ACOUSTOELASTIC EFFECT IN STRESSED ANISOTROPIC PLATES

Ching-Chung Yin, Shih-Ming Hsu, Yu-Ching Lee

Department of Mechanical Engineering, National Chiao Tung University, Taiwan, ROC

Abstract

This paper presents a forward calculation and analytic results of plate wave propagation in stressed plates of cubic materials. The single crystalline Ge films deposited on the Z-cut silicon wafers are investigated. Significant biaxial residual stresses in the film results from the lattice misfit between of the Ge film and the Si substrate. Phase velocity change of the acoustic waves due to mechanical stresses of the media is known as acoustoelastic (AE) effect. The calculated results indicate that the single Ge film has significant AE effect on the Lamb waves because of residual stresses induced in fabrication. The variations of phase velocity change are as small as only several m/s for the Lamb waves and even higher-order modes propagating in the Ge/Si layered system. It is still a challenge to identify the residual stresses in a thin-film heterostructure system using the measured phase velocity data of Lamb waves.

1. Introduction

Determination of residual stresses in manufacturing has been being received intensively attention by the industries of semiconductor, flat panel display, steel, etc. Most previous AE research interests focused on the third-order elastic constants and residual stresses in polycrystalline materials [1-3]. The values of residual stresses in single crystalline heterostructures can exceed the tensile strength of bulk materials due to the lattice misfit between the films on the substrate (Fig.1). The average residual stresses could be reduced as the film becomes thick or pseudomorphic $S_{i1-x}Ge_x$ layers are introduced between the film and the substrate [4].

The variations of bulk waves, surface acoustic waves and Love waves in a stressed Ge/Si system were evaluated by Osetrov et al [5]. Their calculated results show that the relative velocity changes at biaxial stresses of −0.2 GPa and −5 GPa are below ±10 m/s. Wave propagation in bulk piezoelectric material and lithium niobate plate under residual stress was numerically study by Lematre et al [6]. They concluded that it is possible to measure the applied stress at a small frequency-thickness product around 2 MHz-μm.

Acoustic wave propagation in an elastic solid under residual stresses is fundamentally a nonlinear problem. However, the ultrasonic disturbance is assumed to be small so that the Lagrangian description for the particle motion is preferable to the Eulerian. The formulation of acoustoelasticity becomes a linear problem. It is different from the nonlinear acoustic waves, which recently becomes more important in prediction of waveform distortion in the application of laser-induced ultrasound [7].

The AE formulation [1] incorporated with the global matrix method [8] is adapted in this paper. In contrast to surface acoustic waves studied in [5], calculation of the AE effect on Lamb modes in a single stressed thin-film and a multilayered heterostructure under biaxial residual stresses was carried out and investigated. The change of mass density, residual stress, and the modified elastic stiffness tensor by residual strains and third-order elastic constants are included in the formulation.

2. Formulation

The AE problems for acoustic wave propagation in a solid under residual stresses was formulated by Pao *et al* [1] *via* the frame of natural state, initial state, and final state (Fig.2). In the natural state the solid is free of stresses and strains. The pre-stressed state is statically equilibrium in the initial state. The ultrasonic wave motion $u_i(x_j)$ superposed onto the initial state changes the initial state to the final state. The equation of motion observed in the initial state is

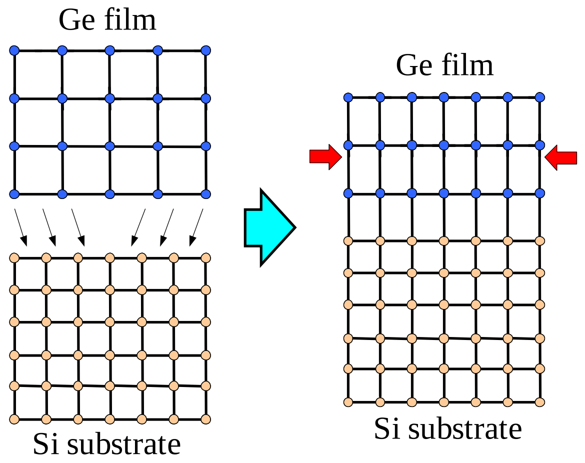

Fig. 1 Schematic of lattice misfit for Ge films deposited onto Si substrate

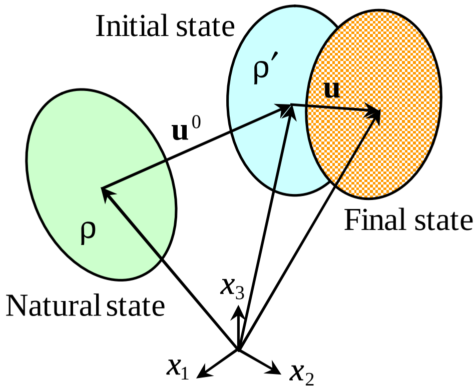

Fig. 2 The displacements and coordinates at the natural, initial, and final states

