Acoustoelastic anomaly in stressed heterostructures

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We investigated the influence of biaxial stress on the acoustic wave propagation in single crystalline heterostructures using a transfer matrix method. Both Rayleigh-type and Sezawa modes exhibit an acoustoelastic anomaly, where the stress induced change of the phase velocity is maximum for a film thickness which is considerably smaller than the acoustic wavelength. For Ge/Si(001) compressed by 1 GPa the velocity shift of Sezawa modes reaches exceptionally high values of about 2%.

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Ultrasonic waves are unique for non-destructive testig of materials. More recently ultrasonic waves have also been employed to measure the elastic properties of polycrystalline and epitaxial thin films. Such measurements are particularly important for heterostructures as the elastic constants play a key role for the understanding of the interdependence of stress and strain with impact for electronic and optoelectronic devices. So far it is not clear whether the elastic constants of thin films deviate from from bulk values. Moreover, an increasing number of technologically interesting materials, such as cubic GaN or AlAs, are stable only in the thin film configuration and therefore require thin film measurements. For thin film investigations the high sensitivity of surface acoustic waves (SAWs) is utilized, which have the vibration energy localized close to the surface, typically within a depth of few wavelengths only. In the presence of a thin film SAWs become dispersive. Moreover, at certain material parameters and film thicknesses new surface guided modes, e.g. Love or Sezawa modes, can arise. Hence, a variety of different acoustic resonances are available to derive the elastic properties of thin films.

It is well known that the phase velocity of acoustic waves is influenced by stress, a phenomenon called AE (acoustoelastic) effect. Usually the relative change of the wave velocity is very small, e.g. $\simeq 10^{-5}$/MPa for aluminum. Hence, stresses as high as 100 MPa typically applied in bulk experiments alter the phase velocity of the acoustic waves only by about 0.1%. In heteroepitaxial thin films, however, due to the misfit between film and substrate the residual stress can easily exceed the 1 GPa limit thus giving rise to phase velocity changes, which no longer are negligible.

For the stress dependence it is widely accepted that maximum change of phase velocity appears when the wave is completely localized within the stressed material. Consequently the wavelength of SAWs in layered structures has to be much smaller than the layer thickness. In contrast to this presumption we recently found that the AE effect in stressed layered system assumes significant values for surface modes with penetration depths considerably larger than the film thickness. Here we report on an anomaly, where the AE effect reaches its maximum value already at film thicknesses considerably smaller than the ultrasonic wavelength. For Rayleigh-type waves we find that the maximum velocity change occurs when the wave is not yet completely localized within the film. The maximum velocity changes being even significantly higher for Sezawa modes.

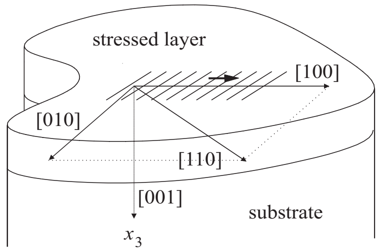

FIG. 1: Sketch of the SAW propagation geometry in a layered system. The $x_3 = 0$ plane is the interface between the layer and the substrate.

The calculations are based on the prototype geometry shown in Fig.1. A stressed layer is deposited onto a substrate. The $x_3 = 0$ plane is the interface between the layer and the substrate while the plane $x_3 = -h$ is the free surface. In the following expressions ξ_i, u_{ij} and σ_{ij} represent the particle displacement, the strain, and the stress, respectively. The notation without superscript describes the acoustic variables and with subscript (0) the residual (static) ones. For the residual stresses we assume the biaxial model $\sigma_{11}^{(0)} = \sigma_{22}^{(0)} = \sigma^{(0)}$, $\sigma_{ij}^{(0)} = 0$, for $i \neq j$. The residual strains are estimated by Hooke's law. Hence, the system contains only the axial strain components $u_{11}^{(0)} = u_{22}^{(0)} \neq 0$, $u_{33}^{(0)} \neq 0$. Then the wave propagation in the system can be described by equation of motion

$$\frac{\partial \sigma_{ij}}{\partial x_j} + \sigma^{(0)} \frac{\partial^2 \xi_i}{\partial x_1^2} = \rho^{new} \frac{\partial^2 \xi_i}{\partial t^2}, \tag{1}$$

where the density

$$\rho^{new} \approx \rho \; (1 - \Delta u^{(0)}), \;\; \Delta u^{(0)} = u_{11}^{(0)} + u_{22}^{(0)} + u_{33}^{(0)} \tag{2}$$

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is modified by the static strain. The wave propagates in the x_1 direction. Furthermore, Hooke's law can be written as $\sigma_{ij} = C_{ijkl}\,(\partial\xi_k/\partial x_l)$ with C_{ijkl} being the modified stiffness modul

$$\begin{aligned} C_{ijkl} &= c_{ijkl}(1 + u_{ii}^{(0)} + u_{jj}^{(0)} + u_{kk}^{(0)} + u_{ll}^{(0)} \\ &- u_{11}^{(0)} - u_{22}^{(0)} - u_{33}^{(0)}) + c_{ijklmn}u_{mn}^{(0)}, \qquad (3) \end{aligned}$$

where c_{ijkl} and c_{ijklmn} are the second and third order stiffness tensor, respectively.

