Proceeding sof the International Congress on Ultrasonics, Vienna, April 9-13, 2007, Paper ID 1431, Session R07: Bulk and surface acoustic waves
doi:10.3728/ICUltrasonics.2007.Vienna.1431_zhang

Guided wave spectra and their asymptotic behaviour in multi-layered plates made of three materials AlN-W-SiO_2

Victor Y. Zhang[1], Bernard Collet[2], Bertrand Dubus[1], Michel Destrade[2], Tadeusz Gryba[1]

[1]Institut d'Electronique, de Microélectronique, et de Nanotechnologie (IEMN), CNRS, France, victor.zhang@iemn.univ-lille1.fr
[2]Institut Jean Le Rond d'Alembert, CNRS/Université Pierre et Marie Curie, Paris, France.

Abstract: A study on guided waves in some layered plates made of tungsten (W) and SiO_2 along with a piezoelectric AlN layer is carried out numerically. Multi-mode dispersion curves are computed up to sufficiently high frequency in order to reveal the asymptotic behaviour of guided waves in the short wavelength regime. The complete spectra were determined without suffering from numerical instability, by combining the surface impedance matrix formalism and a recursive algorithm repeatedly applied at different surfaces/interfaces, and by preserving the basic matrix size. The results reveal that wave-confinement and mode-repulsion phenomena appear in certain spectral domains. Their physical origin is analyzed and interpreted in connection with the characteristic acoustic modes - surface and interface waves at the boundary of one or two half-spaces of the constituent materials. Other asymptotic behaviours associated with classical bulk waves are also highlighted.

Key words: guided wave spectra, impedance matrix, Lamb mode, multilayer plate.

A. Introduction

Engineering applications in *surface acoustic wave* (SAW) device design, composite material characterization, and smart structures require an analysis of acoustic wave interaction with anisotropic and/or piezoelectric multi layers. More recently, analysis of *bulk acoustic waves* (BAW) in multi layered structures composed of stacked piezoelectric, dielectric and metallic materials has once again attracted attention of engineers and researchers working on RF components such as BAW resonators and filters. The development of efficient simulation tools is needed to characterize accurately the electromechanical behaviour of complex stratified structures accounting for realistic electrical and mechanical interface and boundary conditions.

Acoustic wave spectra in multi-layers are rather complex and are difficult to compute, especially in short wavelength regimes and when the layers have strong impedance contrast. By repeatedly using the *surface impedance matrix* [1]-[7] at different surfaces and/or interfaces along with a recursive algorithm for the overall multi layers [3],[4],[6],[7], we were able to determine numerically the full acoustic spectra for plates made of up to 4 layers of 3 materials (W, SiO_2, and AlN), without increasing the basic matrix size and up to extremely short wavelengths [8]. Once the dispersion curves are obtained, the field distributions of any particular mode can be known with more accuracy by selecting the appropriate interface in the neighbourhood of which the electro-mechanical energy flux concentrates.

The model structures consist of a piezoelectric AlN layer, a low impedance dielectric SiO_2, layer, and a high impedance metallic tungsten (W) layer. This choice was motivated by the design of solidly mounted resonators employing AlN as an active resonator and stacked cells made of bi-layer SiO_2/W as a Bragg mirror to isolate the resonator from the substrate (Si, for example). The complete acoustic waves spectra are obtained by locating the zeros of a certain characteristic equation formulated using either the transfer or the impedance matrix, or the hybrid of both, as is more convenient. Starting from the analytical formulation detailed elsewhere [8], we present here the numerical results obtained for the case where only the piezoelectric AlN layer and some SiO_2/W cells in the Bragg coupler are kept, in order to facilitate the analysis of the rather complicated spectrum of guided acoustic modes.