$$\frac{\partial}{\partial x_j}\left[\sigma_{ij}+\sigma^0_{ij}\frac{\partial u_i}{\partial x_k}\right]=\rho'\frac{\partial^2 u_i}{\partial t^2} \quad (1)$$

where the mass density of the strained solid is $\rho' \approx \rho_0(1-\varepsilon^0_{kk})$, ρ_0 is the density of the unstressed solid, ε^0_{kk} is the ratio of volume change from the natural state to the initial state. Assume the solid is hyperelastic. Because of symmetry of material the dynamic stresses σ_{ij} in (1) it follows the stress-train relations in the initial state of the form

$$\sigma_{ij}=C_{ijkl}\frac{\partial u_k}{\partial x_l} \quad (2)$$

where C_{ijkl} are the modified second-order elastic (SOE) stiffness combined the second-order elastic constants c_{ijkl} and the third-order elastic (TOE) constants c_{ijklmn} in the form of

$$C_{ijkl}=c_{ijkl}(1-\varepsilon^0_{mm})+c_{ijklmn}\varepsilon^0_{mn} + c_{mjkl}\frac{\partial u^0_i}{\partial x_m}+c_{imkl}\frac{\partial u^0_j}{\partial x_m} + c_{ijml}\frac{\partial u^0_k}{\partial x_m}+c_{ijkm}\frac{\partial u^0_l}{\partial x_m} \quad (3)$$

where u^0_i is the static displacement from the natural state to the initial state, and its spatial derivatives are $\varepsilon^0_{mn}=\partial u^0_m/\partial x_n$. As an example, the cubic materials [2-3] have 3 non-zero SOE constants, c_{11}, c_{12}, c_{44} and 6 TOE constants, c_{111}, c_{112}, c_{123}, c_{144}, c_{166}, c_{456} if the referred Cartesian coordinate axes identical to the principal axes of materials.

Referring to a Cartesian coordinate system in Fig. 3, the displacement components of plane wave solution are assumed to be of the form

$$u_i=U_i(x_3)\exp[i(\mathbf{k}\cdot\mathbf{x}-\omega t)] \quad (4)$$

where the wave vector is $\mathbf{k}=k_1\mathbf{e}_1+k_2\mathbf{e}_2+\omega\eta\mathbf{e}_3$, and position vector $\mathbf{x}=x_1\mathbf{e}_1+x_2\mathbf{e}_2+x_3\mathbf{e}_3$. The wave vector can be expressed in terms of wave normal $\mathbf{n}$ and wave number $k=\omega/c$ of the form $\mathbf{k}=\mathbf{n}\omega/c=\omega(s_1\mathbf{e}_1+s_2\mathbf{e}_2+\eta\mathbf{e}_3)$, where s_1, s_2, η are the slowness components. Introducing the plane wave solution into the equation of motion (1) yields an eigenvalue problem with eigenvalues η_k $(k=1,2,3)$ in the form of

$$[\Gamma_{ik}-\rho'\delta_{ik}]U_j=0 \quad (5)$$

For the single crystalline heterostrucure made of cubic materials, the lattice misfit induced stresses are assumed to be biaxial such that $\sigma^0_{11}=\sigma^0_{22}\neq 0, \sigma^0_{12}=0$. In addition, the principal axes of materials are identical to those of unstressed state. The modified Christoffel tensor components are $\Gamma_{ik}=(C_{ijkl}+\sigma^0_{jl})n_j n_l$, which can be expressed as

$$\begin{aligned}
\Gamma_{11}&=(C_{11}+\sigma^0_{11})s_1^2+(C_{66}+\sigma^0_{22})s_2^2+C_{55}\eta^2\\
\Gamma_{22}&=(C_{66}+\sigma^0_{11})s_1^2+(C_{22}+\sigma^0_{22})s_2^2+C_{44}\eta^2\\
\Gamma_{33}&=(C_{55}+\sigma^0_{11})s_1^2+(C_{44}+\sigma^0_{22})s_2^2+C_{33}\eta^2 \quad (6)\\
\Gamma_{12}&=(C_{12}+C_{66})s_1 s_2\\
\Gamma_{13}&=(C_{13}+C_{55})s_1\eta\\
\Gamma_{23}&=(C_{23}+C_{44})s_2\eta
\end{aligned}$$

where C_{ij} are the modified second-order elastic constants expressed in Voigt notations. The eigenvalues η^2 satisfy a cubic equation and the

