

# DEPENDENCE OF SURFACE WAVE NONLINEARITY ON PROPAGATION DIRECTION IN CRYSTALLINE SILICON

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## SLIDE NOTES

### Notes on COVER PAGE

- More specifically, the objective of this talk is to demonstrate that the dependence of surface wave nonlinearity on direction is very strong in the sense that relatively small changes in direction can cause dramatic changes in the evolution of the wave as it propagates.
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- Yu. A. Il'inskii and E. A. Zabolotskaya are now employed by MacroSonix Corporation, Richmond, Virginia.

### Notes on ANISOTROPY IN CRYSTALLINE SILICON

- This talk will focus on surface acoustic waves (SAW) in crystalline silicon. Crystalline silicon is a cubic crystal (see "Diamond Cubic Structure" diagram). Cubic crystals have the stress-strain relation shown in the slide. Usually the strains are sufficient small that the linear relation  $\sigma_{ij} = c_{ijkl}e_{kl}$  is valid. However, the strains considered here are large enough that the nonlinear terms contribute significantly and, in fact, give rise to waveform distortion and shock formation.
  - Diamond Cubic Structure: Si has a diamond lattice which can also be considered to be two fcc lattices, one displaced relative to the other by  $(1/4, 1/4, 1/4)$ . Note also that every atom has four nearest neighbors. The lattice spacing for Si is 0.543 nm.
- The material properties of the crystal are expressed via the elastic constants of the material. In particular, 3 SOE and 6 TOE constants are necessary to specify a cubic crystal. For all the simulations presented in this talk, 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).
  - Isotropic Material: In contrast, an isotropic material has only 2 SOE (shear and bulk moduli) and 3 TOE constants. The number of constants is less because the symmetry is higher.
- 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 crystal cut chosen in the experiment is the (001) plane (see diagram). For the experiment and simulations shown in this talk, the pulses propagated in directions measured relative to the  $\langle 100 \rangle$  direction.

### Notes on LINEAR SAW DIAGRAM

- 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 clearly seen, 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 the surface is typically the most experimentally accessible part of the medium, it is the location where SAWs are examined. The particle trajectories at the surface are shown in top and side views. The particle motion is always confined to a plane. For the cases shown here, this plane is generally rotated by some angle  $\phi$  out of the  $xz$ -plane.
  - Isotropic material: In contrast, the particle trajectory of a Rayleigh wave is always confined to the plane perpendicular to the surface that contains the direction of propagation, shown in the figure as the dashed rectangle.
- The particle displacement has a transverse component for most propagation directions in the (001) plane. However, because  $\phi$  is small for most propagation directions, only vertical and longitudinal waveforms will be shown. The transverse component is related to the other components by a relation that can be derived from linear theory.

### 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 was 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 SOE and TOE 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  $\omega$  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,  $\alpha_n$  is the attenuation coefficient for the  $n$ th harmonic,  $\omega$  is the characteristic angular frequency,  $\rho$  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  $\Gamma$  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 SOE and TOE constants of the material (see the section "Notes on Nonlinearity Matrix" for details).
- 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.
  - 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.

### Notes on COMPARISON WITH EXPERIMENT

- The theory described above has been compared with experiment. These results 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] and hence will only be described briefly here.
- The experimental approach used here generates SAW 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. The waves were generated in the (111) plane in  $\langle 112 \rangle$  direction.
- 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  $\mu\text{m}$  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  $\mu\text{m}$  in diameter on the surface at distances 5 mm and 21 mm from the excitation region.
- 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 this experiment.
- To compare the experimental data to theory, the spectral amplitudes from the “source” data at  $x=5$  mm 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.

### Notes on NONLINEARITY MATRIX

- With confidence that the nonlinearity was being described correctly based on the experimental data, the properties of the nonlinearity matrix were investigated in more detail.
- The nonlinearity matrix elements are a complicated function of many quantities. Here the  $d'_{ijklmn}$  values are derived from the second-order elastic constants  $c_{ijkl}$  and third-order elastic constants  $d_{ijklmn}$  as shown in the slide while the values of  $l_3^{(s)}$  and  $q_j^{(s)}$  are parameters of the depth dependence functions  $u_{nj}$  derived by solving the linear problem.
  - 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.
- Physically, the nonlinearity matrix elements can be interpreted in two ways. First, as will be shown on the next slide, they can be related to an effective coefficient of nonlinearity. Secondly, they can be interpreted as describing the strength of the energy coupling between various harmonics of the wave. In particular, the  $S_{mn}$  matrix element describes how energy is transferred from the  $m$ th and  $n$ th harmonics to the  $(m+n)$ th harmonic.

