Theoretical and Experimental study of the Differential Thermal Expansion Effect on the TCD of Layered SAW Temperature Sensors.

Application to Aluminum Nitride based layered structures.

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***Abstract*— In this paper, we show that the stress and strain fields induced in a layered SAW structure by the thermal expansion of the different layers must be taken into account to compute the global structure temperature coefficient of delay (TCD). Experimental and numerical results are provided. The numerical model is described. It is based at the same time on the well-known Campbell and Jones method, the Bolotin equation and a simple way to approximate the strain field in a double layer structure. The model is then applied to test three sets of temperature coefficients for AlN thin film elastic constants. The comparison between AlN/Sapphire already published experimental data and theoretical results leads to the selection of one of the three sets. The recently released AlN 3rd order elastic constants are used here to compute the thermal strain effect. Once chosen, the set is used to compute the TCD of AlN/Diamond structures. The theoretical results are compared with new experimental data. The observed discrepancies are discussed.**

Keywords- TCD; multilayer ; thermal strain ; AlN ; temperature coefficients ;

I. INTRODUCTION

One promising way to develop high temperature SAW sensors is to make use of a layered composite structure. For example, an AlN/Diamond structure can withstand extreme working conditions, it presents a good electromechanical coupling coefficient (K^2) and it is able to operate above 5 GHz. However, in order to develop fully operational SAW sensors based on these layered structures, their behavior with respect to the temperature must be well understood beforehand. It is notably necessary to study further the effect of the stress and strain fields induced within the structure by the differential thermal expansion of the substrate and the film (thermal strain effect). This effect is already non-negligible at room temperature and becomes increasingly strong when the temperature rises. The phenomenon has been commonly ignored up to day and it is quite poorly documented in the literature. We present here the first results of a study carried out to better understand the influence of thermal strain effect on the operating frequency of a layered SAW device, at room temperature. The necessity to take the thermal strain effect into account is demonstrated in the first part of the paper, using ZnO/Quartz and AlN/Quartz experimental results, along with numerical calculations. In a second part, the numerical model is applied to select a set of temperature coefficients for AlN thin film elastic constants, using pre-published AlN/Sapphire data. The choice of such a structure is explained. Recently released AlN 3rd order elastic constants are used to compute the thermal strain effect. Once chosen, the set of temperature coefficients is applied to compute the TCD of AlN/Diamond structures. The theoretical results are compared with newly obtained experimental data. First explanations are given to account for the observed discrepancies.

II. THERMAL STRAIN EFFECT

The TCD of a layered SAW structure depends classically on three distinct parameters: the temperature variation of the acoustical properties for each material, the film normalized thickness (kh) and the substrate coefficient of thermal expansion (α). The two first parameters yield to the temperature coefficient of velocity (TCV). The third parameter gives directly the amount of delay generated by the thermal expansion. The TCD is then given by the following equation:

$$TCD = \alpha - TCV \quad (1)$$

In the conventional approach, the coefficient α is that of the substrate, considering that the thicker substrate can force the elongation of the above thinner layer. The effect of the strain field induced by the substrate within the layer is just ignored. However, the thermal strain effect cannot be neglected in the majority of cases. That can be demonstrated by a comparison between experimental data and numerical results, taking the thermal strain effect into account or not. This effect arises from four distinct causes: the modification of the propagation path length, the density variation when the material is deformed, the variation of the elastic constants under initial strain and the effect of initial stress on the wave propagation itself. The modification of the path length results in a modification of the α coefficient in (1). The calculation of density variation under

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strain is only a matter of geometry. The variation of elastic constants is given by 3rd order coefficients. Finally, the impact of initial stress on the wave characteristics can be obtained, following Bolotin, by directly including the stress field into the equation of motion for a surface acoustic wave in a piezoelectric medium [1]. In order to perform the computations, we have developed a SAW modeling software based on the well-known Campbell and Jones method, with additional function to take in account the four thermal strain effect origins, as described just above. In a first time, the strain field in the film has been approximated by considering only the two orthogonal directions X_1 and X_2 on the surface:

$$S_{f1} = \varepsilon(\alpha_{s1}-\alpha_{f1})(T-T0) \qquad (2)$$

$$S_{f2} = \varepsilon(\alpha_{s2}-\alpha_{f2})(T-T0) \qquad (3)$$

,where α_{fi} and α_{si} are the thermal expansion coefficients of the film and substrate in the X_i direction, ε is an additional factor related to the substrate capability to force the deformation of the above layer. If the substrate is able to fully impose its deformation to the film, ε=1. On the contrary, if the film is able to impose its deformation to the substrate, ε=0. Being given that the strain and stress fields are continuous within the structure, the strain field in the substrate can be approximated as follows:

$$S_{s1} = -(1-\varepsilon)(\alpha_{s1}-\alpha_{f1})(T-T0) \quad (4)$$

$$S_{s2} = -(1-\varepsilon)(\alpha_{s2}-\alpha_{f2})(T-T0) \quad (5)$$

Stress fields can be easily deduced from strain fields, by the mean of classical elasticity laws.