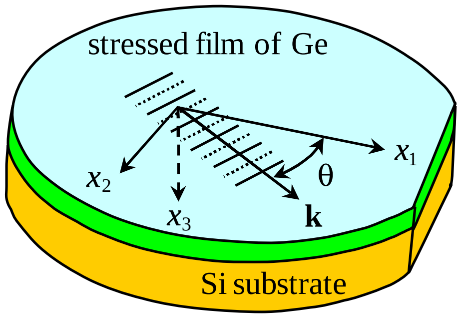

Fig. 3 Lamb wave propagation in a Si/Ge heterostructure

three roots η_i ($i = 1, 2, 3$) might be real or complex. For the single value definiteness they are selected as $\mathrm{Im}(\eta_i) \geq 0$.

The displacement components of the ultrasonic waves and the stress components acting on the x_3 plane in the m-th layer ($z_{m-1} \leq x_3 \leq z_m$) are of the form

$$\mathbf{S} = \begin{Bmatrix} \mathbf{u} \\ \mathbf{t} \end{Bmatrix} = \begin{bmatrix} \mathbf{P}_m^+ & \mathbf{P}_m^- \\ \mathbf{Q}_m^+ & \mathbf{Q}_m^- \end{bmatrix} \begin{bmatrix} \mathbf{E}_m^+ & \mathbf{0} \\ \mathbf{0} & \mathbf{E}_m^- \end{bmatrix} \cdot \begin{Bmatrix} \mathbf{A}_m^+ \\ \mathbf{A}_m^- \end{Bmatrix} \exp[\,i(k_1 x_1 + k_2 x_2 - \omega t)] \quad (7)$$

where

$$\mathbf{P}_m^+ = -\mathbf{P}_m^- = \begin{bmatrix} p_{11} & p_{12} & p_{13} \\ p_{21} & p_{22} & p_{23} \\ p_{31} & p_{32} & p_{33} \end{bmatrix} \quad (8)$$

$$\mathbf{E}_m^+ = diag\left\{ e^{i\eta_1(x_3 - z_{m-1})} \; e^{i\eta_2(x_3 - z_{m-1})} \; e^{i\eta_3(x_3 - z_{m-1})} \right\} \quad (9a)$$

$$\mathbf{E}_m^- = diag\left\{ e^{i\eta_1(z_m - x_3)} \; e^{i\eta_2(z_m - x_3)} \; e^{i\eta_3(z_m - x_3)} \right\} \quad (9b)$$

The state vector **S** composes of the displacement vector **u** and the traction vector **t** acting on the x_3-plane. The elements p_{ij} are the proportional constants of the eigenvectors. The elements in $\mathbf{Q}_m^{\pm}$ are the stress components $\sigma_{13}, \sigma_{23}, \sigma_{33}$ corresponding to the propagators $e^{i\eta_j(x_3 - z_{m-1})}$ and $e^{i\eta_j(z_m - x_3)}$. The superscript "+" denotes the down-going waves and "–" the up-going waves.

The state vector **S** is continuous across the interfaces between the layers. The associated boundary condition becomes

$$\begin{bmatrix} \mathbf{P}_m^+ & \mathbf{P}_m^- \\ \mathbf{Q}_m^+ & \mathbf{Q}_m^- \end{bmatrix} \begin{bmatrix} \mathbf{E}_m & \mathbf{0} \\ \mathbf{0} & \mathbf{I} \end{bmatrix} \begin{Bmatrix} \mathbf{A}_m^+ \\ \mathbf{A}_m^- \end{Bmatrix} = \begin{bmatrix} \mathbf{P}_{m+1}^+ & \mathbf{P}_{m+1}^- \\ \mathbf{Q}_{m+1}^+ & \mathbf{Q}_{m+1}^- \end{bmatrix} \begin{bmatrix} \mathbf{I} & \mathbf{0} \\ \mathbf{0} & \mathbf{E}_{m+1} \end{bmatrix} \begin{Bmatrix} \mathbf{A}_{m+1}^+ \\ \mathbf{A}_{m+1}^- \end{Bmatrix} \quad (10)$$

where the matrix

$$\mathbf{E}_m = diag\{ e^{i\eta_1(m)h_m}, e^{i\eta_2(m)h_m}, e^{i\eta_3(m)h_m} \} \quad (11)$$

and h_m is the thickness in the m-th layer.

