Nonlinear SAW Propagation in Thin-Film Systems with Residual Stress

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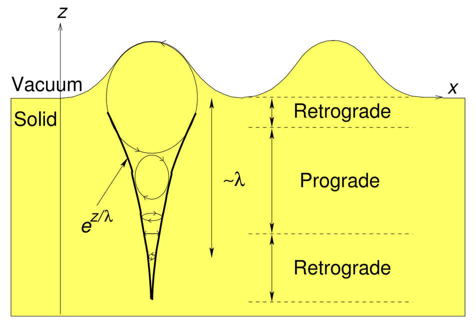
Introduction

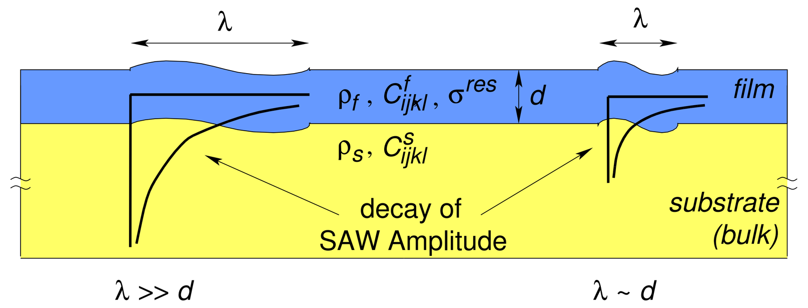
- Thin-film deposition processes can create large residual stresses which change the film's mechanical properties and therefore its performance in a product.
- Residual stress affects the SAW velocity dispersion through the acoustoelastic effect, but the changes are often very small.
- Finite-amplitude SAWs, which nonlinearly generate harmonics as they propagate, may be more sensitive to stress because the combined effects of nonlinearity and dispersion are cumulative with distance.
- Numerical results are presented which compare velocity dispersion, waveform distortion, and harmonic generation for monofrequency SAWs propagating in systems with unstressed and compressively stressed Ge films on a Si substrate.

Surface Acoustic Waves



- Surface acoustic waves are a type of vibrational wave which occur near the surface of a solid half-space.
- Almost all the energy of a SAW is localized within a wavelength λ of the surface, potentially resulting in large surface amplitudes and nonlinear effects.
- Questions:
  How do SAWs propagate in stressed thin films?
  How big are the linear and nonlinear effects?
  Can SAWs evaluate stress in thin films?

SAW Frequency Dispersion



- Without a film, SAWs are nondispersive, i.e., all frequency components travel at the same velocity.
- With a film of thickness d, the lower frequency components ($\lambda \gg d$) travel near the SAW velocity of the substrate, while the higher frequency components ($\lambda \le d$) travel near the SAW velocity of the film.
- Result of film on SAW:
  Various frequencies of the waveform disperse relative to one another.

Linear Theory

Wave equation for the thin film system:

$$C^{\text{eff}}_{ijkl}\frac{\partial^2 u_k}{\partial x_j \partial x_l} + \sigma^{\text{res}}\frac{\partial^2 u_i}{\partial x^2} = \rho^{\text{eff}}\frac{\partial^2 u_i}{\partial t^2},$$

$$\begin{aligned}
C^{\text{eff}}_{ijkl} &= C_{ijkl}(1-\Delta e^{\text{res}} + e^{\text{res}}_{ii} + e^{\text{res}}_{jj} + e^{\text{res}}_{kk} + e^{\text{res}}_{ll}) \\
&\quad + C_{ijklmn}e_{mn},\\
\rho^{\text{eff}} &= \rho(1-\Delta e^{\text{res}}),\\
\sigma^{\text{res}} &\rightarrow \text{equibiaxial residual stress},\\
u_i &\rightarrow \text{SAW displacement components } (i = x, y, z),\\
C_{ijkl(mn)} &\rightarrow \text{2nd and 3rd order elastic constants (unstressed)},\\
\rho &\rightarrow \text{density (unstressed)},\\
e^{\text{res}}_{jk} &\rightarrow \text{linear residual strain tensor},\\
\Delta e^{\text{res}} &\rightarrow \text{linear volume dilatation due to residual strain.}
\end{aligned}$$

- Assumptions include plane wave propagation and equibiaxial, homogeneous, static stress only in film.
- Equations are solved for the SAW velocity c by a Green's function technique to produce the dispersion relations.