- The figure shows the matrix elements  $S_{11}$ ,  $S_{12}$ , and  $S_{13}$  plotted as a function of angle from the  $\langle 100 \rangle$  direction for SAW in Si on the (001) plane. Other matrix elements follow a similar pattern including the same location of zero crossings, but the curves are not multiples of one another.
- 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  $0-5^\circ$  and  $25-30^\circ$  regions. On the other extreme, the waveform evolution is predicted to be linear (to third order in the wave variables) around  $21^\circ$  and  $32^\circ$ . While the matrix elements go to zero near  $45^\circ$ , the wave also degenerates into an exceptional bulk shear 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. Thus the sensitivity to changes in direction is much greater for the nonlinearity matrix elements than in the case of the linear SAW speed.

### Notes on SHOCK FORMATION DISTANCE

- While the nonlinearity matrix may be a unfamiliar concept, it may be related to a quantity that is more familiar: the shock formation distance.
- For an initially sinusoidal wave, the shock formation distance can be estimated by the expression shown on the slide where  $\beta_x$  is the coefficient of nonlinearity,  $\epsilon_x$  is the acoustic Mach number or, equivalently, peak strain, and  $k$  is the wavenumber. The coefficient of nonlinearity contains the nonlinearity matrix element  $S_{11}$ , the density  $\rho$ , and the SAW sound speed  $c$ .
  - In general the nonlinearity matrix elements are complex. Hence the coefficient of nonlinearity may also be complex. The interpretation of a complex-valued coefficient of nonlinearity is not clear and is a topic of current research.
- Hence the shock formation distance is inversely proportional to the magnitude of the nonlinearity matrix element  $S_{11}$ . The figure shown plots this estimate of the shock formation distance on the (001) plane of silicon as a function of direction for the case of  $\omega/2\pi=50$  MHz and  $v_{x0} = 36$  m/s ( $\epsilon_x \approx 0.007$ ).
- Where the nonlinearity matrix element  $S_{11}$  approaches zero, the waveform evolution is linear and, correspondingly, the shock formation distance approaches infinity. Where the nonlinearity matrix element  $S_{11}$  is maximized, the shock formation distance is minimized.
- The importance of the relationship between the nonlinearity matrix elements and the shock formation distance is that it allows for the prediction of regions where experiments would be most likely to measure significant nonlinear waveform distortion.

### Notes on SIMULATIONS WITH SINUSOIDS

- 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  $S_{11}$  matrix element as a function of propagation direction. Waveforms are examined for two directions,  $10^\circ$  and  $26^\circ$  degrees, that exhibit distortion characteristic of propagation in their respective regions.
- First look at the  $26^\circ$  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. Here the distance is scaled such that  $X=1$  corresponds to the estimated shock formation distance of 10 mm.
- 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  $S_{11}$  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 LINEAR SAW DIAGRAM).
- Now look at the  $10^\circ$  direction in Region I. Here  $S_{11}$  is lower in magnitude and negative. The reduced magnitude of the nonlinearity results in an increase of the shock formation distance to 23 mm. Because  $S_{11}$  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  $45^\circ$  direction is approached (see Notes on Supplement: RESULTS FROM LINEAR THEORY and Notes on Supplement: WAVEFORMS: REGION III) As this occurs, the energy of the wave penetrates deeper and deeper into the solid and is correspondingly weaker at the surface. This reduced amplitude then makes the nonlinear effects weaker.

### Notes on CONCLUSION

- The nonlinear wave propagation of surface acoustic waves in crystalline silicon was investigated on the (001) plane over all directions. Due to the symmetries of the crystal in this plane, only the range  $0^\circ < \theta < 45^\circ$  from the  $\langle 100 \rangle$  direction need be studied. This is the first systematic theoretical study of nonlinear SAW of its kind.
- It was found that the behavior of the nonlinearity matrix elements allows the waveform distortion to be classified into into three distinct regions:

Region	Angular range	Waveform Behavior
I	$0^\circ < \theta < 21^\circ$	Steepens "backward"
II	$21^\circ < \theta < 32^\circ$	Steepens "forward"
III	$32^\circ < \theta < 45^\circ$	Steepens "backward"

- The theory predicted that SAW propagation in two particular directions ( $\theta \approx 21^\circ$  and  $\theta \approx 32^\circ$  from the  $\langle 100 \rangle$  direction) will be linear to within the accuracy of the theory even for finite amplitude SAW.
- Nonlinearity effects vary more than linear SAW speed as a function of direction (see the Notes on Supplement: RESULTS FROM LINEAR THEORY).