The boundary values of the state vector **S** on the top surface of the first layer and the bottom surface of the N-th layer are

$$\begin{bmatrix} \mathbf{Q}_1^+ & \mathbf{Q}_1^- \mathbf{E}_1 \end{bmatrix} \begin{Bmatrix} \mathbf{A}_1^+ \\ \mathbf{A}_1^- \end{Bmatrix} = 0 \quad (12)$$

$$\begin{bmatrix} \mathbf{Q}_N^+ \mathbf{E}_N & \mathbf{Q}_N^- \end{bmatrix} \begin{Bmatrix} \mathbf{A}_N^+ \\ \mathbf{A}_N^- \end{Bmatrix} = 0 \quad (13)$$

respectively. As an example, the combination of (10) and (12-13) for a 2 layered system yields a system equations of the form

$$\begin{bmatrix} \mathbf{Q}_1^+ & \mathbf{Q}_1^- \mathbf{E}_1 & \mathbf{0} & \mathbf{0} \\ \mathbf{P}_1^+ \mathbf{E}_1 & \mathbf{P}_1^- & -\mathbf{P}_2^+ & -\mathbf{P}_2^- \mathbf{E}_2 \\ \mathbf{Q}_1^+ \mathbf{E}_1 & \mathbf{Q}_1^- & -\mathbf{Q}_2^+ & -\mathbf{Q}_2^- \mathbf{E}_2 \\ \mathbf{0} & \mathbf{0} & \mathbf{Q}_2^+ \mathbf{E}_2 & \mathbf{Q}_2^- \end{bmatrix} \begin{Bmatrix} \mathbf{A}_1^+ \\ \mathbf{A}_1^- \\ \mathbf{A}_2^+ \\ \mathbf{A}_2^- \end{Bmatrix} = 0 \quad (14)$$

The zero determinant of the matrix in (14) leads to the dispersion equation for Lamb wave traveling in a layered heterostructure system.

2. Numerical Results and Discussion

The material properties of Ge film and Si substrate are listed in Table 1. The lattice constants of Ge and Si are 5.658 Å and 5.431 Å, respectively. Once upon the Ge film was deposited on the Si substrate, the lattices of Ge are compressed by the in-plane biaxial stresses such that the lattices of film and substrate have the same length. The strain components in Ge film become $\varepsilon_{11}^0 = \varepsilon_{22}^0 = (5.431 - 5.658)/5.658 = -0.0401$, $\varepsilon_{33}^0 = -\nu\,\varepsilon_{11}^0$, where the Poisson's ratio $\nu = 2c_{12}/c_{11} = 0.7494$. If the Ge film is very thin, then the biaxial residual stresses in the film are $\sigma_{11}^0 = \sigma_{22}^0 = (c_{11} + c_{12} - 2c_{12}^2/c_{11})\,\varepsilon_{11}^0 = -5.654\,\mathrm{GPa}$. The value of the residual stresses in the single crystalline Ge film and Si substrate are much higher than ordinary cases of polycrystalline metals.

Table 1 2nd-order and 3rd-order elastic constants (GPa) and mass density (kg/m^3) of Silicon and Germanium [2, 9]

Silicon (Si) density &		Germanium (Ge) density &		TOE	
				c_{111}	-710
ρ	2332	ρ	5322	c_{112}	-389
c_{11}	165.7	c_{11}	128.9	c_{123}	-18
c_{12}	63.9	c_{12}	48.3	c_{144}	-23
c_{44}	79.56	c_{44}	67.1	c_{166}	-292
				c_{456}	-53

Fig. 4 depicts the dispersion curves of the Lamb wave propagation along the [100] axis in a 1 μm Ge/500 μm Si wafer. Two cases were calculated. The first case ignores the lattice misfit between Ge film and Si substrate and the residual stresses. Both materials are assumed to be bonded perfectly. In the second case, the Ge film is assumed to be a single layer under homogeneous biaxial stresses of −5 GPa and deposited on the Si substrate.

Since the Ge film is much thinner than the Si substrate, we assume that the residual stresses only appear in the Ge film. The TOE constants and the compression due to lattice misfit are considered only in the Ge film so that the elastic stiffness constants are modified in the thin-film using (3). Material constants in the substrate are still the same. The velocity changes of the Lamb waves are below ±5 m/s for both cases in a broad frequency range form 0 to 20 MHz. The result indicates the AE effect on the Lamb modes of a multilayered heterostructure is too small to determine the residual stressed in the thin-film.