Fig. 1 shows a comparison between experimental and theoretical results, for the fundamental Rayleigh mode in a ZnO/Quartz ST-X+35° structure. The three theoretical curves correspond respectively to the classical approach (solid line), to the results obtained by considering only the effect of a small deformation induced by the layer in the substrate (dashed line) and to the results obtained by considering the effect of this same deformation at the same time in the layer and in the substrate (dotted line). In both latter cases, ε = 0.7. This is a value we think to be close from the actual experimental value. Because of the non-availability of the 3rd order ZnO elastic coefficients, the dotted line doesn't take into account the modification of the elastic constants under thermal strain. Therefore, the dotted line can only be taken as a tendency. Nevertheless, Fig. 1 seems to confirm the necessity to consider the thermal strain effect to explain the observed TCD values. A consequence is that the thickness h becomes a parameter as relevant as the kh, because it defines the value of ε, together with the materials stiffness coefficients. Fig. 2 shows other evidences to confirm the importance of h to account for the experimentally observed TCD. This time, an AlN/Quartz ST-ψ structure is considered.

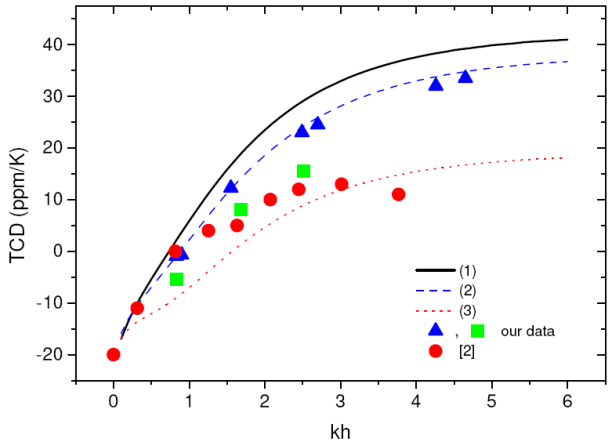

Figure 1. TCD=f(kh) for the fundamental Rayleigh mode in a ZnO/Quartz ST-X+35° structure. (1) classical approach (2) ε=0.7 / thermal strain effect in the substrate only (3) ε=0.7 / thermal strain effect in the whole structure.

The experimental kh values are willingly small and similar (0.24 < kh < 0.4) in order to attenuate the classical thin film influence on the TCD and to magnify the thickness influence. One can see that the experimental results are close to the theoretical values when h is very small. This was expected because a very thin layer is not stiff enough to resist the substrate thermal expansion. But, when h increases, the discrepancies do the same.

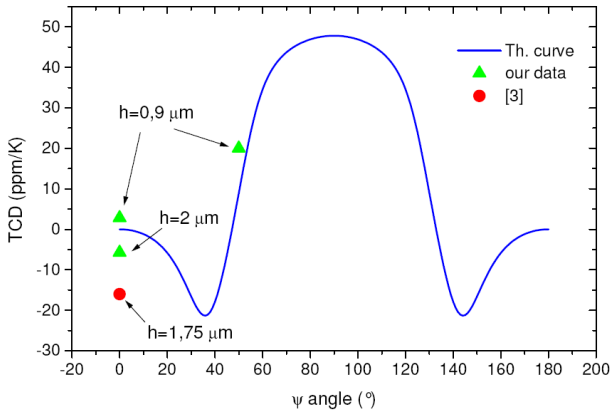

Figure 2. Comparison between experimental AlN/Quartz ST-ψ TCD values and theoretical TCD values for naked Quartz ST--ψ substrate.

