

A SIMPLE METHOD FOR COMPARING WAVEFORM DISTORTION OF NONLINEAR SURFACE WAVES IN DIFFERENT CUBIC CRYSTALS

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SLIDE NOTES

Notes on COVER PAGE

- Finite amplitude waves propagating in crystals exhibit a wide diversity of nonlinear waveform distortion. The objective of this talk is to demonstrate that there exists a method for characterizing and comparing waveform distortion in cubic crystals which is simpler than performing a full integration of the model equations for every case.
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Notes on NONLINEAR SURFACE WAVES

- Surface waves are elastic waves which occur at stress-free surface of a semi-infinite solid. They 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 the estimated shock formation distance.
- 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 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 wave propagation in crystals," *Nonlinear Acoustics in Perspective*, R. J. Wei, ed. (Nanjing University Press, Nanjing, China, 1996), pp. 64–69.
 - 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 j th 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 n th harmonic of the j th 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

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

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 n th harmonic, α_n is the attenuation coefficient for the n th 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. However, in the more general lower symmetry cases, the matrix elements are complex-valued.

Notes on CRYSTALLINE GEOMETRY

- Before presenting experimental results, it is necessary to introduce some of the notation used to describe crystalline geometry. This discussion will also show the wide diversity possible in cubic crystals (as compared to isotropic media).
- Unlike isotropic media, crystalline media can have many different structures. Two common examples are shown in the top set of figures.
 - The left figure is the face-centered cubic structure, which is characteristic of NaCl and KCl. The right figure is the diamond cubic structure, which is characteristic of Si and Ge.
- Because these systems 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.
 - In both cases, the propagation properties of the surface wave changes with direction, as will be seen in later slides. The variation of the nonlinearity with direction in the (001) plane of Si, Ni, and KCl has been presented in a previous talk [R. E. Kumon, M. F. Hamilton, Yu. A. Il'inskii, and E. A. Zabolotskaya, *J. Acoust. Soc. Am.* **104**, 1815(A) (1998)].

Notes on COMPARISON WITH EXPERIMENT

- The theory described above has been compared with experiment. The data for the (111) plane were presented previously at the Seattle ASA/ICA meeting during June 1998 [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], while the data for the (001) plane were presented at the Göttingen ISNA meeting during September 1999 [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," *Proceedings of the 15th International Symposium on Nonlinear Acoustics* (2000) (in press)]. Hence these experiments will only be described briefly here.
- The experimental approach used here generates SAWs via photoelastic laser excitation. This method was described previously by 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. Measurements were made at locations closer and farther from the "source" excitation region.
 - 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 5 mm and 21 mm from the excitation region.
 - The longitudinal velocity components were computed from the directly measured vertical velocity components by a linear transformation. In particular, if the velocity components have the form

$$v_i(x, \tau) = \sum_{n=-\infty}^{\infty} v_n(x) |B_i| e^{i(n/|n|)\phi_{B_i}} e^{-in\omega_0\tau}, \quad (1)$$

in the frequency representation, then they can be related to one another by the time domain transformation

$$v_j(x, \tau) = \text{Re}(B_j/B_i)v_i(x, \tau) - \text{Im}(B_j/B_i)\mathcal{H}[v_i(x, \tau)], \quad (2)$$

where \mathcal{H} is the Hilbert transform.

- As can be seen in the figures, the surface wave pulses had durations of 25–40 ns and peak-to-peak velocity changes of 40–60 m/s. These values were typical for the pulses generated by these experiments.
- To compare the experimental data to theory, the spectral amplitudes from the "source" data at the close measurement locations were propagated using the model equations shown on the previous slide. The dashed line shows the theoretical result of this propagation. The waveforms match closely.
- Pulse data is shown here for the longitudinal velocity waveforms for the two cases shown in the slide. First, look at the data in the left column from the (001) plane. The nonlinearity is of the "positive real" kind, which means that the peaks of the waveform should advance and the troughs should recede. This behavior is seen in the lower left plot.

- Next, look at the data in the right column from the (111) plane. First, notice that, even though the generation mechanism is identical between the two cases, the waveforms measured at the close location is substantially different. Second, if this pulse had the same “positive real” nonlinearity like the other set of data, then the peaks of the waveform should advance, the troughs should recede, and a shock should form. Instead, a broad “U-shaped” distortion occurs. Nevertheless, the shape of the waveform is reproduced by the theory.
- In both cases, the theory is corroborated by experiment.

