DEPENDENCE OF SURFACE WAVE NONLINEARITY ON PROPAGATION DIRECTION IN CRYSTALLINE SILICON

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OUTLINE

- Anisotropy in Crystalline Silicon
- Linear Surface Acoustic Waves
- Nonlinear Theory
- Comparison with Experiment
- Nonlinearity Matrix & Shock Formation Distance
- Simulations with Sinusoids
- Conclusion

ANISOTROPY IN CRYSTALLINE SILICON

Stress-strain relation for cubic crystal:

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

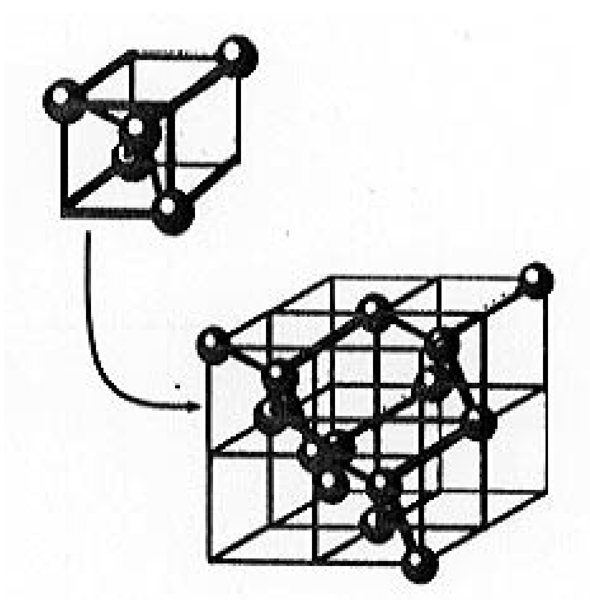
c_{ijkl} $\rightarrow$ 3 Second Order Elastic (SOE) constants

d_{ijklmn} $\rightarrow$ 6 Third Order Elastic (TOE) constants

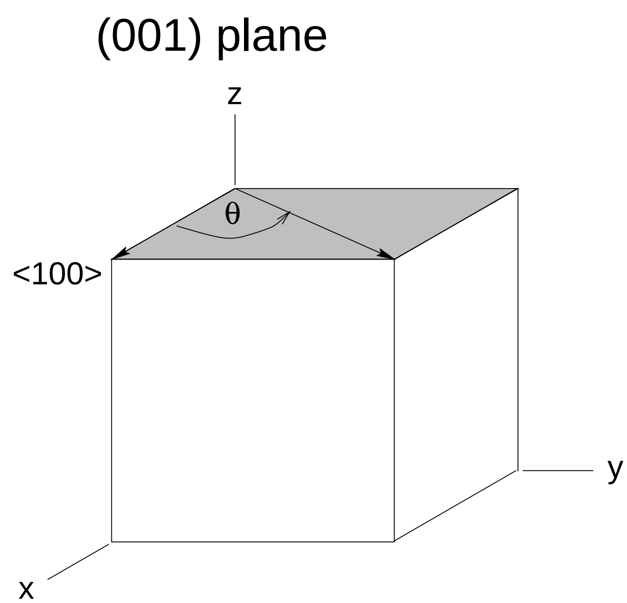
Data for Si elastic constants:

- McSkimin, H. J. and Andreatch, Jr., P., J. Appl. Phys. **35**, 3312–3319 (1964).

Diamond Cubic Structure:

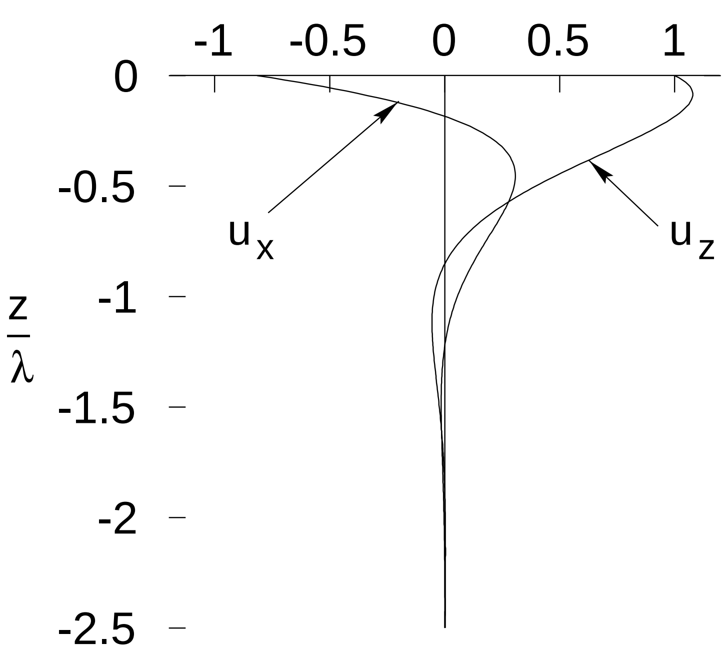


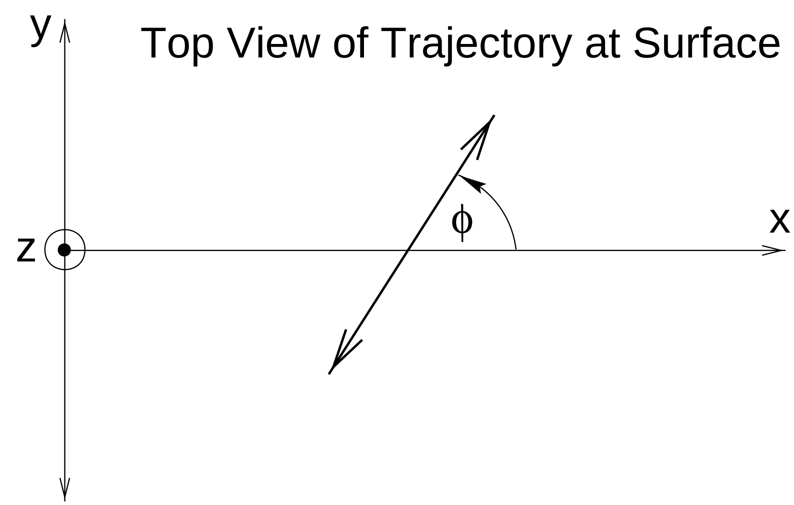
Crystal Cut in Simulations:

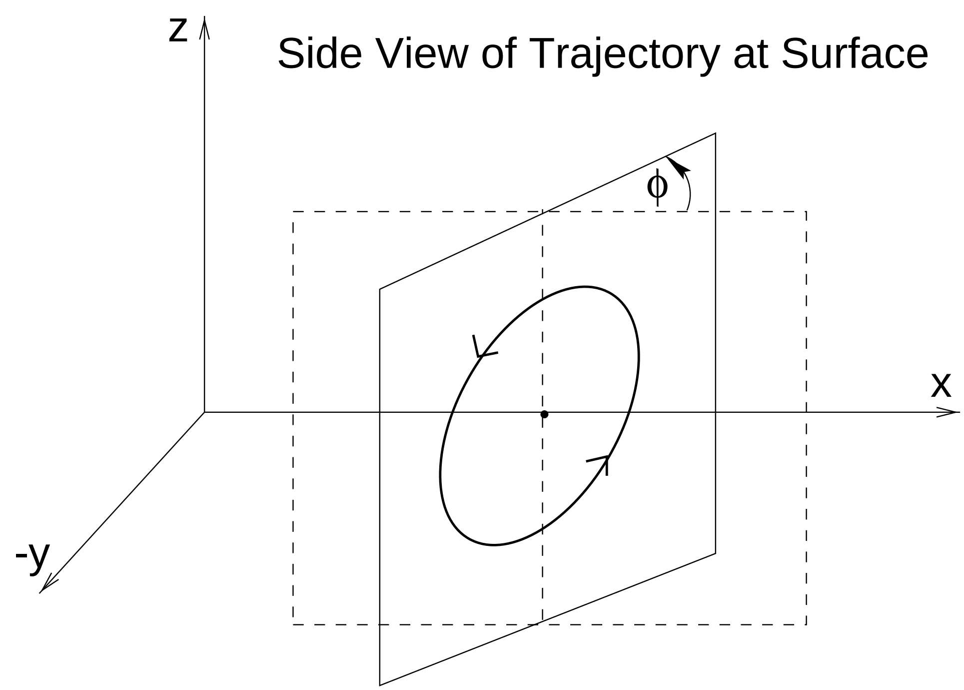


Linear Properties of a Surface Acoustic Wave in an Anisotropic Medium

Displacement Depth Profile







NONLINEAR THEORY

Approach: Hamiltonian mechanics formalism
(Hamilton, Il'inskii, Zabolotskaya, 1996)

Velocity waveforms in solid:

$$v_j(x,z,t) = \sum_{n=-\infty}^{\infty} v_n(x) u_{nj}(z) e^{in(kx-\omega t)}$$
$$u_{nj}(z) = \sum_{s=1}^{3} q_j^{(s)} e^{inkl_3^{(s)} z}$$

Coupled spectral evolution equations:

$$\frac{dv_n}{dx} + \alpha_n v_n = \frac{n^2\omega}{2\rho c^4} \sum_{l+m=n} \frac{lm}{|lm|} S_{lm} v_l v_m$$

