sort of "U-shaped" distortion.

- The top right plot shows the vertical velocity waveform. If the wave were to distort with the "positive" or "negatively" nonlinearity seen previously, then a sharp peak would be expected to form at one of the peaks of the wave. Instead, an asymmetric shock front forms around $\omega\tau = 3\pi/2$ in a sort of "N-shaped" distortion.
- Note that the components exhibit distortion which is opposite to the same components in isotropic media.
- Due to the symmetry of this particular direction, there is no transverse velocity component.
- One major difference between this case and the previous cases is that the matrix elements are generally complex-valued.
- The bottom left plot shows the magnitude of the nonlinearity matrix elements $\widehat{S}_{11}$, $\widehat{S}_{12}$, and $\widehat{S}_{13}$as a function of angle from the $\langle 11\bar{2}\rangle$ direction, while the bottom right plot shows the phase of the same matrix elements over the same range.
- As will be shown in subsequent slides, the phase of the nonlinearity matrix elements provides the key to understanding the asymmetric distortion process. Previous cases have shown only positive (phase of 0 radians) and negative (phase of $\pm\pi$ radians) real-valued matrix elements. Here the phase of the matrix elements is around 0.59π radians.
- As will shown in subsequent slides, it is possible to relate the phase of the nonlinearity elements to the type of waveform distortion. Given that the waveform distortion appears to quite complicated in many cases, this can be a useful tool.

Notes on EXPERIMENT FOR SI (111)

- This slide shows the evolution of the experimental waveforms from the first probe beam location ($x = 5$ mm) to the second probe beam location ($x = 21$ mm). The experimental (solid line) and theoretical (dashed line) waveforms are also compared at the second beam location. [This data was first reported in R. E. Kumon, M. F. Hamilton, P. Hess, A. Lomonosov, and V. G. Mikhalevich, "Dependence of surface acoustic wave nonlinearity on propagation direction in crystalline silicon," in *Nonlinear Acoustics at the Turn of the Millennium: Proceedings of the 15th International Symposium on Nonlinear Acoustics*, Vol. 524 of *AIP Conference Proceedings*, edited by W. Lauterborn and T. Kurz (American Institute of Physics, Melville, New York, 2000), pp. 265–268.]
- The comparison shows that the theory is in close quantitative agreement with the experiment, and the waveforms evolve generally as expected based upon the discussion of the sinusoidal waveform simulations above. Here the experimental waveforms have a bandwidth of 500 MHz (from the photodiodes) while the theoretical waveforms were reconstructed with bandwidth of 700 MHz. Comparison of the longitudinal velocity waveforms shows the distinct lengthening of the pulse. This lengthening is also reflected in the lowering of the frequency of peak amplitude.
  - One aspect of the waveforms that does not seem to match the sinusoidal simulations is that the pulse height does not increase significantly. It can be shown that this is probably due to the fact that the bandwidth limitations of the photodiodes exclude the higher frequency terms necessary to record steep shocks and narrow peaks. In other words, the temporal resolution of the experiment (1 ns) is probably insufficient to resolve the very short peaks in the evolved waveforms.
- Notice that both the vertical velocity waveform distorts as would be expected from the sinusoidal simulations (formation of an "N-shaped" waveform for the vertical, "U-shaped" distortion for the horizontal). In addition, the pulses observed at the initial location are different in shape than those in the (001) plane of Si.

Notes on PHASE OF MATRIX ELEMENTS

- To investigate the relationship between the phase of the nonlinearity matrix elements and the spectral components, consider the effect of the phase shift shown in Eq. (1). Where n is positive, Eq. (1) represents a uniform phase shift by the angle ψ. Note that the signum function must be included to enforce consistency with the model equations.

- The evolution equations for a material with the transformed matrix S^{ψ}_{lm} are shown in the equation below Eq. (1), where the notation v^{ψ}_{n} designates that these spectral components are the solutions associated with the matrix S^{ψ}_{lm}.

- By inspection, it can be seen that if the transformed spectral amplitudes v^{ψ}_{n} are related to the untransformed spectral amplitudes v_n by Eq. (2), then the model equations for all the untransformed quantities are reobtained.

- The result is that a relationship has been established between the phases of the matrix elements and spectral amplitudes which keeps the underlying physics unchanged.

Notes on PHASE TRANSFORMED WAVEFORMS

- This slide shows how the abstract, analytical result derived in the previous slide can be used to gain insight into the waveform distortion process for different phases.

- For example, start with the well known waveform distortion of Rayleigh waves in steel. The waveforms and spectral components for these Rayleigh waves can be computed by integrating a simplified set of the model equations shown previously on the NONLINEAR THEORY slide. The matrix elements for Rayleigh waves in steel are positive and real-valued.