Nonlinear Theory

Frequency domain evolution of a SAW velocity waveform is described by the coupled system:

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

$$\begin{aligned}
v_n(x) &\rightarrow n\text{th harmonic amplitude},\\
\gamma_n &= \alpha_n + i\delta_n,\\
\alpha_n &\rightarrow \text{attenuation coefficient of } v_n,\\
\delta_n &\rightarrow \text{dispersion coefficient of } v_n,\\
\omega &\rightarrow \text{fundamental angular frequency},\\
S_{lm} &\rightarrow \text{nonlinearity matrix.}
\end{aligned}$$

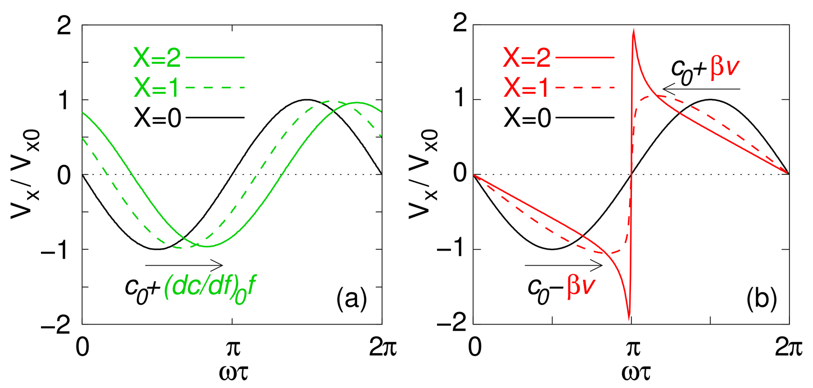
- Physically, S_{lm} describes coupling of the lth and mth harmonics to generate the $n = (l+m)$th harmonic.
- A coefficient of nonlinearity can be defined

$$\beta = 4S_{11}/\rho c^2,$$

which is interpreted physically below.

Dispersion and Nonlinearity

Consider the following snapshots of evolving waveforms in the retarded frame (moving at c_0):



- Figure (a): Dispersion, No Nonlinearity
  Waveforms experience a phase shift in the retarded frame because they have a different velocity $c(f)$ relative to c_0:

$$c(f) = c_0 + (dc/df)_0 f + \cdots.$$

- Figure (b): Nonlinearity, No Dispersion
  Parts of the waveforms move at different velocities $c(v)$ relative to c_0 depending on their local particle velocity amplitude:

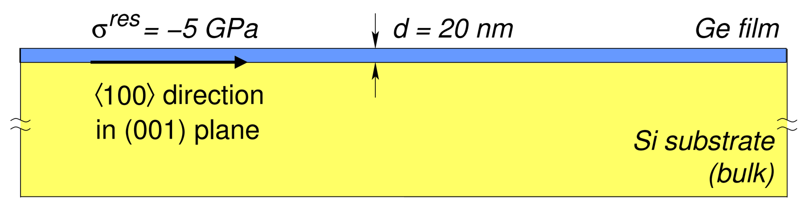
$$c(v) = c_0 + \beta v + \cdots.$$

- Relative contributions of dispersion to nonlinearity can be characterized by dimensionless parameter

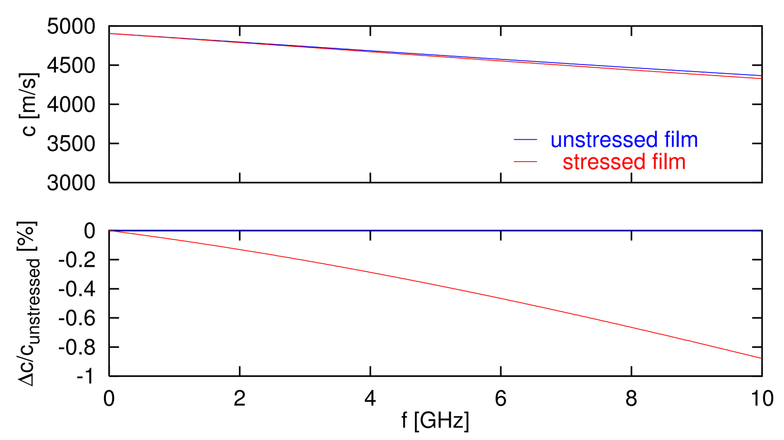
$$D = \frac{(dc/df)_0 f}{\beta v}.$$

- Assume monofrequency source with frequency $f = 30$ MHz and peak acoustic particle velocity $v = 50$ m/s (peak strain $\epsilon = 0.01$). With $\beta = -0.12$ for the chosen system, these values result in a characteristic length scale for nonlinear distortion of $x_0 = 20$ mm ($X = x/x_0$).
- Thin film assumptions:
  Film only causes dispersion of harmonics, film does not affect harmonic generation, and negligible stress exists in the substrate.

