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To cite this article: V Zhang et al 2007 J. Phys.: Conf. Ser. 92 012017

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True and pseudo surface acoustic phonons in piezoelectric (001)-GaAs/AlAs superlattice

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Abstract. Dispersion curves and coupling coefficients of surface acoustic phonons propagating in a semi-infinite periodic GaAs/AlAs super-lattice (SL) are numerically studied considering the materials’ anisotropy and piezoelectricity. It is shown that a linear combination of some Floquet modes gives rise to true surface modes propagating without attenuation along the layering with a velocity higher than the bulk modes and decaying into the SL depth. They exist below the lowest pass bands and within some stop bands. The pseudo surface phonons appear in some pass bands. Field profiles of a few selected modes are drawn to identify the phonon polarization. Floquet model is exploited to normalize the wave amplitude and to resolve the numerical instability in computing field profiles.

1. Introduction
The purpose of the present work is to investigate theoretically the existence and propagation characteristics of both true and pseudo surface acoustic phonons on the surface parallel to the layering of a semi-infinite and periodic super lattice (SL). In addition to the elastic anisotropy, we explicitly take into account the piezoelectricity of the constituent layers. A perfectly periodic SL (infinitely long) made of piezoelectric materials allows eight independent Floquet modes to exist, resulting from superposition of the classical bulk modes in a homogeneous solid [1-6]. When the SL is semi infinite in thickness with a stress-free surface, general wave motion can be constructed by linearly combining Floquet modes [2, 5-7]. True surface modes are particular solutions which propagate along the layering without attenuation and exponentially decay into the SL depth. Pseudo surface modes are those which must contain some growing partial modes and decay with propagation in order to satisfy the stress-free boundary condition (BC) [8, 9]. In section 2, we remind some basic concepts and connections between the classical bulk and Floquet modes. Numerical investigation was performed in section 3 for the (001) AlAs/GaAs SL. Dispersion curves of the surface phonons, determined for various propagation directions, are presented along with the Floquet band structures. Field profiles for some selected modes are plotted to check the mode polarization and to highlight advantages and drawbacks of the Floquet approach. Conclusions are given in section 4.

2. Surface solutions for a semi-infinite periodic SL based on Floquet modes
A plane wave (phonon) propagating in an arbitrary piezoelectric layer or a layered structure can be described by a state vector $\tau$ expressed as a linear combination of the classical bulk waves (modal solutions) [6, 7]. For a SL structure which is periodic and semi infinite, this approach, which is
associated to the transfer matrix formalism, is impractical because the layer number is infinite and the numerical instability appears at high frequencies. We express $\tau$ for a SL using a linear combination of Floquet modes defined by the eight eigenvalues ($\lambda_m=1$ to 8) and eigenvectors of the unit cell transfer matrix $P_c$ of the SL when it is piezoelectric. The number of decaying modes ($|\lambda_m|<1$) varies from 1 to 4 depending on the value of pair ($\omega_k$) for a given period $H$, with the same number of growing modes ($|\lambda_m|>1$). Both are called evanescent and form the stop bands. The remaining ones are homogeneous ($|\lambda_m|=1$) which form the so-called Floquet pass bands. For the resultant mode to be a surface one, all of its components should decay with depth. Thus we construct the surface modes using only the 4 decaying Floquet modes. This number is reduced in some decoupling configurations. The effective surface permittivity $\varepsilon_s$ and the usual mechanical impedance matrices $Z_{m,f}$, which account for the electrical BC on the SL surface, can be expressed in terms of the elements of the generalized surface impedance matrix $G$ for a semi infinite SL [6, 7]. Locating the zeros and poles of $\varepsilon_s$ as a function of $s_1 \equiv k/\omega$ at a given $\omega$ fixes slowness values of the piezo-active surface modes for that frequency. Similarly, locating the determinant zeros of matrices $Z_{f,m}$ yields all surface modes including piezo-inactive ones. Repeating this for all interested frequencies yields the dispersion curves of surface modes. The velocity is somewhat slowed down when the SL surface is metallized, and the velocity shift $\Delta V=V_f-V_m$ is a qualitative indication of the electromechanical coupling coefficient.

3. Numerical results for (001)-GaAs/AlAs SL

3.1. Dispersion curves and Floquet band structures

We consider a semi-infinite SL made of (001)-oriented alternative AlAs and GaAs layers of same thickness $h_1=h_2=H/2$. Some surface solutions (velocity and coupling coefficient $K^2=2\Delta V/V_f$) found in this SL for propagation in [100] and 45° from this axis are plotted in figure 1 assuming the top layer to be GaAs. For acoustic phonons propagating in these two particular directions, their polarization either lies in the sagittal plane (SP) or is pure shear horizontal (SH). When the phonons propagate in the direction $\psi=20°$ from the [100]-axis, the polarization of surface modes involves both SP ($U_{1,2}$) and SH ($U_3$) components and they are all coupled to the electrical potential ($\phi$). Given in figure 2 are both true and pseudo surface modes, along with the band structure of the Floquet modes which would exist if the SL was perfect instead of semi infinite. Two true surface branches exist below the pass bands (subsonic region), of which one is quasi-SH and the other quasi-SP polarized. True surface modes are also found in the interior of some stop bands (transonic and supersonic regions, where they propagate faster than the bulk modes). However, when the top surface is AlAs, only one subsonic surface branch exists, and this true surface branch becomes pseudo one at high frequencies. The pseudo modes, which were approximately determined by canceling the real part of the $Z_{f,m}$ determinants because no real value of pair ($\omega_k$) can exactly cancel them, are found within some pass bands.