## Notes on Supplement: NONLINEARITY MATRIX & LINEAR THEORY

- This procedure will be more fully described in the forthcoming paper [M. F. Hamilton, Yu. A. Il'inskii, and E. A. Zabolotskaya, "Nonlinear surface acoustic waves in crystals," J. Acoust. Soc. Am. (in review)].
- The elastic constants with the tilde are transformed into the coordinate system in which the  $x$ -axis is the direction of propagation and the  $z$ -axis is perpendicular to the surface of the solid.

## Notes on Supplement: RESULTS FROM LINEAR THEORY

- Non-piezoelectric crystals have three bulk acoustic modes (one longitudinal or quasi-longitudinal and two shear or quasi-shear) and one surface acoustic wave mode. The wave speed for each mode is generally a non-constant function of the direction of propagation.
  - The acoustic modes in a crystal and isotropic solid differ in two ways: (1) for an isotropic solid the wave speeds for all modes are independent of the direction of propagation and (2) for an isotropic solid the two shear modes are always degenerate in wave speed and have polarizations that are mutually perpendicular.
  - While some of the individual particle velocity polarizations of the bulk acoustic modes may not be parallel or perpendicular to the direction of propagation, the polarizations of the three modes are always mutually perpendicular [B. A. Auld, *Acoustic Fields and Waves in Solids*, 1st ed. (John Wiley & Sons, New York, 1973), pp. 219–220.].
- In this case, silicon has one quasi-longitudinal, one pure shear ([001]-polarized), and one quasi-shear mode. Because the pure shear mode has constant wave speed for all directions, it was used as a reference velocity. Here the wave speed of the acoustic modes relative to the pure shear wave speed are plotted as a function of the angle of propagation  $\theta$  from the  $\langle 100 \rangle$  direction. Because of the symmetry of the crystal for this particular cut and direction, the wave speeds are periodic every  $90^\circ$  and symmetric about  $\theta = 45^\circ$ .
  - At  $\theta = 0$ , the bulk acoustic waves are similar to those in an isotropic solid with a pure longitudinal mode and two degenerate pure shear modes.
  - For reference, the bulk shear wave speed for Si at  $\theta = 0$  is 5829 m/s while the bulk longitudinal wave speed is 8413 m/s (based upon the McSkimin and Andreatch data).
- The surface acoustic wave (SAW) is shown as the dashed line. It is always less than the lowest bulk wave speed. For reference, the SAW speed at  $0^\circ$  is 4902 m/s. As  $\theta \rightarrow 0$ , the SAW speed approaches the speed of the quasishear bulk mode. At  $\theta = 45^\circ$ , the modes become degenerate thereby allowing for a bulk shear wave that satisfies the surface boundary conditions. This wave is usually called an exceptional bulk wave or “surface-skimming” bulk wave.
- Note that the variation in the wave speed from  $0^\circ$  to  $45^\circ$  is relatively small for all the modes:

Mode	Variation
Quasilongitudinal	+5%
Pure shear	0%
Quasishear	–20%
SAW	–8%

In contrast, it will be shown subsequently that the nonlinear effects change more than this linear effect as a function of direction.