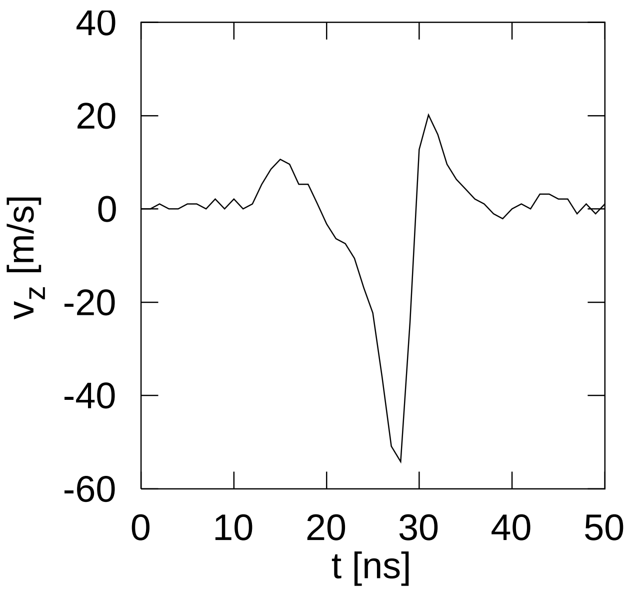
$v_n \rightarrow$ nth harmonic amplitude
$S_{lm} \rightarrow$ nonlinearity matrix elements
$\alpha_n \rightarrow$ weak attenuation

COMPARISON WITH EXPERIMENT

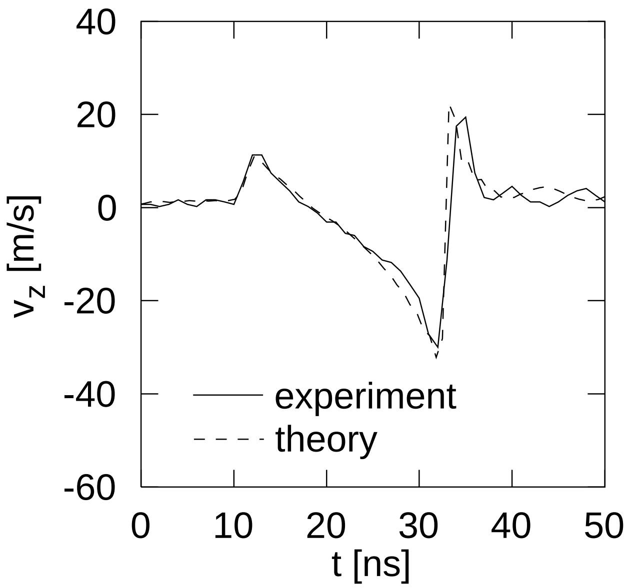
[from Kumon *et al.*, Seattle ICA/ASA, June 1998]

Experiment: Laser-excited pulses in Si on (111) plane in $\langle 11\bar{2} \rangle$

Velocity waveform at $x = 5$ mm from source:



Velocity waveform at $x = 21$ mm from source:



NONLINEARITY MATRIX

Nonlinearity matrix elements:

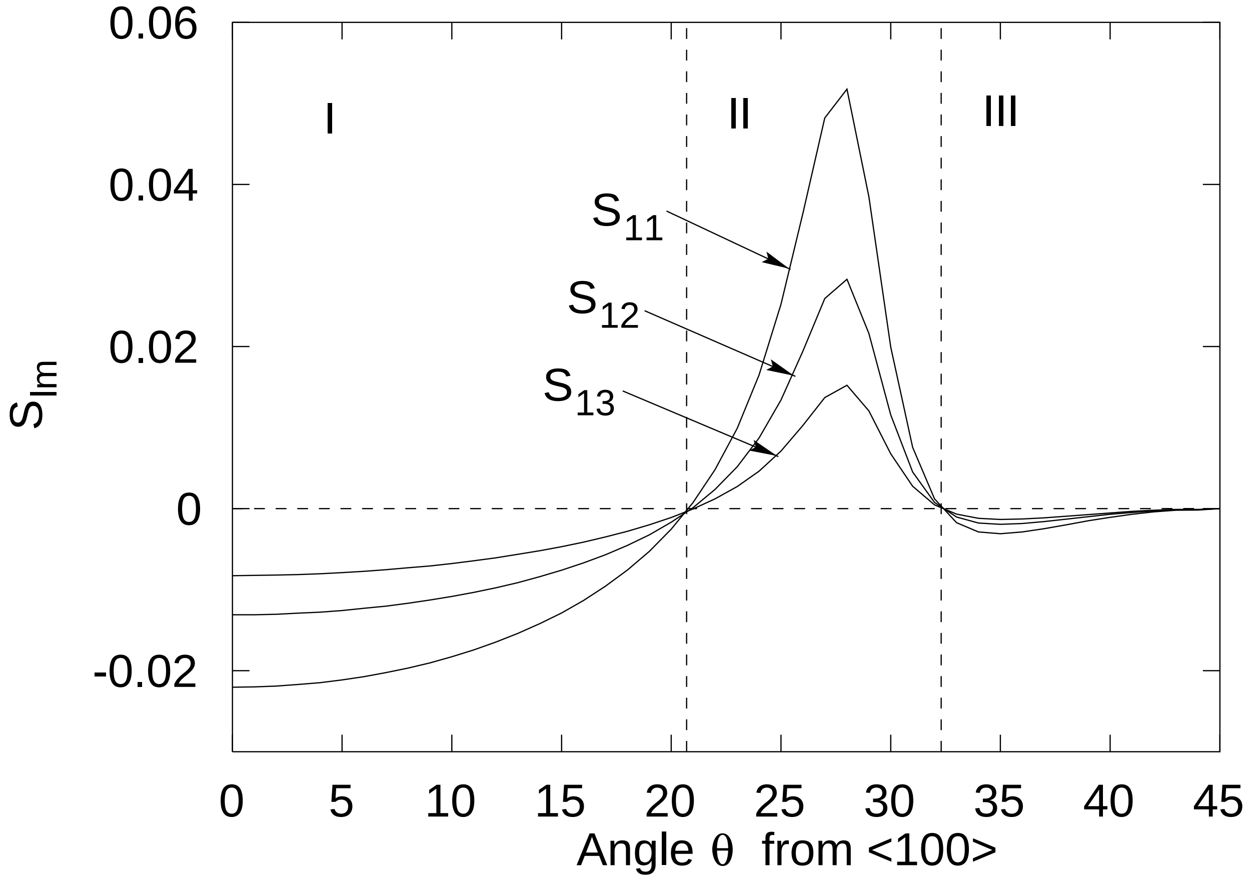
$$S_{n_1 n_2} = \sum_{s_1,s_2,s_3=1}^{3} \frac{\frac{1}{2} d'_{ijklmn} q_i^{(s_1)} q_k^{(s_2)} [q_m^{(s_3)}]^* l_j^{(s_1)} l_l^{(s_2)} [l_n^{(s_3)}]^*}{n_1 l_3^{(s_1)} + n_2 l_3^{(s_2)} - (n_1 + n_2)[l_3^{(s_3)}]^*}$$

$l_3^{(s)} \rightarrow$ eigenvalues of linear problem

$q_j^{(s)} \rightarrow$ eigenvectors of linear problem

$d'_{ijklmn} \rightarrow$ SOE and TOE constants

Selected matrix elements for Si on (001) plane:



SHOCK FORMATION DISTANCE

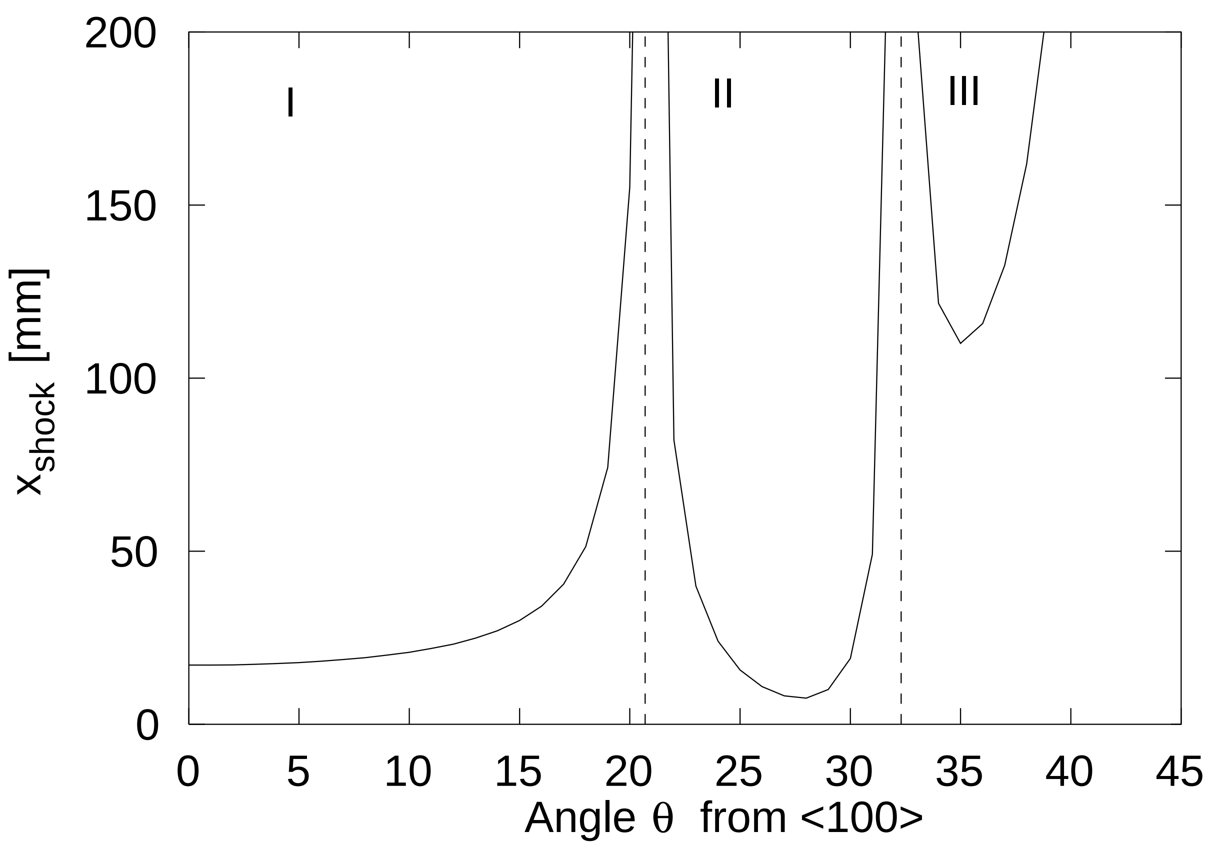
Estimate of shock formation distance:

$$\overline{x} = \frac{1}{|\beta_x|\epsilon_x k}, \qquad \beta_x = \frac{4S_{11}}{\rho c^2}$$

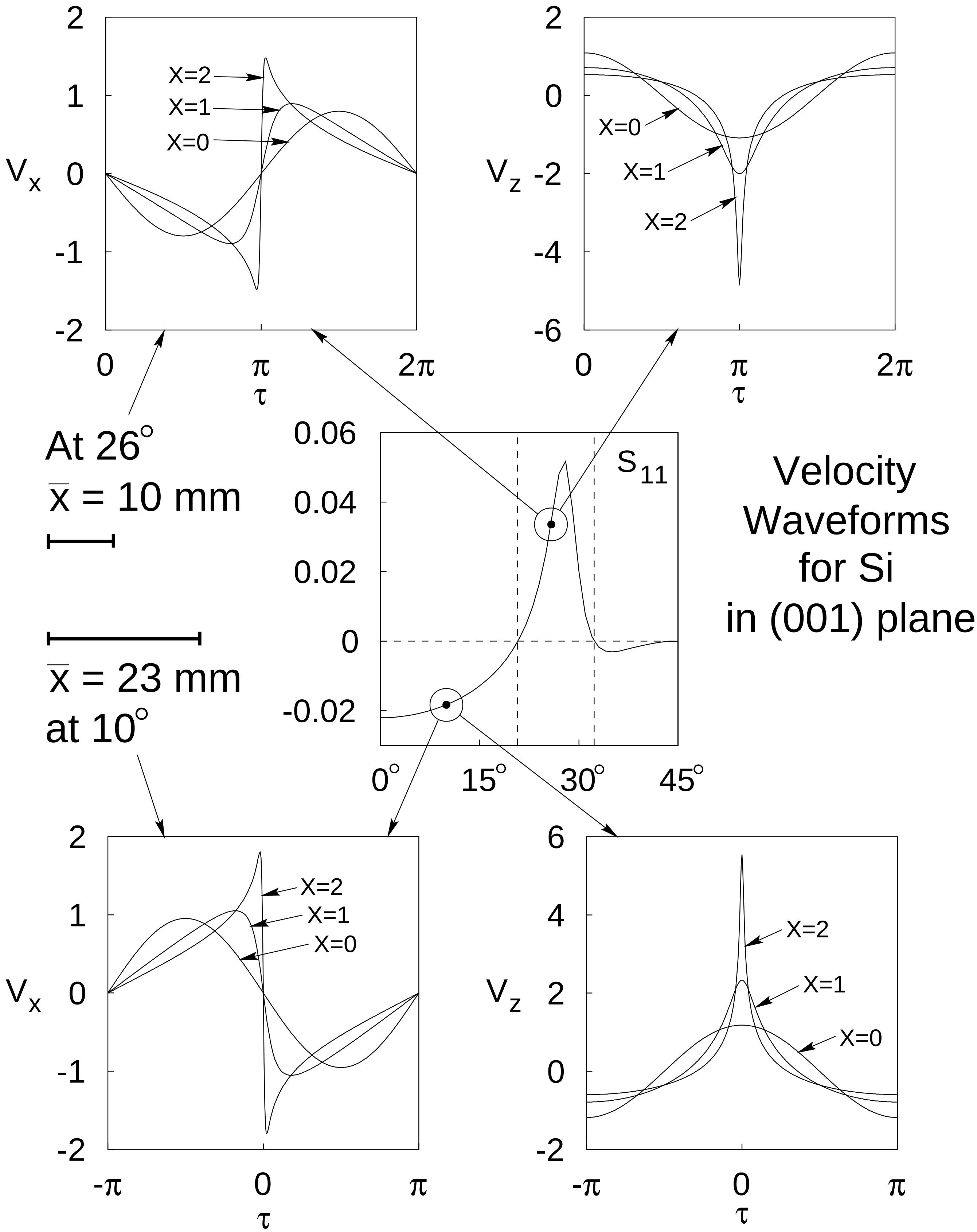
where $\epsilon_x = v_{x0}/c$, and $v_x = v_{x0}\sin\omega t$ at $x = 0$.