Figure 1. Dispersion curves (up panel) and coupling coefficient (bottom) for a few of lowest-order surface modes in a semi-infinite GaAs/AlAs SL, top layer is GaAs. Left panel is for 0° or [100]-propagation, where SH is piezo-active; right panel for 45°, where SH is purely elastic and SP is piezo-active. Dots (lines) are purely elastic (piezo-active) surface modes.
3.2. Field profiles based on Floquet and classical models

Floquet model consists in expressing the field in the entire SL in a unique expression based on the Floquet eigenmodes. We apply the same linear combination of the 4 decaying Floquet modes to define surface solutions by considering the SL as an equivalent fictive homogeneous medium. The classical model combines the 8 bulk modes in every layer and imposes the field continuity at the layer interfaces. The wave amplitude is usually normalized with respect to the total wave power. For a semi infinite SL, it is impractical to count this later by summing powers layer by layer. Since the Floquet model field is a function unique of $x_2$ value, independent of the layer number $n$, and its power flow density ($p_1$) parallel to the wave vector in the SL plane ($x_1$) and varying with depth ($x_2$) is readily written out for being integrated in the entire half space, we take these advantages in obtaining the total power in order to normalize the mode amplitude. Figure 3 shows the profiles computed by both models and normalized by a total power equal to 1mW per acoustic beam $\lambda$ (wavelength) for two surface modes (metallized surface, top layer GaAs, $k_H=2$): one with $V_m=3158$ (which is preponderantly SH-polarized) and another with $V_m=2899$ m/s (preponderantly SP-polarized). We note that all physical fields decay with $x_2$, satisfying the primary characteristic of a surface mode. The difference in both types of profiles is hardly observable on the $U_{1,2}$ curves, but noticeable on $U_3$ and becomes particularly significant on the $\phi$-curve. In particular, no slope-discontinuity on $\phi$-curve of the Floquet model is observed at layers interfaces, as it should be according to the classical continuum theory. Figure 3(c) shows that the electric field $E_2$-component given by Floquet model does not exhibit discontinuity. This fact implies that the field profiles based on the Floquet model we proposed do not totally conform to the physical laws. By contrast, discontinuities of the slope of $E_1$, which is proportional to $\phi$, and those of $E_2$ at $x_2=nH/2$ are clearly restored by the classical model, as expected. We observe that both models give common values on the surface and at the interfaces $x_2=NH$ of the unit cells. In effect, though our Floquet model gives right field values only at the cell interfaces, it uses the same function regardless the layer number. Another Floquet model as proposed in [3] guarantees the right field values at all layer interfaces but the field function had to be written for every layers of a unit cell. Discrepancy in the $p_1$-profile of both approaches is small as seen from figure 3(d) up to $x_2=12H$. This justifies the use of power of Floquet model in normalizing the modes amplitude. For $x_2>12H=4\lambda$, numerical instability occurs with the transfer matrix based classical model, as shown in figure 3(d) for $p_1$ profile. Similar phenomenon exists for all other field variables at the same depth.
3.3. Numerical instability in computing field profiles with classical approach and transfer matrix

Though our Floquet model is stable for any \( x_2 \), it is not accurate enough for the profiles of electrical fields. The classical approach enables exact field profiles but suffers from numerical instability as the value of \( x_2 \) increases. We attribute this to the imprecision in calculating the n-power of \( P_c \) when n is large and \( P_c \) contains both very large and small elements when its eigenmodes are evanescent. To resolve these drawbacks, we compute the field profiles by combining both models. Namely, we use the Floquet modes to compute the state vector at the cell interfaces and then use it to deduce the mode amplitude in a layer belonging to that cell instead of evaluating the power of \( P_c \). Since the Floquet modes can be evaluated with desired accuracy for any depth, cf. equation (71) in [1], this allows fields to be computed without numerical instability even at very large n. For the same mode as in figure 3(b), stable results were obtained for depth up to \( x_2 = 20H \approx 6\lambda \). For the mode with \( V_m = 2751 \) m/s and \( kH = 10 \), no instability occurs up to \( x_2 = 4H \approx 7\lambda \).

Figure 3. (color online) Field profiles of two surface modes propagating along 20°, \( kH = 2 \), top surface is metallized GaAs, total power is 1 mW/\( \lambda \). Dash-dotted red lines = Floquet model; Solid blue lines = classic model. (a) Displacement and potential (enlarged 20 times) for \( V_m = 3158 \) m/s. (b) Same as (a) but for the mode with \( V_m = 2899 \) m/s. (c) Electrical field \( E_{1,2} \) of the mode in (a). (d) Power flow density \( p_1 \) of the mode in (b) showing numerical instability for \( x_2 > 12H \) with classical model.

4. Conclusions

Surface modes in a semi-infinite periodic SL are studied. True surface modes exists in the subsonic region of the Floquet spectral domains and also in certain transonic regions where all of the Floquet modes are evanescent (stop bands). The same dispersion branches become pseudo modes when crossing a pass band. This is the case of the subsonic surface branch at high frequencies when the AlAs is the top layer of the SL. Exact field profiles should be computed with the classical approach along with the help of the Floquet model instead of cascading the layers’ transfer matrices in order to avoid the numerical instability and to have exact field values at any depth.

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