Another structure of the stressed thin-film system shown as Fig. 5 was considered to get rid of the influence of thicker substrate on the AE effect in the stressed thin-film. The Si substrate is partially etched from the bottom so that the thin-film is suspended as a single plate fixed by the remaining substrate. No change appears in the stressed state of the film. Fig. 6 shows the phase velocities of Lamb modes propagating along the [100] axis in a single Ge film. In contrast to previous results in Fig. 5, the AE effect is significant for stressed film according to the comparison between the dispersion curves calculated for the Ge film under biaxial stresses of −1 GPa and those of stress-free state.

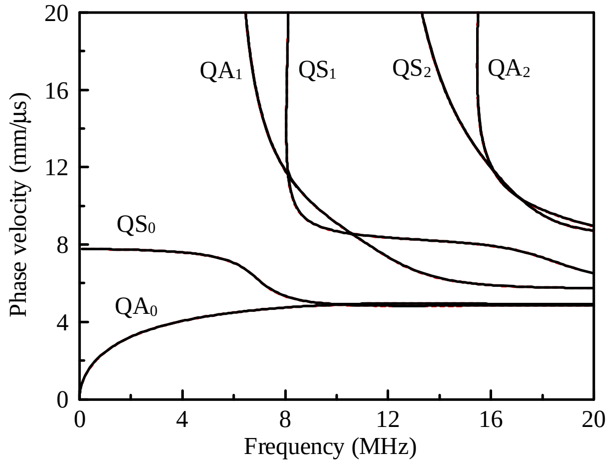

Fig. 4 Dispersion curves of Lamb wave propagation along the [100] axis in a 1 μm Ge/500 μm Si wafer. Dashed lines are calculated for the Ge film under biaxial stresses of −5 GPa. Solid lines are for stress-free Ge film and almost identical to the dashed lines.

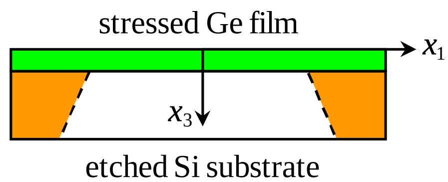

Fig. 5 Lamb wave propagation in the Ge film

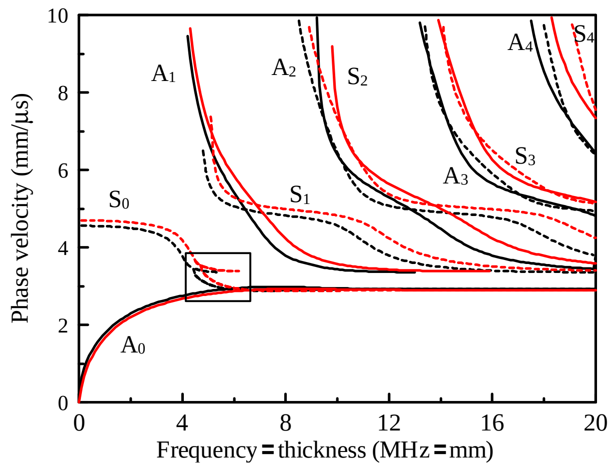

Fig. 6 Phase velocities of Lamb wave propagation along the [100] axis in a 1 μm Ge film. Black lines are calculated results for the Ge film free of stresses. Red lines are those for Ge film under biaxial stress of −1 GPa.

4. Conclusion

A matrix method incorporated with the acoustoelasticity formulation and the global matrix method is used to calculate the AE effect on Lamb wave propagation in a single stressed thin-film and a multilayered heterostructure under biaxial residual stresses. The change of mass density, residual stress, and the modified elastic stiffness tensor by residual strains and third-order elastic constants are considered.

The lattice misfit between Ge film and Si substrate induces significant biaxial stresses in the Ge film. The stress value can exceed the tensile strength of bulk materials. The AE effect on phase velocities of Lamb waves becomes significant for the single Ge film on an etched Si substrate. However, the relative velocity changes on phase velocities of Lamb waves in stressed Ge/Si layered heterostructures are within only several m/s. The AE effect on Lamb modes decreases since the Ge film is comparatively thinner than the Si substrate. The calculated results evident Lamb modes and even higher-order modes in Ge/Si layered heterostructure cannot provide as a sensitive technology to distinguish the influence of residual stresses in a thin film. Further investigation will be needed for understanding the azimuthal dependence of the relative phase velocity changes on Lamb waves in multilayered stressed systems.

5. Acknowledgement

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6. References

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