Example: $\omega/2\pi$ = 50 MHz
v_{x0} = 36 m/s ($\epsilon_x \approx$ 0.007)

Shock formation distance for Si on (001) plane:



SIMULATIONS WITH SINUSOIDS



CONCLUSION

Summary:

- Thorough theoretical study of nonlinear properties of SAWs in (001) plane of crystalline silicon.

Results:

- Nonlinearity matrix properties divide the waveform distortion into three 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"

- Wave propagation for $\theta \cong 21^\circ$ and $\theta \cong 32^\circ$ is linear even for finite amplitude SAW.

NONLINEARITY MATRIX & LINEAR THEORY

The nonlinearity matrix is given by

$$S_{n_1 n_2} = \sum_{s_1,s_2,s_3=1}^{3} \frac{\frac{1}{2} d'_{ijklmn} q_i^{(s_1)} q_k^{(s_2)} [q_m^{(s_3)}]^* l_j^{(s_1)} l_l^{(s_2)} [l_n^{(s_3)}]^*}{n_1 l_3^{(s_1)} + n_2 l_3^{(s_2)} - (n_1 + n_2)[l_3^{(s_3)}]^*}$$

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

$$d'_{ijklmn} = d_{ijklmn} + c_{ijln}\delta_{km} + c_{jnkl}\delta_{im} + c_{jlmn}\delta_{ik} \ .$$

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

Start with linearized wave equation

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

Next assume SAW solution of form

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

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

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

Solve Eq. (3) subject to the stress-free surface bound. cond.

$$\sigma_{i3} \, \big|_{x_3=0} = 0 \ . \tag{4}$$

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

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

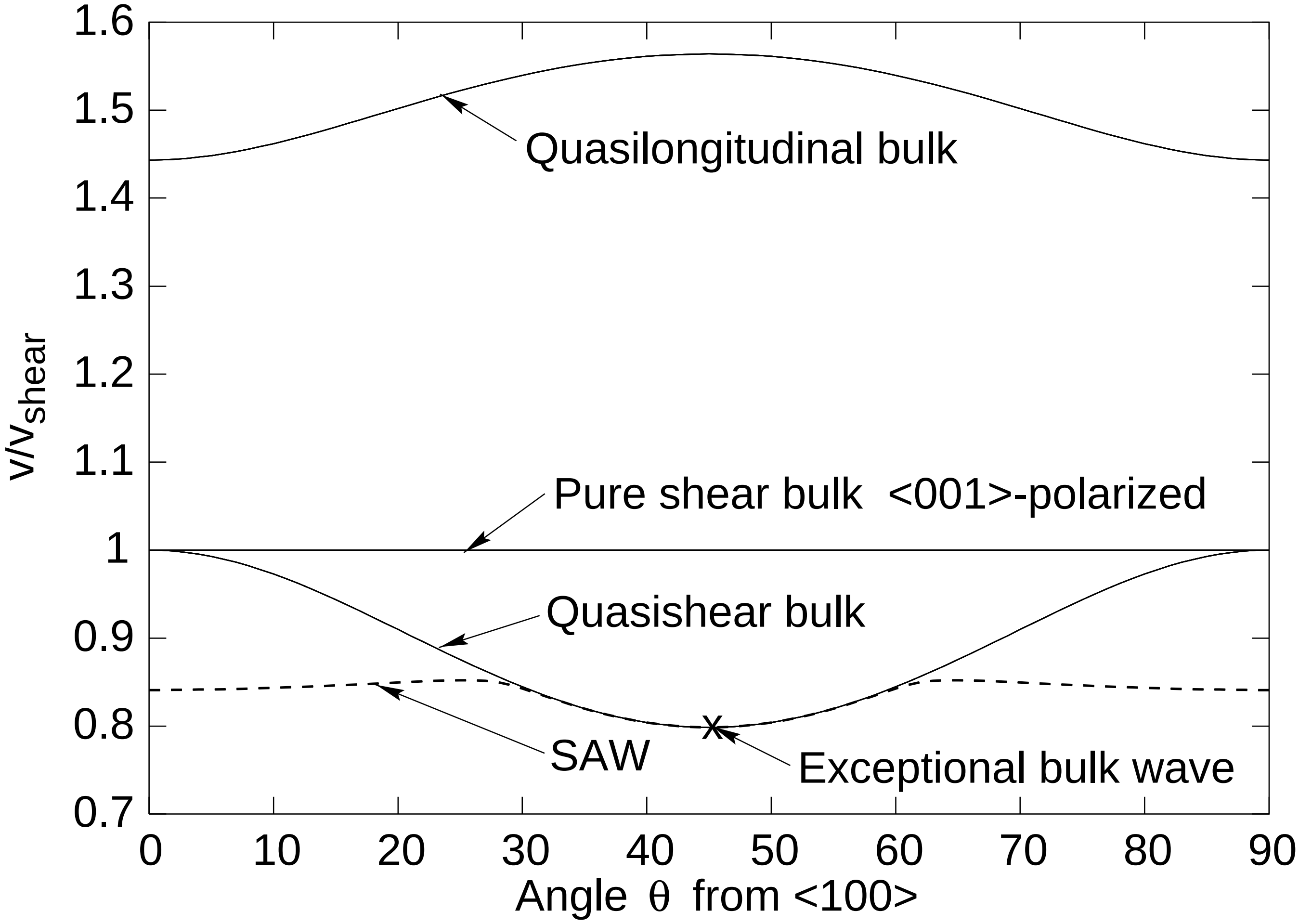
These equations can be solved numerically for $l_i^{(s)}$, $\alpha_i^{(s)}$, and C_s.

