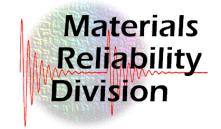
Nonlinear SAW Propagation in Thin-Film Systems with Residual Stress

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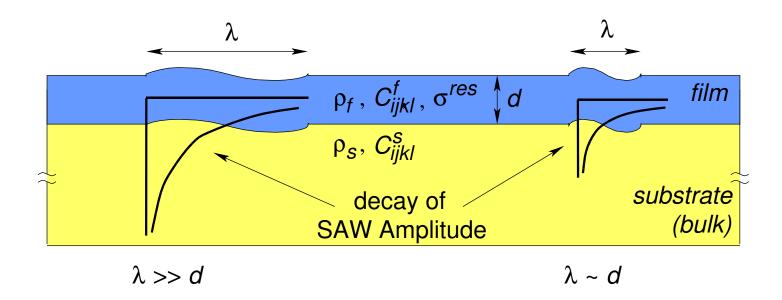




Introduction

- Thin-film deposition processes can create large residual stresses in the film which changes its 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.

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 $(\lambda \leq d)$ 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:

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

- 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 dispersion relations.

Nonlinear Theory

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

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

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

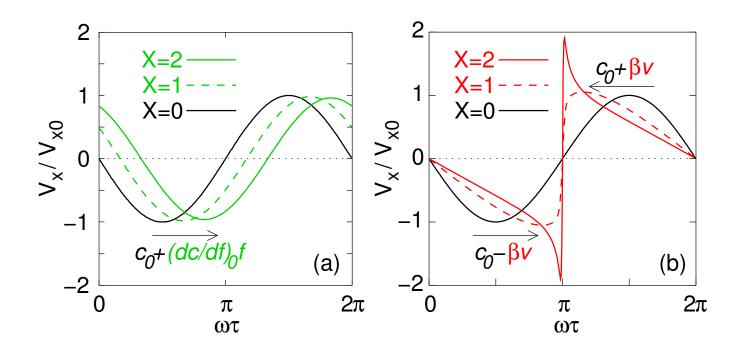
- Physically, S_{lm} describes coupling of the lth and mth harmonics to generate the n=(l+m)th harmonic.
- A coefficient of nonlinearity can be defined

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

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 v:

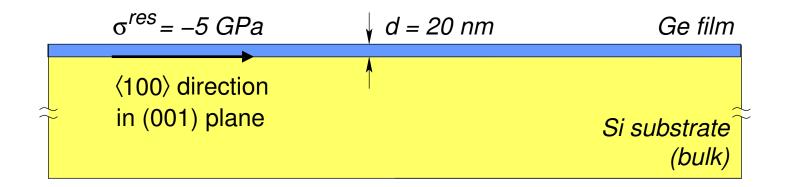
$$c(v) = c_0 + \beta v + \cdots.$$

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

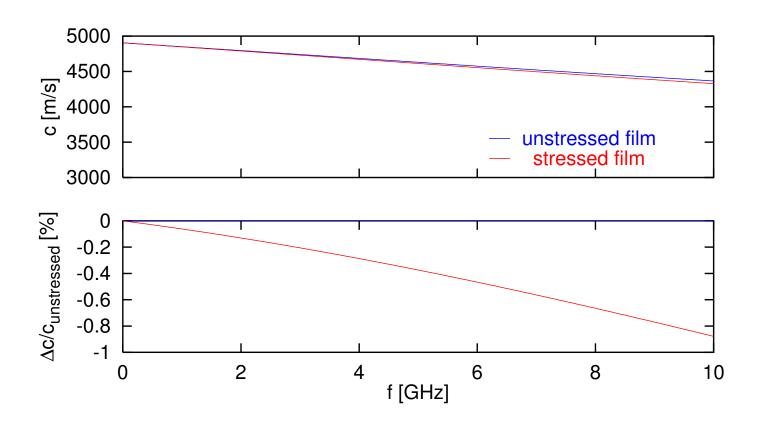
$$D = \frac{(dc/df)_0 f}{\beta v}.$$

- 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:
 - (1) Film only causes dispersion of harmonics.
 - (2) Film does not affect harmonic generation.
 - (3) Negligible stress exists in the substrate.