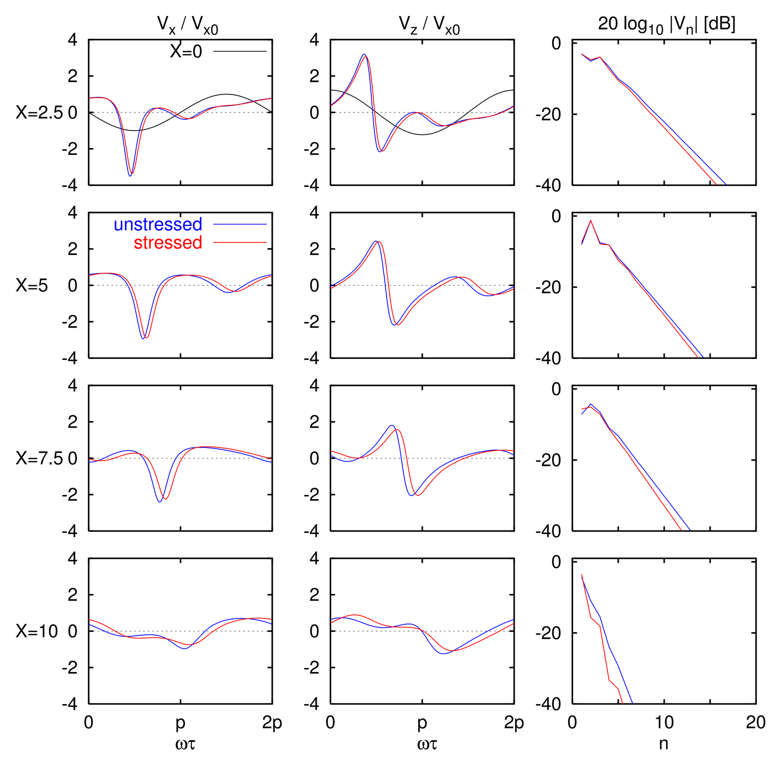
Moderate Dispersion ($D = 0.26$)



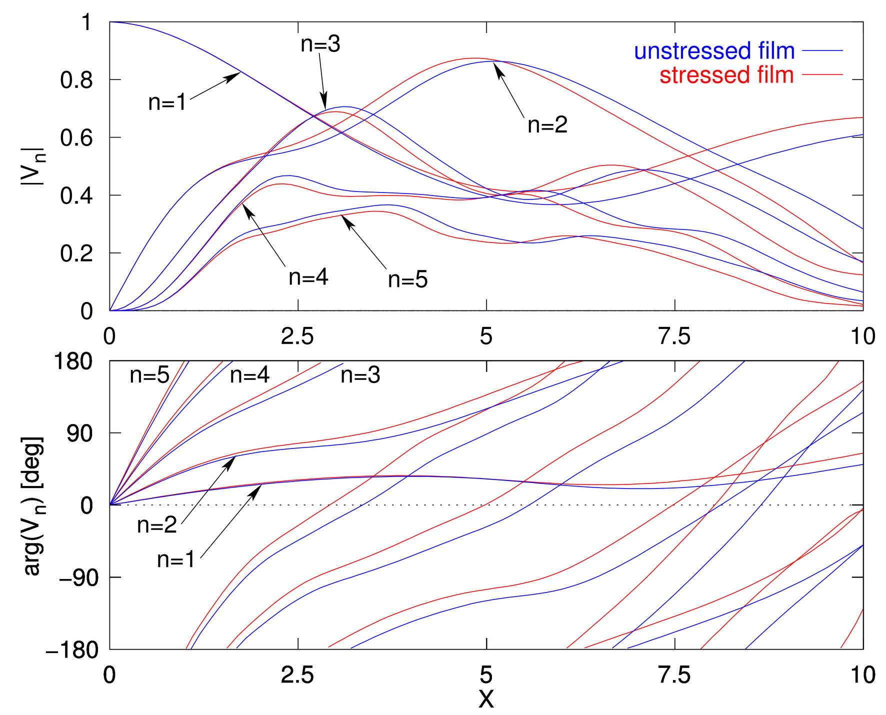
- Small SAW velocity shift: $|\Delta c/c| < 1\,\%$.
- $|D| < 1$ implies nonlinearity is dominant.