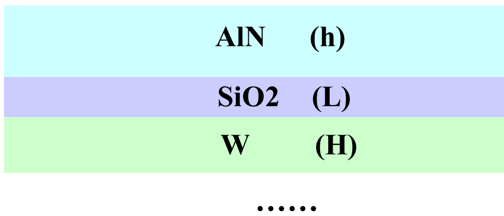

Fig.1. Layered plate composed of a piezoelectric AlN layer together with some additional layers of W and SiO_2.

B. Numerical results

We have calculated the solutions for structures consisting of a piezoelectric c-axis oriented AlN layer and a Bragg coupler having different unit cells of SiO_2/W (see Fig.1). Owing to the isotropy of the coupler materials and to the special orientation of the AlN layer, the shear horizontal (SH) partial modes are decoupled from the sagittal plane (SP) ones and are piezo-inactive. In what follows, we focus only on the SP vibrations which are coupled with the electrical field. In all numerical examples, the thickness h of the AlN layer was taken to be 1 μm. For W (SiO_2), the thickness H (L) was chosen to be $\lambda/4$-thick when the wavelength λ of the longitudinal thickness-mode in AlN is $\lambda=2h$; this leads to H=238.79 nm and L=278.81 nm. The characteristic wave speeds for the three materials involved in our study are calculated first and the results are given in Table 1 using some set of materials constants. They show that AlN is the fastest

doi:10.3728/ICUltrasonics.2007.Vienna.1431_zhang

material and W the slowest one.

Fig.2 presents the acoustic spectra calculated for a 3-layer AlN/SiO_2/W plate. Two branches exist for all frequencies, and higher order branches only appear for $f \geq f_c$, with a few of them exhibiting negative slope in the *f-k* plot of the dispersion curves near cut-off f_c. No mode in the full spectra is symmetric nor anti-symmetric because the plate does not exhibit any symmetry in thickness. The enlarged views of the dispersion curves V_p-f plot, in a restricted velocity range but in a more extended frequency range (up to $f_n = 25$), allows us to observe more easily some plateaux where the wave speed seems to reach an asymptotic limit (horizontal line). An analysis of the origin of these peculiar behaviours enables us to get a deeper physical insight into the wave motion in this 3-layer plate. A plateau appears clearly in the V_p-f plot for $f_n \geq 3$, situated at $V_p / V_0 \approx 0.9$ which corresponds to the speed of SAW in massive AlN. Another plateau exists for $f_n \geq 5$, situated at the lowest wave speed at $V_p / V_0 = 0.479$ which does not correspond to the speed of SAW in massive SiO_2 nor in W. Here a careful analysis reveals that the plateau tends to the wave speed of the interfacial, also called Stoneley mode which would exist and propagate at the interface of W and SiO_2 were both materials to fill up the half-spaces. Another asymptotic limit is observed just above the interface mode for $f_n > 10$, which corresponds to the shear BAW in massive W. At higher frequencies ($f_n > 17$), some branches reach a plateau-like zone just below $V_p / V_0 = 0.9$ and over a finite frequency range, which is relative to the longitudinal BAW in massive W; the branches then undergo a sharp decrease in phase velocity; after that, they approach first the asymptotic limit of shear BAW speed of massive SiO_2 ($V_p / V_0 \approx 0.63$) and then the shear BAW speed of massive W ($V_p / V_0 \approx 0.5$).

Another peculiar feature worth noticing is that the horizontal asymptotic line does not cross any branch when they approach each other. This is illustrated in Fig.3 which shows some zoomed views of Fig.2 in some selected zones. In particular, the line for SAW in AlN around the very beginning of its existence (corresponding to the red-circled part) is enlarged in the top-right quarter of Fig.3. The others two subplots for shear bulk waves in AlN (at $V_p / V_0 \approx 1$) and in SiO_2 (at $V_p / V_0 \approx 0.63$) show clearly that the branches do not cross but instead exhibit a sharp slop-change whenever they get near one each other. This feature indicates the energy interchange between various modes, a property known as mode-repulsion when many modes co-exist.