It's worth noting that the experimental data for h=2µm and h=1.75µm are extracted from recently published works aimed to define a value for the TCD of AlN thin films [3-4]. The idea was to use zero TCD substrate in order to infer directly the TCD of AlN from the TCD of the whole AlN/substrate structure. As a well-known zero TCD substrate, the Quartz ST-X was chosen in both cases. But, it is now clear that these results cannot be fully trusted. Indeed, the kh were too small to make the wave sensitive enough to the AlN parameters and the thermal strain effect was fully neglected. But, given the film thickness and the great stiffness and small thermal expansion of AlN compared to Quartz, thermal strain should play a role. The experimental TCD in the case h=2µm could be for example explained by a reduction of the coefficient α in (1)

due to the presence on the substrate of a rigid and less thermal expanding film. In this case, there would be no need for a classical TCD of AlN, which might as well be zero… However, the idea and its limitations led us to a possible solution to evaluate correctly AlN TCD. Such knowledge is strongly needed to design high temperature SAW sensors.

The solution is to find firstly a substrate with a thermal expansion coefficient similar to that of AlN, in order to avoid or to diminish the thermal strain effect (a low effect is easier to simulate correctly, because no extra effect appears). A mono-crystalline substrate is preferable, because such a substrate is homogeneous and there are no micro or nano-crystalline parts, with strongly (or even slightly) different physical properties. The knowing of 3rd order elastic coefficients is a plus, because this allows the fully computing of the thermal strain effect in the AlN/substrate structure. Indeed, the 3rd order coefficients of AlN have been recently published [5]. Secondly, we have to grow a layer thick enough to relax the residual strains in the film and to achieve a large kh value. The relaxation of strain allows getting a coefficient α in (1) close to that of natural AlN. The large kh value allows getting a wave influenced only by the AlN parameters.

Fortunately enough, at least one possible substrate exists. This is Sapphire (Al_2O_3). Its thermal expansion coefficient is close to that of AlN, high quality mono-crystalline Sapphire wafers are commercially available and the 3rd order elastic constants of the bulk material are known [9]. Moreover, the velocity of Rayleigh wave in this material is either higher or close enough to that of AlN, thus avoiding numerical simulation troubles.

III. Determination of the Right Set of Thermal Coefficients for Aluminium Nitride Thin Films

The Tab. 1 presents three sets of temperature coefficients for AlN elastic constants. Among the three sets, two have been recently published [7-8]. As far as our knowledge, these two sets have never been applied to compute AlN SAW properties. The corresponding theoretical TCD for the fundamental Rayleigh mode in the (0001) plane (z-cut) are presented at the end of the table. The thermal expansion coefficients are always those of [6] ($\alpha_1=\alpha_2=5.27*10^{-6}$; $\alpha_3=4.15*10^{-6}$).

TABLE I. Thermal Coefficients of ALN Thin Films

Coeff.	Elastic constants temperature coefficients		
	Tsubouchi *et al.* [6] -1-	**Reeber *et al.* [7] -2-**	**Bjurström *et al.* [8] -3-**
C11	0.8 ($*10^{-4}$)	-0.28	-0.37
C12	1.8	-0.35	-0.018
C13	1.6	-0.4	-0.018
C33	1	-0.3	-0.65
C44	0.5	-0.11	-0.5
C66			-0.57
TCD	-29.6 (ppm/K)	5.6	24.3

Fig. 3 presents a comparison between experimental and theoretical results for (0001) [11-20] AlN / (0001) [1-100] Sapphire structures. The Sapphire physical constants needed for the calculations come from [6] and [9]. The classical approach gives the solid lines. The dashed lines include the thermal strain effect. The curve -1- appears to be far from the experimental values for kh>3. The curve -2- seems to fit quite correctly the experimental data but, when the thermal strain effect is taken in account, it deviates from the experimental data while the curve -3- comes closer to them.

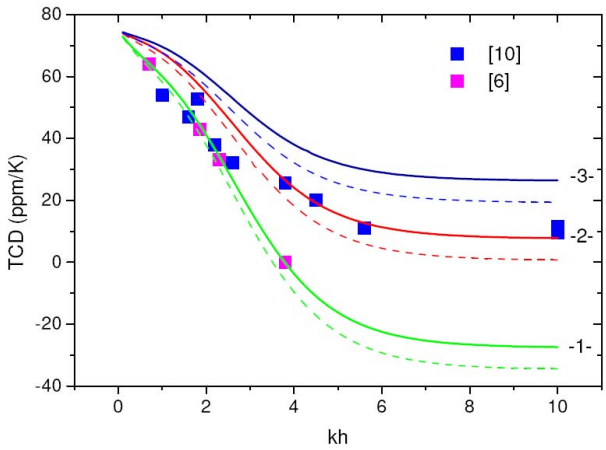

Figure 3. TCD=f(kh) for (0001) [1 1 -2 0] AlN / (0001) [1 -1 0 0] Sapphire structures. Compaison between experimental and theoretical values. Solid lines correspond to classical results. Dashed lines include the thermal strain effect in the thin film. A number refer to the set of temperature coefficients used for the computation.