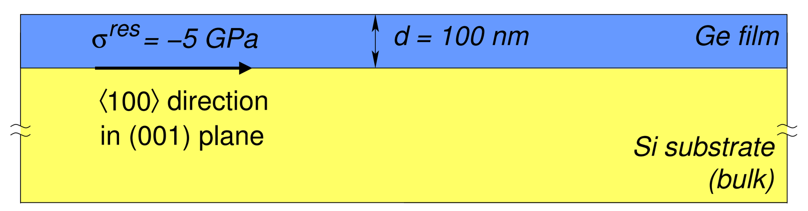
- Waveforms exhibit significant distortion and harmonic generation with some dispersion.



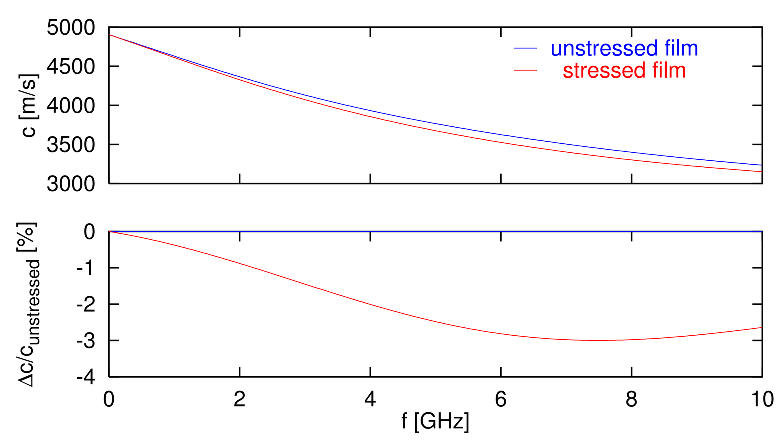
- Harmonic magnitudes and phases between the stressed and unstressed cases start to differ noticeably for $X > 1.5$.



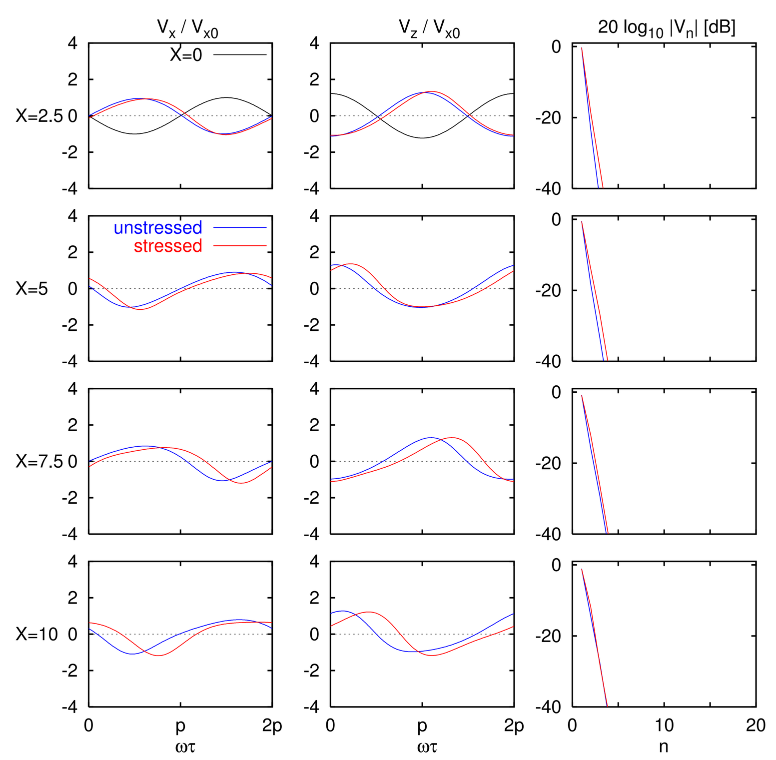
Strong Dispersion ($D = 1.30$)