If the same three layers are arranged differently, say as AlN/W/SiO_2, a sandwich with the slowest layer embedded between two faster ones, then the plateau attributed to the SAW in massive AlN appears as soon as $f_n \geq 2$, and a supplementary plateau exists above $V_p / V_0 = 0.5$, which corresponds to the SAW speed in massive SiO_2. Other characteristics remain rather similar [8].

To go further, we also calculated the dispersion curves, as shown in Fig.4, for a 4-layer plate AlN/SiO_2/W/SiO_2. The characteristics of higher-order modes cut-off, no symmetry, and negative slope are similar to the previous 3-layer plates, except that here the number of modes is larger (58 instead of 47 in Fig.2) within the same frequency range ($f_n \leq 15$). The lowest limit of the spectra is still the interface mode speed (though the SAW in massive W is the lowest one among all possible modes in these materials). Notice that two branches approach this limit from respectively the upper- and lower-side. We interpret this phenomenon by saying that there exists two interfaces between the W and SiO_2 materials within the structure. The lower one is attributed to the W and the outside SiO_2 layers, and the higher one to the W and the embedded SiO_2 layers.

The third lowest mode tends to the SAW speed of massive SiO_2 ($V_p / V_0 \approx 0.568$) after mode-exchanging (crossing) near $f_n \approx 2.2$ with $V_p / V_0 \approx 0.9$, a value near the characteristic plateau visible for $f_n > 3$ and attributed to the SAW in massive AlN. The plateau relative to the SAW in SiO_2 is well constructed as soon as $f_n > 4$. Higher modes get divided into two families in the very short wavelength regime. The lower family approaches the shear bulk speed limit of W (just above the interface mode), and the upper family tends to the shear bulk speed limit of SiO_2 by pair, owing to the couple of SiO_2-layer in the structure. A barely visible single-mode plateau appearing for $f_n > 15$ and just below $V_p/V_0 \approx 0.9$ is due to the intermediate confinement originated from the longitudinal bulk-like mode in the W-layer. The single mode plateau appearing for $f_n > 7$ and just above $V_p/V_0 \approx 1$ is due to the confinement originated from the shear bulk-like mode in the AlN-layer. The interface mode speed is the bottom limit of the phase velocity in the whole spectra of guided waves in the 4-layer AlN/SiO_2/W/SiO_2 plate. No mode tends to the SAW speed of massive W in neither 3- and 4-layer cases involving only one W-layer in Figs. 2 and 3, and this is true whether the W is or is not an exterior layer.

When the roles of the W and SiO_2 layers are interchanged in the 4-layer system, the lowest branch is the SAW speed of massive W ($V_p / V_0 = 0.454$). We point out that it is not sufficient to have the W-layer as an exterior one, as in Fig.2, but that another W-layer embedded in the structure is also required for the SAW in W to exist in the very short wavelength regime. The next lowest branch approaches rapidly (for $f_n \geq 2$) the speed of the interfacial mode. Another branch also tends to the interface mode speed, but at a much higher frequency, $f_n \geq 8$. This phenomenon is logically explained by the presence of two W/SiO_2 interfaces in the current configuration. The branch which reaches the interfacial wave speed first is essentially at the interface of SiO_2 with the outside W-layer, while the other one is mainly at the interface of SiO_2 with the embedded W-layer. No mode tends to the SAW speed of massive SiO_2 because this layer has no stress-free surface.