It is then impossible to choose between the two remaining sets of coefficients. In order to actually make a choice, more information is needed.

Crucial information is given by experimentally observed TCD for AlN-based F-BAR. Indeed, in addition of being available, these data give the TCD of BAW, which react differently from SAW for a same set of temperature coefficients. Dubois *et al.* have notably obtained a TCD value of 33 ppm/K for a (0001) AlN-based F-BAR [11]. The theoretical value obtained for the longitudinal wave which propagates along the c-axis with the set -2- is 10.9 ppm/K. With the set -3-, one obtains a TCD of 27.5 ppm/K, which is a lot closer to the experimental value. The set -3- is definitely validated when used to compute the TCD for another AlN/Sapphire configuration, as shown on Fig 4. This time, an (11-20) [0001] AlN / (01-12) [0-111] Sapphire structure is considered. Again, the solid line corresponds to the classical approach, while the dashed line includes the thermal strain effect in the thin film. The results seem to confirm at the same time the relevance of the third set of temperature coefficients and the necessity to consider the thermal strain effect.

Once selected a good set of temperature coefficients for the AlN thin film, it becomes possible to apply it to compute theoretical values for various layered SAW structures. We can notably compute TCD for AlN / Diamond structures.

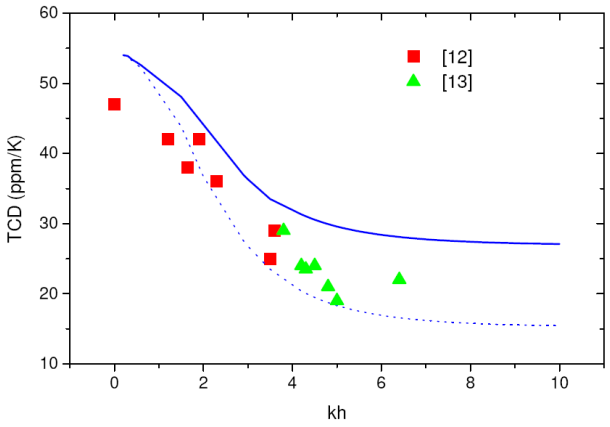

Figure 4. TCD=f(kh) for (1 1 -2 0) [0 0 0 1] AlN / (0 1 -1 2) [0 -1 1 1] Sapphire structure. Compaison between experimental and theoretical values. Solid lines correspond to classical results. Dashed lines include the thermal strain effect in the thin film. The thermal constants used for the computation are those of Bjurström *et al.*(2007) [8]. The AlN 3rd order coefficients are those of Pandey *et al.* (2007) [5].

IV. TCD OF ALN / DIAMOND STRUCTURES

Fig. 5 presents the results obtained for a (0001) AlN / (001) Diamond structure. The diamond physical constants needed for the calculations are extracted from [14-15] (the thermal strain effect is not considered here). If the theoretical results for mode 1 and mode 2 are not too far from experimental results, there is a big discrepancy between theoretical and experimental values for the mode 0. Because a compression of AlN results in an increase of TCD, taking the thermal strain effect into account would even worsen the situation…

The trouble could arise from the microstructure of the diamond substrate. Indeed, the experimental data have been obtained with AlN thin films deposited on the nucleation side of home grown diamond. But this side exhibits a nano-crystalline character and its elastic constants differ quite drastically from those of the growth side, which is structurally closer to mono-crystalline phase [16]. Hence, it seems highly probable that a sub layer just below the AlN / Diamond interface could present thermal properties quite different to those tabulated for the mono crystalline diamond. Moreover, the problem is complicated by the fact that different modes don't propagate at the same depth for a given kh. For example, the mode 1 (Sezawa) propagates more deeply than the mode 0 (fundamental Rayleigh mode). The mode 1 is then concentrated closer to the nano crystalline domain and must be more influenced than mode 0 by its parameters. Further studies are then needed to better understand the TCD of AlN/Diamond SAW structures. It's notably essential to characterize the physical parameters of the nano crystalline phase (elastic constants, temperature coefficients…), if possible with respect to depth inside a home grown diamond sample.