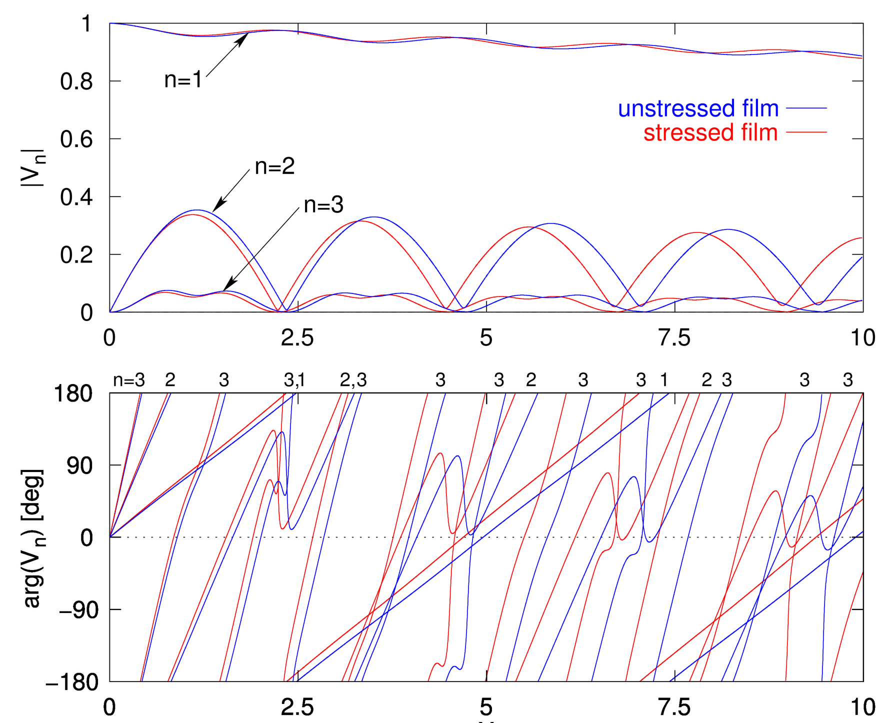
- Small SAW velocity shift: $|\Delta c/c| < 3\,\%$.
- $|D| > 1$ implies dispersion is dominant.



- Waveforms exhibit primarily dispersion (180° phase shifts for shown positions) with some distortion.

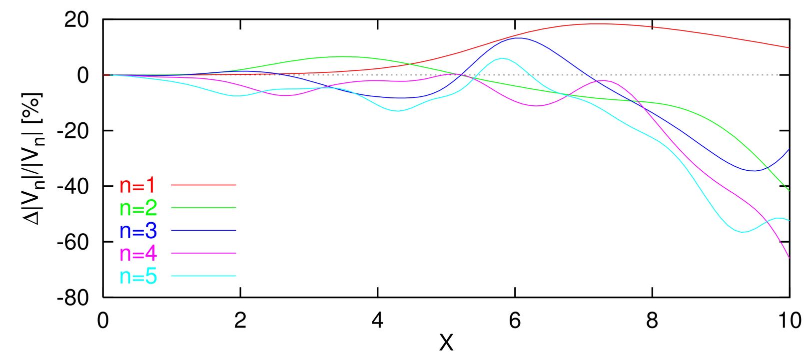


- Harmonic magnitudes exhibit growth and decay cycles, while the phases show much dispersion.

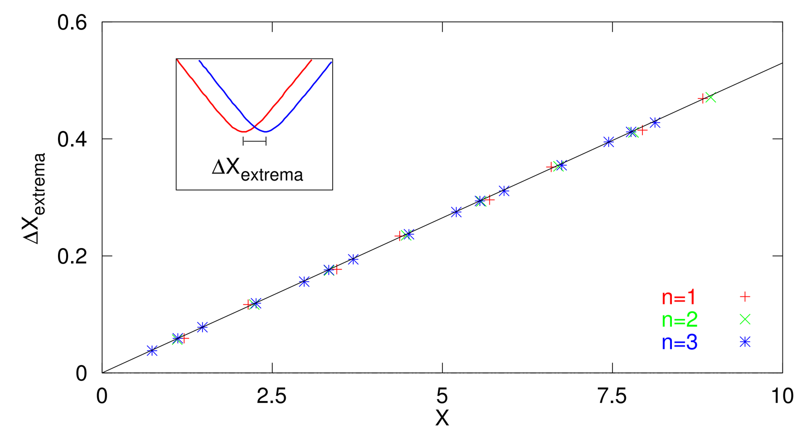


Conclusions

- Thin films cause dispersion (phase shifts) between frequency components of SAWs. With finite-amplitude SAWs, nonlinearly generated harmonics disperse relative to one another causing complicated evolution of waveforms and harmonics.
- Linear SAWs: Stress causes small changes in wave velocity (1 to 3 %).
- Nonlinear SAWs: Moderate dispersion
  Stress causes a shift in magnitudes and phases of the harmonics. Maximum effects occur at longer propagation distances and higher harmonics (20 to 60 %):



- Nonlinear SAWs: Strong dispersion
  Strong dispersion results in only limited harmonic generation but with spatial oscillations in magnitude. Stress causes extrema of the harmonic curves to shift around 5 % for every nonlinear length scale traversed:



Future Work

(1) Other film/substrate combinations, (2) Broadband sources, (3) Different cuts and directions, (4) Inversion for stress, (5) Effects of applied stress.

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