C. Conclusion

Full acoustic spectra in some plates consisting of layers having strong impedance and/or velocity contrast are numerically studied. It is found that in a 3-layer plate of either AlN/W/SiO_2 or AlN/SiO_2/W, the lower limit of the wave spectra is the interface wave existing between SiO_2 and W layers. The asymptotic line standing for the speed of SAW in an AlN half space always exists, but the

doi:10.3728/ICUltrasonics.2007.Vienna.1431_zhang

line for the SAW in SiO_2 only exists in the case of $AlN/W/SiO_2$. No SAW in W was found whether the W-layer is or is not an exterior one in the 3-layer plates. In a 4-layer $AlN/SiO_2/W/SiO_2$ plate, the 2-fold interface wave speed remains the bottom limit of the whole spectra, lying below the SAW speed of massive SiO_2, and no SAW in W was found. When the layers are arranged in the order $AlN/W/SiO_2/W$, the SAW in W does exist and becomes the low limit of the whole wave spectra lying below the 2-fold asymptote associated with the interface wave between W and SiO_2. There is no SAW in massive W in any structure possessing only one W-layer, even if it is an exterior layer, and no interface wave exists between AlN and W or SiO_2, though the SAW in AlN exists anyway. The results made evident in the present study can be useful for structure optimization in BAW filter and Lamb wave guide design.

D. Literature

[1] B. Honein, A.M.B. Braga, P. Barbone, G. Herrmann, "Wave propagation in piezoelectric layered media with some applications," J. Intell. Mater. Syst. Struct. **2** (1991) 542–557.

[2] V.Y. Zhang, T. Gryba, J. M. Orellana, B. Collet, "Surface impedance matrix for the study of acoustical propagation in multilayered structures," Acta. Acust.- Acust. **88**, 218–230 (2002).

[3] T. Pastureaud, V. Laude, S. Ballandras, "Stable scattering-matrix method for surface acoustic waves in piezoelectric multilayers," Appl. Phys. Lett. **80** (2002) 2544–2546.

[4] S.I. Rokhlin and L. Wang, "Stable recursive algorithm for the elastic propagation in layered anisotropic media: stiffness matrix method," J. Acoust. Soc. Am. **112** (2002) 822–834.

[5] E.N. Tan, "A concise and efficient scattering formalism for stable analysis of elastic wave in multilayered anisotropic solids," Ultrasonics **41** (2003) 229–236.

[6] L. Wang and S.I. Rokhlin, "A Compliance/Stiffness Matrix Formulation of General Green's Function and Effective Permittivity for Piezoelectric Multilayers," IEEE Trans. UFFC **51** (2004) 453–463.

[7] B. Collet, "Recursive surface impedance matrix methods for ultrasonic wave propagation in piezoelectric multilayers," Ultrasonics **42** (2004) 189–197.

[8] V.Y. Zhang, B. Dubus, B. Collet, M. Destrade, "Piezoacoustic wave spectra in high impedance-contrast layered plates, using improved matrix formalisms," (submitted for publication).

Table 1 Characteristic wave speeds for the studied materials (SC=short-circuit, OC=open circuit, L, T=longitudinal, shear BAW):

	V_L (m/s)	Y-polar-V_T	2^{nd} V_T (m/s)	V_{SAW} (m/s)
c-axis AlN: SC/OC	10605/10939	5796	5796	5395/5402
X-propagation	9911 (non-piezo)	5597	5796/5867	5417/5437
W (High-impedance)	5224	2888		2669
SiO_2 (Low-impedance)	6100	3655		3342