RESULTS FROM LINEAR THEORY

Description of acoustic modes for Si with SAW on (001) plane:

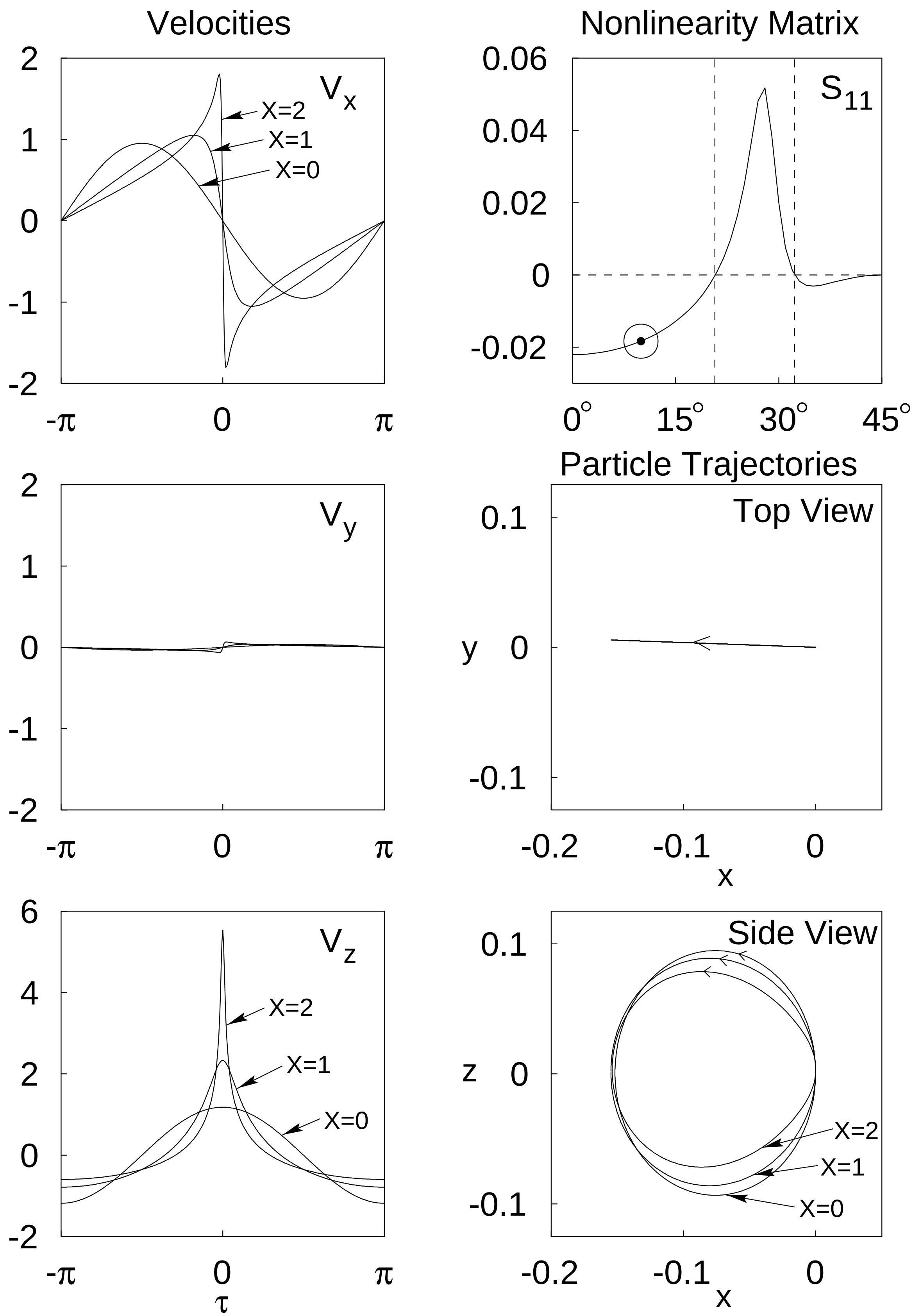
- Three bulk modes, one surface mode
- Surface mode $\rightarrow$ exceptional bulk shear wave as $\theta \rightarrow 45^\circ$
- Change in wave speeds is relatively small (5% to 20%) for $0^\circ < \theta < 45^\circ$