## Notes on Supplement: WAVEFORMS: REGION I

- These plots show the waveform distortion due to nonlinear processes for Si in the (001) plane in the direction  $10^\circ$  from  $\langle 100 \rangle$  for **the waveforms at the surface**. It is a typical example of surface waveforms in the region  $0^\circ < \theta < 21^\circ$ . For convenience, the plot of the nonlinearity matrix element  $S_{11}$  is reproduced in the upper right graph. The thick solid line marks the location of  $10^\circ$  on the graph.
- The graphs in the left column show the  $x$ -,  $y$ -, and  $z$ -components of the velocity. In each waveform, the non-dimensional velocity 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 imaginary part of the Fourier amplitude of the fundamental is unity, and the retarded time  $\tau$  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 (see the slide on Shock Formation Distance). The estimate of the shock formation distance  $\bar{x}=23$  mm.
  - Because the nonlinearity matrix elements are different in each direction, the shock formation distance is also different in each direction. Hence it is not possible to directly compare the waveforms at the same non-dimensional distance  $X$  for waveforms propagating in different directions.
- The waveforms clearly exhibit significant distortion and shock formation. The longitudinal velocity component  $V_x$  has the cusps near the shock front while the vertical velocity component  $V_z$  has a sharp peak. Both of these effects are similar to those observed in SAW in isotropic media [E. A. Zabolotskaya, "Nonlinear propagation of plane and circular waves in isotropic solids," *J. Acoust. Soc. Am.* **91**, 2569–2575 (1992)].
- Due to the symmetry of this cut, the waveform distortion is symmetric. However, this is not generally true for any cut and direction (e.g., Si in the (111) plane in the  $\langle 11\bar{2} \rangle$  direction).
- Because the nonlinearity matrix element  $S_{11}$  is negative, the coefficient of nonlinearity  $\beta$  is also negative. This causes the longitudinal velocity waveform to steepen "backward" from the way a sinusoid would steepen in a fluid with nonlinear distortion modelled by the Burgers equation. Here the "peaks" of the waveform move slower than the SAW speed while "troughs" move faster.
- Unlike an isotropic medium, here the wave has a transverse velocity component  $V_y$ . This effect can be more clearly visualized by looking at a top view of the particle trajectory (projected into the (001) plane) as shown in the figure. Looking from above the (001) plane, the plane of the particle motion is rotated clockwise out of the sagittal plane by approximately  $\phi = 2^\circ$ .
- The overall motion of the wave can be seen in the side view of the particle trajectory (projected into the (100) plane). The motion is retrograde at the surface. It begins as an ellipsoid with eccentricity  $e = 0.590$  and distorts to more asymmetric "egg-like" shape due to the nonlinear effects. The decrease in the in the path length visible in the graph is due to energy loss at the shock front.
- Each waveform was generated from a numerical calculation using 200 harmonics. However, in order to minimize the effects of numerical aliasing due to the finite spectral width taken only the first 150 harmonics were used to reconstruct the time waveform from the harmonic amplitudes (the remaining 50 harmonics set to zero before the inverse Fourier transform was taken).

## Notes on Supplement: WAVEFORMS: REGION II

- These plots show the waveform distortion due to nonlinear processes for Si in the (001) plane in the direction  $26^\circ$  from  $\langle 100 \rangle$  for **waveforms at the surface**. It is a typical example of surface waveforms in the region  $21^\circ < \theta < 32^\circ$ . For convenience, the plot of the nonlinearity matrix element  $S_{11}$  is reproduced in the upper right graph. The thick solid line marks the location of  $26^\circ$  on the graph.
- The graphs in the left column show the  $x$ -,  $y$ -, and  $z$ -components of the velocity. In each waveform, the non-dimensional velocity is plotted versus a non-dimensional retarded time. **Note that for purposes of plotting the waveform in a clearer way, the phase of the wave has been shifted by  $\pi$  from the  $10^\circ$  case.** The initial waveform is a single frequency, continuous wave. The velocity  $V$  is scaled such that the imaginary part of the Fourier amplitude of the fundamental is unity, and the retarded time  $\tau$  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 (see the slide on Shock Formation Distance). The estimate of the shock formation distance  $\bar{x} = 10$  mm.
  - Because the nonlinearity matrix elements are different in each direction, the shock formation distance is also different in each direction. Hence it is not possible to directly compare the waveforms at the same non-dimensional distance  $X$  for waveforms propagating in different directions.
- The waveforms clearly exhibit significant distortion and shock formation. The longitudinal velocity component  $V_x$  has the cusps near the shock front while the vertical velocity component  $V_z$  has a sharp peak. Both of these effects are similar to those observed in SAW in isotropic media [E. A. Zabolotskaya, "Nonlinear propagation of plane and circular waves in isotropic solids," *J. Acoust. Soc. Am.* **91**, 2569–2575 (1992)].
- Due to the symmetry of this cut, the waveform distortion is symmetric. However, this is not generally true for any cut and direction (e.g., Si in the (111) plane in the  $\langle 11\bar{2} \rangle$  direction).
- Because the nonlinearity matrix element  $S_{11}$  is positive, the coefficient of nonlinearity  $\beta$  is also positive. This causes the longitudinal velocity waveform to steepen "forward" in the same way that a sinusoid would steepen in a fluid with nonlinear distortion modelled by the Burgers equation. Here the "peaks" of the waveform move faster than the SAW speed while "troughs" move slower.
- Unlike an isotropic medium, here the wave has a transverse velocity component  $V_y$ . This displacement is significantly greater than in the  $10^\circ$  case. This effect can be more clearly visualized by looking at a top view of the particle trajectory (projected into the (001) plane) as shown in the figure. Looking from above the (001) plane, the plane of the particle motion is rotated counterclockwise out of the sagittal plane by approximately  $\phi = 13^\circ$ .
- The overall motion of the wave can be seen in the side view of the particle trajectory (projected into the (100) plane). The motion is retrograde at the surface. It begins as an ellipsoid with eccentricity  $e = 0.659$  and distorts to more asymmetric "egg-like" shape due to the nonlinear effects. The decrease in the path length visible in the graph is due to energy loss at the shock front. Note that the small end of the "egg" shape of the  $X = 2$  trajectory is on the opposite side to the similar trajectory in the  $10^\circ$  case.
  - Because the particle motion is rotated out of the sagittal plane, the side view as a projection is distorted so that the elliptical motion looks narrower in the horizontal direction.
  - While the dimensionless value of the attenuation  $A_1 = \alpha_1 \bar{x} = 0.025$  is held constant in all the cases shown, the physical attenuation coefficient  $\alpha_n$  is changing as the shock formation distance changes. Hence for this case the physical attenuation coefficient is approximately twice as high as in the previous case because the shock formation distance is approximately half as much.
- Each waveform was generated from a numerical calculation using 200 harmonics. However, in order to minimize the effects of numerical aliasing due to the finite spectral width taken only the first 150 harmonics were used to reconstruct the time waveform from the harmonic amplitudes (the remaining 50 harmonics set to zero before the inverse Fourier transform was taken).