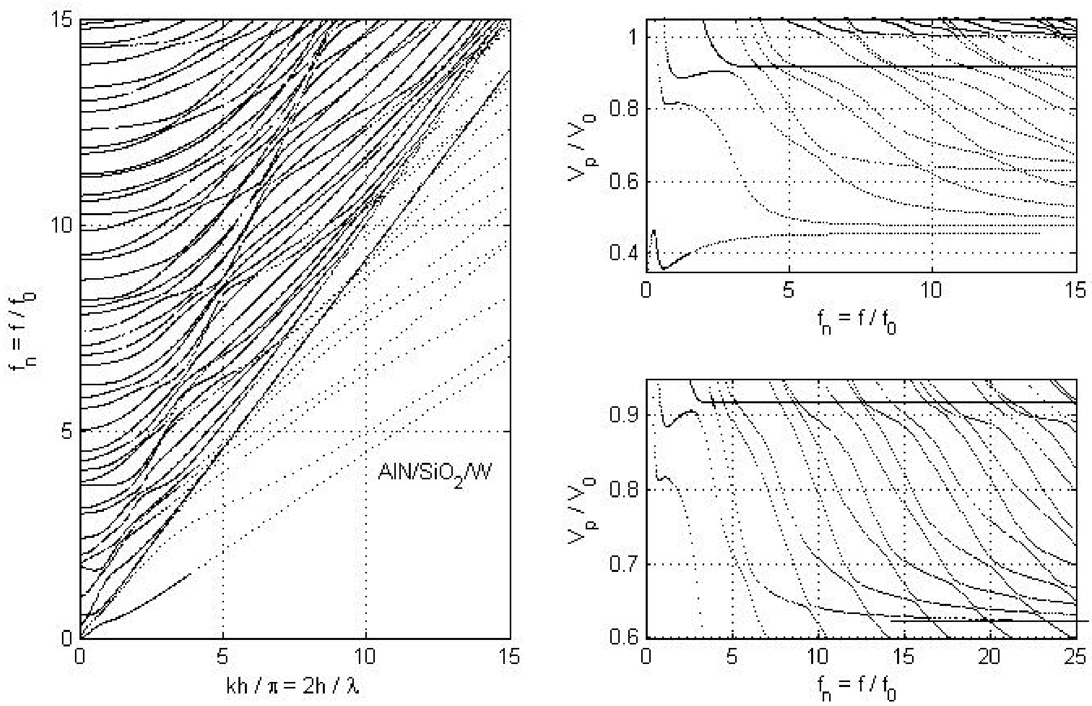

Fig.2. Acoustic spectra of guided waves in a 3-layer plate $AlN/SiO_2/W$: global view (left panel) and enlarged partial views of normalized phase velocity plotted vs. frequency in two particular spectral regions (right panel).