Relative velocity vs. angle for all modes:



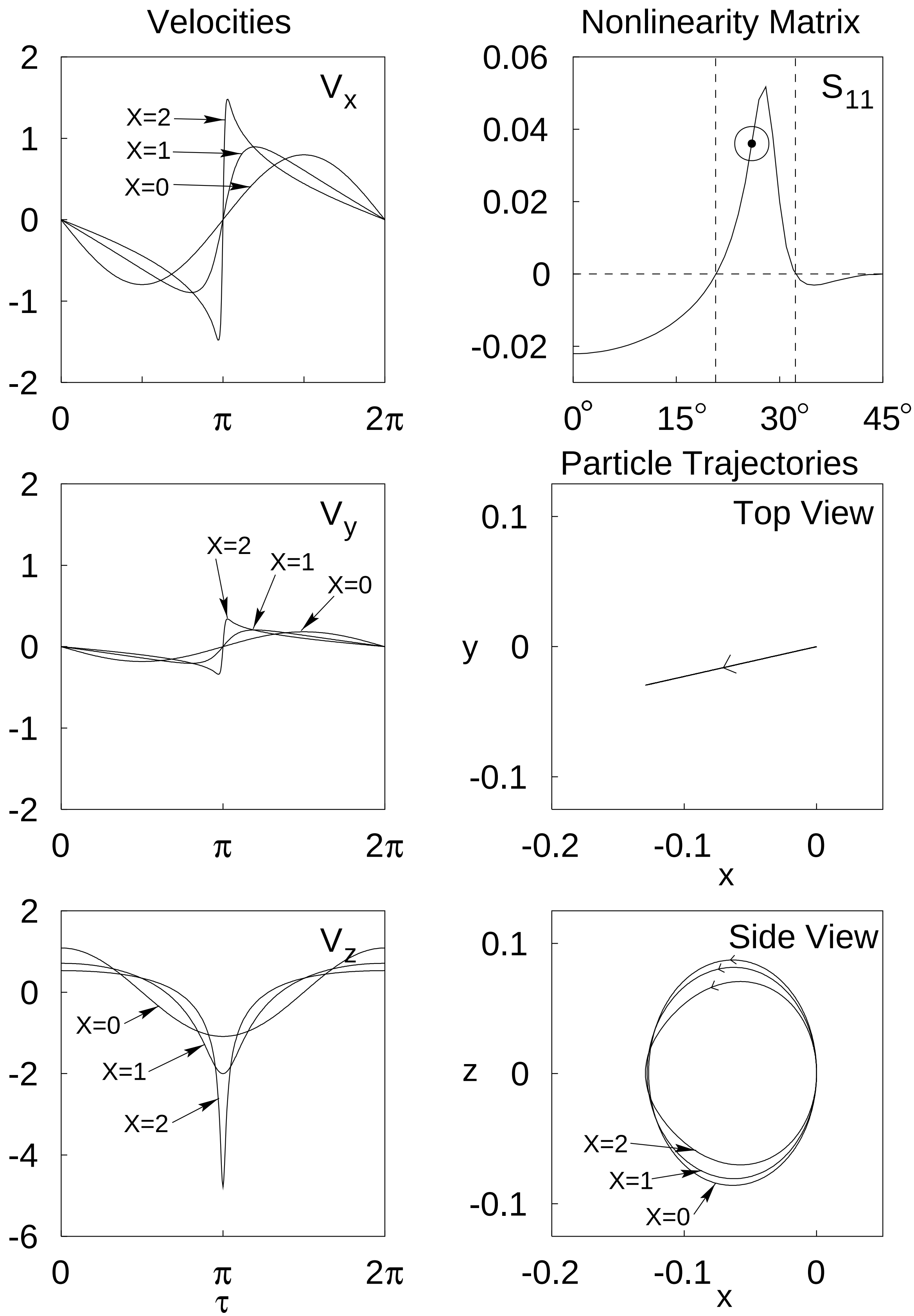
WAVEFORMS: REGION I

Waveform Distortion in direction 10° from <100>



WAVEFORMS: REGION II

Waveform Distortion in direction 26° from <100>



WAVEFORMS: REGION III