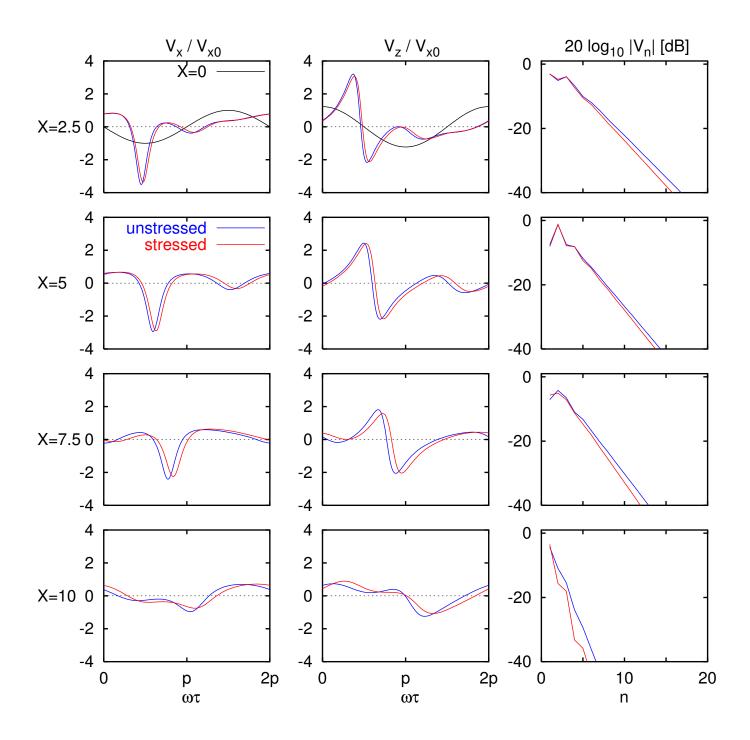
Moderate Dispersion (D = 0.26)



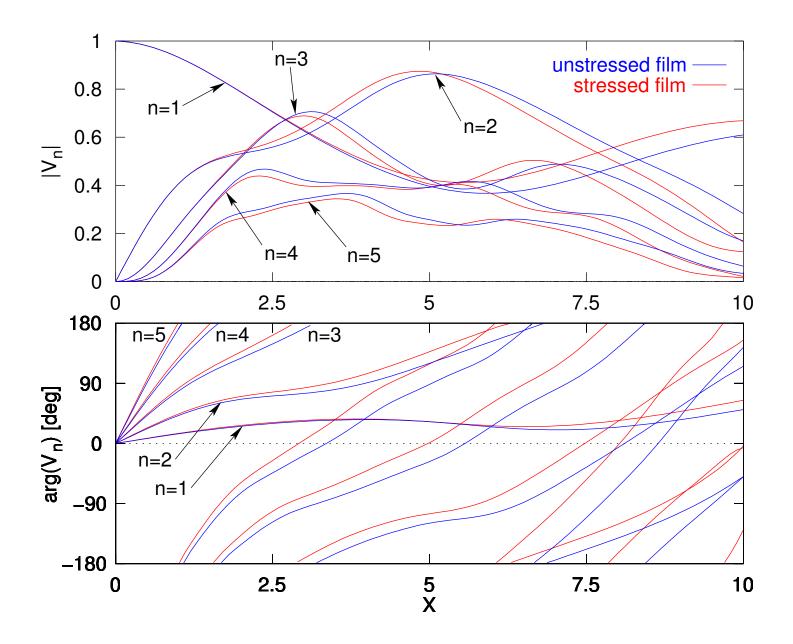
- Small SAW velocity shift: $|\Delta c/c| < 1\%$.
- |D| < 1 implies nonlinearity is dominant.



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



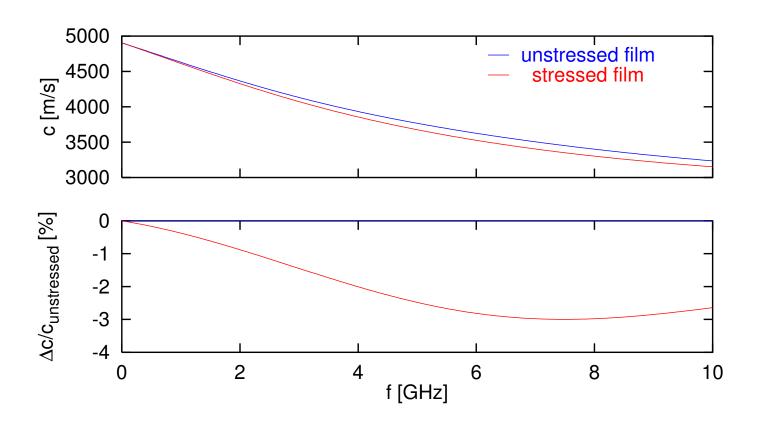
• Harmonic magnitudes and phases between the stressed and unstressed cases start to differ noticeably for X > 1.5.



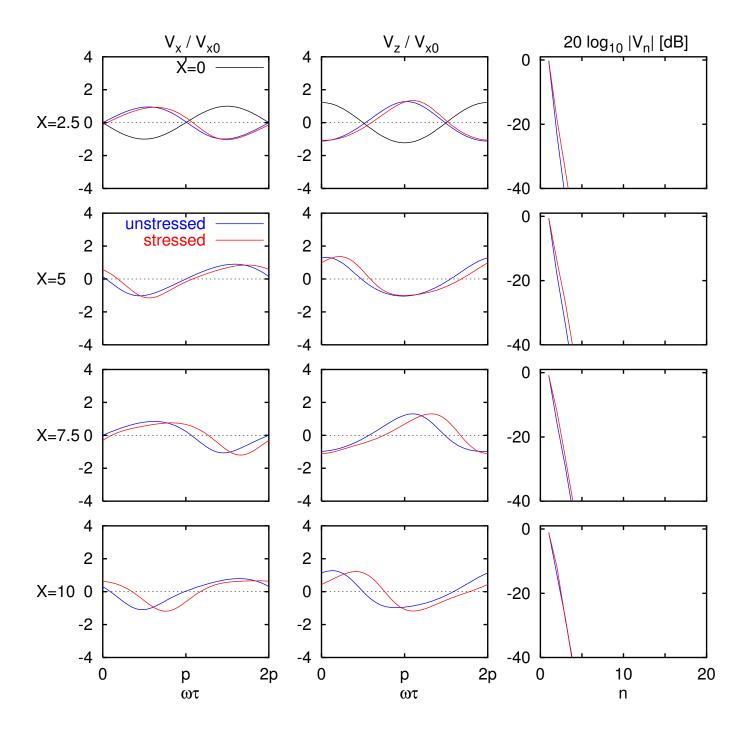
Strong Dispersion (D = 1.30)