doi:10.3728/ICUltrasonics.2007.Vienna.1431_zhang

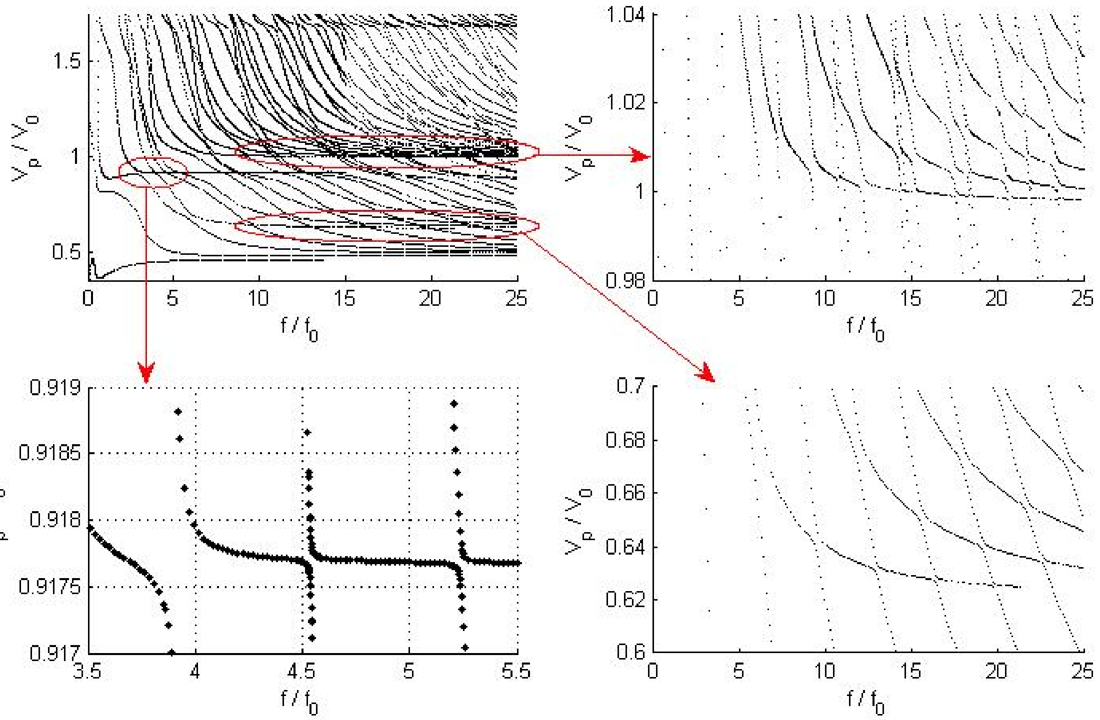

Fig.3. Enlarged views of guided waves spectra for the plate AlN/SiO_2/W showing the mode-repulsion, namely no branches cross one each other, near the asymptotes associated to the SAW (bottom-left subplot) and shear BAW in massive AlN (top-right subplot), as well as the one to the shear BAW in SiO_2 (bottom-right subplot). Red ellipses and arrows indicate approximate zoomed regions.

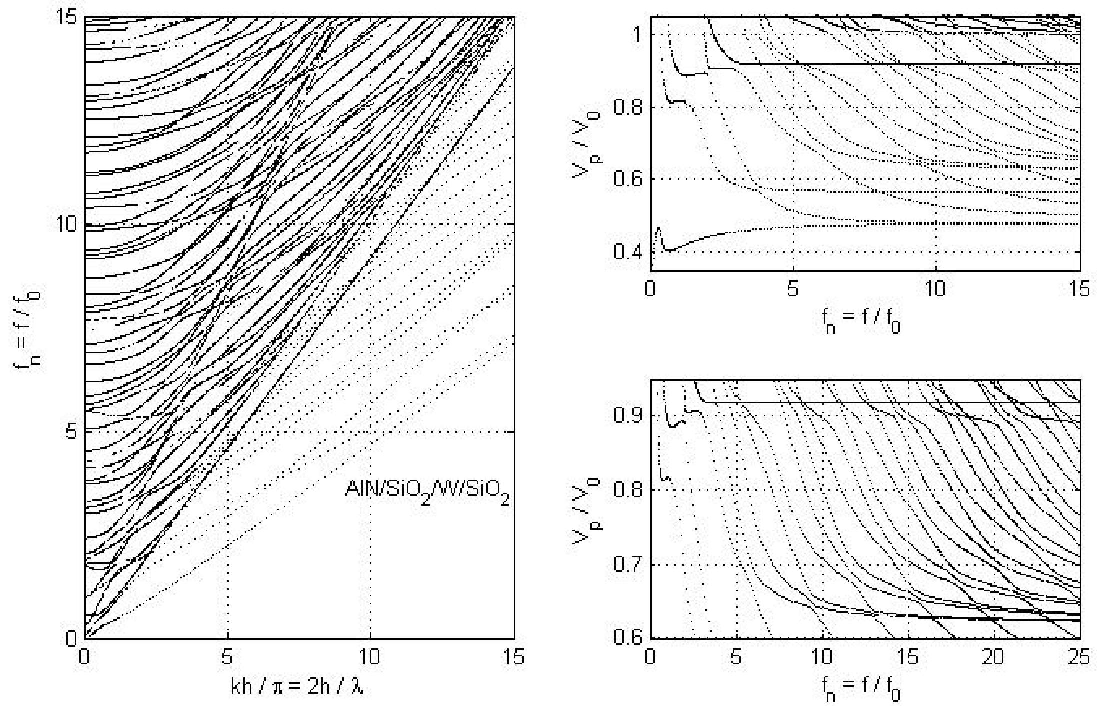

Fig.4. Acoustic spectra of guided waves in a 4-layer plate AlN/SiO_2/W/SiO_2: global view (left panel) and enlarged partial views of normalized phase velocity plotted vs. frequency in two particular spectral regions (right panel).