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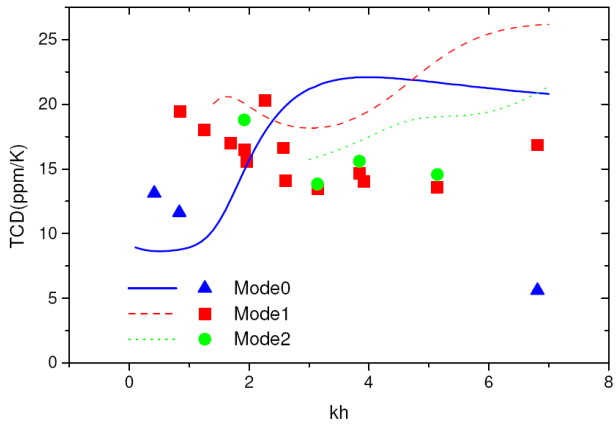

Figure 5. TCD=f(kh) for AlN/Diamond structure. Comparison between experimental and theoretical data.

REFERENCES

[1] A.L. Nalmwar and M. Epstein, Surface Acoustic Waves in Strained Media, J. Appl. Phys., Vol. 47, No. 1, pp. 43-48, 1976.

[2] M. Kadota, Combination of ZnO Films and Quartz to Realize High Coupling Factor and Excellent Temperature Coefficient for SAW Devices, Proc. IEEE Ultrasonics Symp., pp. 261-266, 1997.

[3] K. Kao, Y. Chen, Y. Lee, C. Cheng, Temperature Coefficients of SAW Velocity for AlN Thin Film Sputtered on ST-X Quartz, Proc. IEEE Ultrasonics Symp., pp. 239-242, 2002.

[4] M.B. Assouar, O. Elmazria, M. Elhakiki and P. Alnot, Study of structural and microstructural properties of AlN films deposited on silicon and quartz substrates for surface acoustic wave devices, J. Vac. Sci. Technol. B 22(4), pp. 1717-1722, 2004.

[5] D.K. Pandey, D. Singh, R.R. Yadav, Ultrasonic wave propagation in IIIrd group nitrides, Applied Acoustics 68, pp. 766-777, 2007.

[6] K. Tsubouchi and N. Mikoshiba, Zero-Temperature-Coefficient SAW Devices on AlN Epitaxial Films, IEEE Trans. on Sonics and Ultrasonics, Vol. SU-32, No. 5, pp. 634-644, 1985.

[7] R. Reeber, K. Wang, High Temperature Elastic Constant Prediction of Some Group III-Nitrides, MRS Internet J. Semicond. Res. 6, 3, 2001.

[8] J. Bjurström, G. Wingqvist, V. Yantchev and I. Katardjiev, Temperature compensation of liquid FBAR sensors, J. Micromech. Microeng., 17, pp. 651-658, 2007.

[9] J.M. Winey and Y.M. Gupta, r-axis sound speed and elastic properties of sapphire single crystals, J. Appl. Phys., Vol. 90, No. 6, pp. 3109-3111, 2001

[10] K. Uehara, C.M. Yang, T. Shibata, S.K. Kim, S. Kameda, H. Nakase and K. tsubouchi, Fabrication of 5-GHz-Band SAW Filter with Atomically-Flat-Surface AlN on Sapphire, Proc. IEEE Ultrasonics Symp., pp. 203-206, 2004.

[11] M.A. Dubois and P. Muralt, Properties of aluminium nitride thin films for piezoelectric transducers and microwave filter applications, Appl. Phys. Lett., Vol. 74, No. 20, pp. 3032-3034, 1999.

[12] J.K. Liu, R.B. Stokes and K.M. Lakin, Evaluation of AlN films on sapphire for surface acoustic wave applications, Proc. IEEE Ultrasonics Symp., pp. 234-237, 1975.

[13] R.S. Kagiwada, K.H. Yen and K.F. Lau, High frequency SAW devices on AlN/Al2O3, Proc. IEEE Ultrasonics Symposium, pp. 598-601, 1978.

[14] H.J. McSkimin, W.L. Bond, Elastic Moduli of Diamond, Phys. Rev., Vol. 105, pp. 116-121, 1957.

[15] E.S. Zouboulis, M. Grimsditch, A.K. Ramdas and S. Rodriguez, Temperature dependance of the elastic moduli of diamond : A Brillouin-scattering study, Phys. Rev. B, Vol. 57, No. 5, pp. 2889-2896, 1998.

[16] R.J. Jimenez Rioboo and M. Belmahi, Brillouin spectrosocpy and elastic properties of the nucleation and growth faces of synthetic diamond films, J. Appl. Phys, Vol. 97-073509, 2005.