Equations (1)–(3) represent the total system of equations for the wave propagation in a stressed body. For the surface wave propagation in a layered system additionally the boundary conditions at the interface between substrate and layer, and at the free surface have to be fulfilled. For the calculation of the phase velocity dispersion

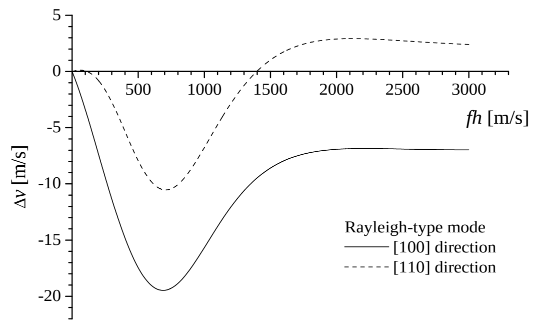

FIG. 2: Phase velocity change Δv vs. frequency-thickness product fh for Rayleigh-type waves propagating parallel to the [100] and [110] direction in biaxially compressed ($\sigma^{(0)}$ = 1 GPa) Ge films on Si(001). The AE effect is maximum when the wave is still penetrating into the unstressed substrate (cf. Fig. 3). For [110] propagation the AE effect changes sign.

and the AE effect we have used second order elastic constants and density of Si (c_{11} = 165 GPa, c_{12} = 64 GPa, c_{44} = 79.2 GPa, ρ = 2329 kg/m^3), and Ge (c_{11} = 129 GPa, c_{12} = 48 GPa, c_{44} = 67.1 GPa, ρ = 5323.4 kg/m^3), as well as third order elastic constants of Ge (c_{111} = −720 GPa, c_{112} = −380 GPa, c_{123} = −30 GPa, c_{144} = −10 GPa, c_{155} = −305 GPa, c_{456} = −45 GPa), respectively. When the Ge film is biaxially stressed the phase velocity dispersion changes. Since this change is very small compared with the dispersion itself we introduce the phase velocity shift $\Delta v = v^{new} - v$, where v and v^{new} is the phase velocity for the system without and with residual stresses and strains, respectively.

In Fig.2 the calculated velocity change Δv is displayed for Rayleigh-type waves propagating parallel to the [100] and [110] direction when the Ge film is biaxially compressed by 1 GPa. For thick films and high frequency limit the velocity change approximates a constant value. But, in contrast to previous discussions, this is not the maximum velocity change of this system, which appears at $fh \simeq 700$ m/s. For the [100] direction the maximum of the AE effect is almost twice the value for a wave completely localized within the stressed film. For the [110] propagation direction the maximum of Δv is even opposite in sign with respect to the high frequency limit.

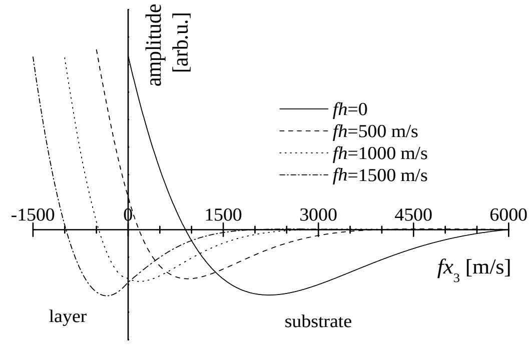

FIG. 3: Dependence of the amplitude of the longitudinal displacement component for the Rayleigh-type wave in the [100] direction vs. the product of the frequency and penetration depth fx_3. The interface between the substrate and the layer corresponds to $fx_3 = 0$, while $fx_3 < 0$ and $fx_3 > 0$ represent the layer and substrate region, respectively.

In order to explain this surprising phenomenon the amplitude dependence of the longitudinal particle displacement component into substrate is shown in Fig.3 for four fh values , starting at an infinitesimal film thickness (solid line). The amplitude of the longitudinal oscillation decreases rapidly when the wave penetrates into the substrate. For certain threshold values the oscillation phase changes its sign. When the layer thickness increases, the threshold approaches the interface. For $fh \gtrsim 700$ m/s the longitudinal oscillation with opposite phase enters the region of residual stress. This, however, causes a local velocity change in the opposite direction. Hence the integral AE effect is reduced. Consequently a maximum velocity change is observed. For the Sezawa mode, however, the AE effect exceeds the value of the Rayleigh wave significantly. Along [110] a velocity change of 82 m/s is calculated for a Ge film biaxially compressed by 1 GPa, i.e. almost 2% with respect to the unstressed system.

In conclusion, the change of the phase velocity of Rayleigh-type and Sezawa waves due to residual stresses reveal an anomalous frequency dispersion exhibiting a maximum at finite layer thickness, where the wave is still penetrating into the unstressed substrate. For Sezawa modes where the longitudinal oscillation component exceeds the vertical component we found a huge increase of the AE effect. Since the maximum AE effect can appear even for quite thin layers, i.e. when the layer thickness is much smaller then the acoustic wavelength, this has significant consequences for GHz acoustic phonon measurements.