- The spectral amplitudes from the solution of the Rayleigh wave problem are then used to compute the transformed spectral amplitudes for a variety of phases ψ and then the time waveforms are reconstructed.

- The results are shown in the matrix of plots in the slide. At $\psi = 0$, the plot shows the distortion of the Rayleigh wave without an phase shift (identity transformation). As ψ increases, the waveform distortion becomes increasing asymmetric and changes from (1) the forming of distinct shocks in the "positive sense" (peaks advance and troughs recede in retarded time frame) to (2) sharp peaking to (3) the forming of distinct shocks in the "negative sense" (peaks recede and troughs advance in retarded time frame).

- Admittedly, the model equations have to be integrated once to use this procedure, but only once. In this sense, the determination of the various other waveforms is significantly simpler. This approach also provides a clear interpretation of the meaning of the phase of a complex-valued nonlinear matrix element.

- In the method above, the phase of all the untransformed matrix elements was taken to be the same and a uniform phase increment was applied. But, as it has already been seen, real crystals have matrix elements with differing phases. Thus, the question remains: Is this useful for real crystals or just a nifty mathematical trick?

- The answer is that it does work well in cases where the phases of the dominant matrix elements are similar, but not so well where they are dissimilar. However, the computation of the matrix elements over the full range of directions can determine where the regions of dissimilar phase lie.

Notes on APPROXIMATE AND FULL SOLUTIONS

- First, consider cases where the phases of the matrix elements are similar. The left column of plots shows results for propagation in the direction 0° from $\langle 11\bar{2} \rangle$ in the (111) plane of Si. small circles on each curve.

- Choose the phase angle ψ for transforming the spectral amplitudes to be the phase of the $\widehat{S}_{11}$ matrix element. The transformed waveforms based on the nonlinear Rayleigh waves in steel are shown in the second row, and the result from integrating the full set of model equations is given in the third row (except for a phase shift of π, these are the same graphs shown on the SIMULATIONS OF SINUSOIDS FOR SI (111) slide).

- For the Si, the agreement is reasonable in terms of the overall shape and location of the peaking, although the finer features (like the steep shock) are not quite reproduced.

- In contrast, consider cases where the phases of the matrix elements are dissimilar. The left column of plots shows results for propagation in the direction 20° from $\langle 11\bar{2} \rangle$ in the (111) plane of KCl. The selected directions are marked on the matrix element graphs by the small circles on each curve.

- Again choose the phase angle ψ for transforming the spectral amplitudes to be the phase of the $\widehat{S}_{11}$ matrix element. The transformed waveforms based on the nonlinear Rayleigh waves in steel are shown in the second row, and the result from integrating the full set of model equations is given in the third row.
- For the KCl 20° case, the approximate waveform does reproduce the approximate location of the peak, but does not reproduce the low frequency oscillations of the waveform from the full simulation.
- Nevertheless, it is clear from the graphs of the nonlinearity matrix element phase where the matrix elements are significantly dissimilar. For these regions, a simulation using the full model equations must be performed to obtain accurate results.

Notes on SUMMARY

- Investigations were undertaken for nonlinear SAWs propagating in different materials, cuts, and directions.
- The nonlinearity matrix was shown to be a useful tool for characterizing the waveform distortion. It has the advantage that it can be computed only using only basic physical constants for the system (density, second- and third-order elastic constants) and the solution of the linear problem.
- Results of investigations in the (001) plane included:
  - It was demonstrated that wide variations of waveform distortions occur between different materials and that the nonlinearity depends sensitively on the direction of propagation.
  - In particular, distinct regions were shown to exist with nonlinearity of alternating sign. Positive nonlinearity gives rise to compression shocks, while negative nonlinearity gives rise to rarefaction shocks.
  - The theory indicates that there exist directions where the generation of certain harmonics are suppressed or greatly reduced. Other directions exist where energy is rapidly transferred to higher harmonics.
  - The theory was corroborated by presenting a comparison of predictions with data from external experiments.
- Results of investigations in the (111) plane included:
  - Initially sinusoidal waveforms were shown to exhibit asymmetric waveform distortion.
  - In some cases oscillations occurred near peaks and shocks due to the nonlinearly generated phase difference between lower harmonics.
  - The theory was corroborated by presenting a comparison of predictions with data from external experiments.
  - An approximate method for estimating waveform distortion was developed based upon a simple mathematical transformation. The approximate method is most effect when the dominant nonlinearity matrix elements are similar.