$$\sigma^{res}$$
 = −5 GPa d = 100 nm Ge film $\langle 100 \rangle$ direction in (001) plane Si substrate $\langle bulk \rangle$

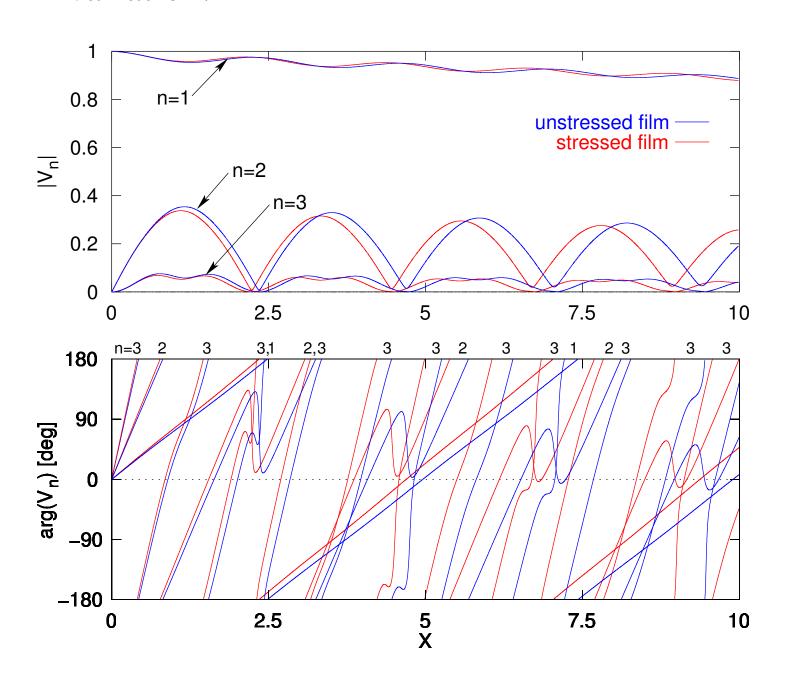
- Small SAW velocity shift: $|\Delta c/c| < 3\%$.
- |D| > 1 implies dispersion is dominant.



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

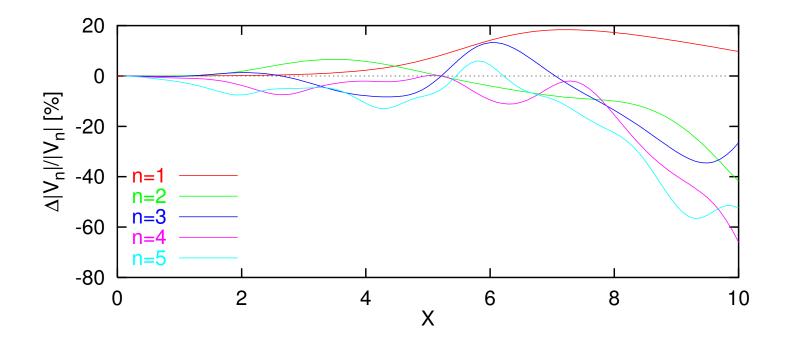


• Harmonic magnitudes exhibit growth and decay cycles, while the phases show much variation.

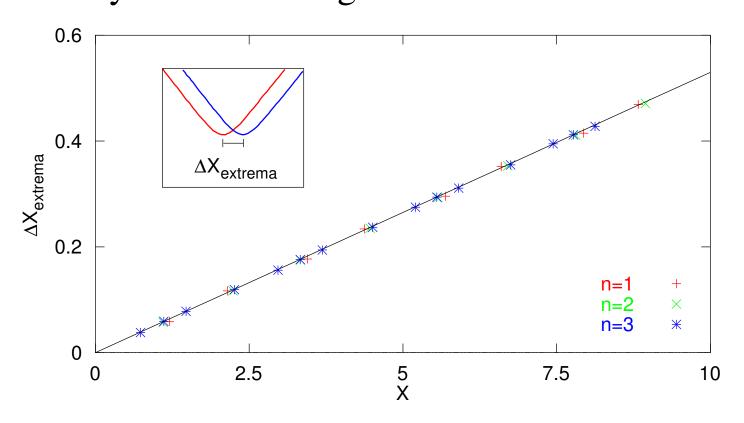


Conclusions

- Thin film causes harmonics to disperse relative to one another, resulting in 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.

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