Notes on WAVEFORM DISTORTION DIVERSITY

- This slide shows examples of the diversity of the more general nonlinear distortion predicted for propagation in the (111) cut of two real crystals.
- The top two rows show the nonlinear waveform distortion and shock formation for KCl and Si in the (111) plane in the $\langle 11\bar{2} \rangle$ direction. The left column contains the longitudinal velocity waveform while the right column contains the vertical velocity waveform. Due to the symmetry of this particular case, there is no transverse velocity component.
 - In each waveform, a non-dimensional velocity component is plotted versus a non-dimensional retarded time. The initial waveform is a single frequency, continuous wave. The velocity v is scaled such that the total initial velocity amplitude is unity, and the retarded time is scaled by the period of the initial sinusoidal signal. The propagation distance X is scaled such that $X = 1$ corresponds to approximately one shock formation distance.
- KCl: In its longitudinal waveform, cusps form near the shock front while in its vertical waveform, a peak forms. Note that the wave distorts asymmetrically. Interestingly, the longitudinal waveform looks similar to the waveform distortion of an acoustic wave in a fluid except that here peaks move slower and troughs, faster in contrast to the behavior in fluids where peaks move faster, and troughs, slower.
 - For the computation of these matrix elements, the data for the Si elastic constants was taken from the paper by J. R. Drabble and R. E. B. Strathen, “The third-order elastic constants of potassium chloride, sodium chloride and lithium fluoride,” Proc. Phys. Soc. (London) **92**, 1090–1095 (1967).
- Si: In contrast to KCl, here the *vertical* waveform forms a shock and *longitudinal* waveform forms a peak. there also seem to be some mixed features. For example, the vertical waveform forms a shock but the cusping is so asymmetrical that one side also looks like a peak.
 - For the computation of these matrix elements, the data for the Si elastic constants was taken from the paper by H. J. McSkimin and P. Andreatch, Jr., J. Appl. Phys. **35**, 3312–3319 (1964).
- Next, consider what happens when the crystal, cut, and propagation distance are held constant and only the direction of propagation is changed.
- Here the longitudinal velocity waveforms are plotted for KCl in the (111) plane for a variety of directions relative to the $\langle 11\bar{2} \rangle$ direction. Each individual waveform shown is the waveform that results after an initially sinusoidal signal is propagated to a distance of $X = 2$ for that case. The scaling is the same as in the previous set of graphs.
- Here the mixing of features between the various components is seen even more than in the previous plots. The longitudinal waveform at 0° starts in a shock, and turns into more of a peaked waveform as the angle is increased to 5° .
 - Over the same change in direction, the peak in the vertical waveform turns into an asymmetric peak with one side steepened. Finally, the transverse component (which is zero at 0°) appears as a peak and grows in amplitude as the angle increases.
- As can be seen, the distortion of these waveforms is diverse and complicated. The question is: “Is it possible to develop a simple (or at least relatively simpler), approximate method to characterize the waveform distortion and predict trends without having to integrate the full set of model equations for every different crystal, cut, and direction?” The answer is “sometimes,” as will be demonstrated in subsequent slides.

Notes on NONLINEARITY MATRIX

- As mentioned previously, the matrix elements for surface waves in the (111) plane are generally complex-valued. This slide shows the magnitude and phase of the dimensionless matrix elements \widehat{S}_{11} , \widehat{S}_{12} , and \widehat{S}_{13} ($\widehat{S}_{ij} = -S_{ij}/c_{44}$) for silicon in the (111) plane over the range 0° to 30° from the $\langle 11\bar{2} \rangle$ direction. Due to the symmetries of this plane, the matrix elements are symmetric about the 30° direction and periodic every 60° .
- First consider the magnitudes. The magnitudes peak at 0° and monotonically decrease toward 30° . The magnitude of the matrix elements give a relative measure of the strength of the nonlinear interactions. In cases where shocks form, the strength of nonlinear interaction can be shown to be inversely proportional to the shock formation distance (if shocks form!). Hence the effect of the magnitude of the nonlinearity matrix elements is well understood.
- Next consider the phases. For this particular case, the phase goes from around 105° to 180° (negative real). The question which remains is: How the the phase of the matrix elements is related to the shape of the waveform distortion? How can the phase be interpreted physically?

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 θ . 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_{lm}^θ are shown in the equation below Eq. (1), where the notation v_n^θ designates that these spectral components are the solutions associated with the matrix S_{lm}^θ .
- By inspection, it can be seen that if the transformed spectral amplitudes v_n^θ 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 θ and then the time waveforms are reconstructed.
- The results are shown in the matrix of plots in the slide. At $\theta = 0^\circ$, the plot shows the distortion of the Rayleigh wave without an phase shift (identity transformation). As θ 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 ELEMENTS WITH SIMILAR PHASE

- 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, while the right column shows results for the same direction for KCl. The selected directions are marked on the matrix element graphs by the small circles on each curve.
- Choose the phase angle θ for transforming the spectral amplitudes to be the phase of the \hat{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 WAVEFORM DISTORTION IN (111) PLANE 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.
- For KCl, the agreement is also reasonable, but again the fine features near the shock are not reproduced (e.g., the small cusp on the left side of the graph from the full simulation). Note also that the graph of the nonlinearity matrix element clearly shows that the phase of the elements is changing rapidly as a function of direction. This latter result is consistent with the simulations shown previously on the WAVEFORM DISTORTION IN (111) PLANE slide.

Notes on ELEMENTS WITH DISSIMILAR PHASE

- 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, while the right column shows results for 28° for KCl. The selected directions are marked on the matrix element graphs by the small circles on each curve.
- Again choose the phase angle θ for transforming the spectral amplitudes to be the phase of the \hat{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.
- For the KCl 28° case, the agreement is even worse as not even the location of the peak is reproduced. This result should be expected though because \hat{S}_{11} differs substantially from \hat{S}_{12} and \hat{S}_{13} .
- 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.