## Notes on Supplement: WAVEFORMS: REGION III

- These plots show the waveform distortion due to nonlinear processes for Si in the (001) plane in the direction  $35^\circ$  from  $\langle 100 \rangle$  for **waveforms at the surface**. It is a typical example of surface waveforms in the region  $32^\circ < \theta < 45^\circ$ . For convenience, the plot of the nonlinearity matrix element  $S_{11}$  is reproduced in the upper right graph. The thick solid line marks the location of  $35^\circ$  on the graph.
- The graphs in the left column show the  $x$ -,  $y$ -, and  $z$ -components of the velocity. In each waveform, the non-dimensional velocity is plotted versus a non-dimensional retarded time. **Note that for purposes of plotting the waveform in a clearer way, the phase of the wave has been shifted back by  $\pi$  so that it is the same as in the  $10^\circ$  case.** The initial waveform is a single frequency, continuous wave. The velocity  $V$  is scaled such that the imaginary part of the Fourier amplitude of the fundamental is unity, and the retarded time  $\tau$  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 (see the slide on Shock Formation Distance). The estimate of the shock formation distance  $\bar{x} = 110$  mm.
  - Because the nonlinearity matrix elements are different in each direction, the shock formation distance is also different in each direction. Hence it is not possible to directly compare the waveforms at the same non-dimensional distance  $X$  for waveforms propagating in different directions.
- The waveforms clearly exhibit significant distortion and shock formation. This is true even though the wave is almost degenerate with the quasishear mode.
- Due to the symmetry of this cut, the waveform distortion is symmetric. However, this is not generally true for any cut and direction (e.g., Si in the (111) plane in the  $\langle 11\bar{2} \rangle$  direction).
- Because the nonlinearity matrix element  $S_{11}$  is negative, the coefficient of nonlinearity  $\beta$  is also negative. This causes the longitudinal velocity waveform to steepen “backward” from the way a sinusoid would steepen in a fluid with nonlinear distortion modelled by the Burgers equation. Here the “peaks” of the waveform move slower than the SAW speed while “troughs” move faster.
- The top view of the particle trajectory (projected into the (001) plane) is shown in the figure. Looking from above the (001) plane, the plane of the particle motion is rotated clockwise out of the sagittal plane by approximately  $\phi = 83^\circ$ .
- The overall motion of the wave can be seen in the **front view** of the particle trajectory (projected into the (010) plane). The motion is retrograde at the surface. It begins as an ellipsoid with eccentricity  $e = 0.956$  and distorts to more asymmetric “egg-like” shape due to the nonlinear effects.
  - While the dimensionless value of the attenuation  $A_1 = \alpha_1 \bar{x} = 0.025$  is held constant in all the cases shown, the physical attenuation coefficient  $\alpha_n$  is changing as the shock formation distance changes. Hence for this case the physical attenuation coefficient is approximately eleven times less than in the  $10^\circ$  case because the shock formation distance is approximately eleven times more.
- Each waveform was generated from a numerical calculation using 200 harmonics. However, in order to minimize the effects of numerical aliasing due to the finite spectral width taken only the first 150 harmonics were used to reconstruct the time waveform from the harmonic amplitudes. (the remaining 50 harmonics set to zero before the inverse Fourier transform was taken).