Available online at www.sciencedirect.com

SCIENCE DIRECT®

Sensors and Actuators A 115 (2004) 456–461

SENSORS AND ACTUATORS A PHYSICAL

www.elsevier.com/locate/sna

Numerical calculation of SAW sensitivity: application to ZnO/LiTaO$_3$ transducers

David A. Powell [a,b,*], Kourosh Kalantar-zadeh [a,b], Wojtek Wlodarski [a,b]

[a] *School of Electrical and Computer Engineering, RMIT University, Melbourne, Australia*
[b] *CRC for Microtechnology, Melbourne, Australia*

Received 1 September 2003; accepted 13 May 2004
Available online 2 July 2004

Abstract

A technique for analysing the sensitivity of a surface acoustic wave (SAW) device is presented, based on the numerically obtained Green's function. It is applied to devices based on a 36°-YX LiTaO$_3$ substrate with a ZnO guiding layer. The capability of these devices for gas and liquid sensing is shown by studying parameters such as mass sensitivity and electromechanical coupling coefficient. Devices were fabricated with film thicknesses ranging from 0 to 8 μm yielding operating frequencies between 101.5 and 78.5 MHz. Phase velocity is calculated as a function of ZnO guiding layer thickness by searching for singularities of the Green's function in wavenumber domain. The calculations were confirmed by measuring the change in centre frequency of fabricated devices. Electromechanical coupling coefficient was measured and found to have a maximum of 7.5% at thickness of $h/\lambda_0 = 0.05$. Mass sensitivity was measured as a function of layer thickness, and found to have a maximum of 70 cm^2/g.

Keywords: SAW sensor; LiTaO$_3$; ZnO; Sensitivity; Layered media

1. Introduction

Layered surface acoustic wave (SAW) devices have previously been developed as high sensitivity gravimetric sensors due to their strong surface acoustic energy confinement. Those with shear-horizontal (SH) particle displacement are suitable for operation in both gas and liquid media. The change in acoustic wave velocity due to mass, elasticity, viscosity, permittivity or conductivity change is measured as a change in frequency response of the device. Due to the complicated nature of SAW propagation in anisotropic materials, modelling the sensitivity of these devices typically requires simplifying assumptions or use of numerical methods. For example, [1,2] demonstrate numerical and experimental analysis of layered devices fabricated on 90° rotated ST-quartz with SiO$_2$ guiding layer.

A ZnO guiding layer has previously been shown to yield higher sensitivity when used with a 90° rotated ST-X quartz substrate [3]. Although devices fabricated on a lithium tantalate (LiTaO$_3$) substrate have lower mass sensitivity than those on quartz [4], their higher electromechanical coupling increases sensitivity to conductometric changes, and allows for smaller devices with low insertion loss.

2. Fabrication

Devices were fabricated on 36°-YX LiTaO$_3$ wafers, using an Al metallisation layer and Cr adhesion layer deposited by electron beam evaporation. Inter-digital transducers (IDTs) with a periodicity of 40 μm were fabricated using a wet-etch process to create delay line devices. ZnO films were deposited by RF magnetron sputtering.

Fig. 1 shows an SEM micrograph of the thin film ZnO grown on LiTaO$_3$. As was previously reported [5], the grain growth and corresponding crystal orientation of ZnO is (0 0 1) on the metallised region and (1 1 0) on the bare substrate. This implies that acoustic wave properties will also differ. Devices were fabricated with film thickness (h) ranging from 0 to 8 μm, with corresponding operating frequencies between 101.5 and 78.5 MHz.

3. Green's function

A common method for calculating SAW parameters is to obtain the Green's function for the desired substrate

---

[*] Corresponding author. Tel.: +61 3 9925 3690; fax: +61 3 9925 2007.
E-mail address: david.powell@ieee.org (D.A. Powell).

0924-4247/$ – see front matter © 2004 Elsevier B.V. All rights reserved.
doi:10.1016/j.sna.2004.05.031

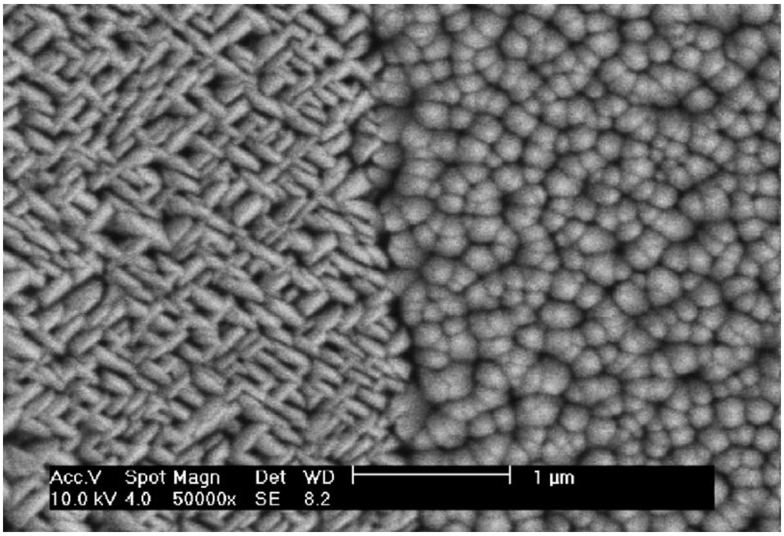

Fig. 1. ZnO growth on bare $LiTaO_3$ (left) and metallised area (right).

[6]. Referring to Fig. 2, the wave propagation is assumed to be in the x_1 direction, with all variation in the x_2 direction being neglected. Each layer of the structure is homogeneous, may be anisotropic and piezoelectric, and occupies a region $x_n < x_3 < x_{n+1}$. Boundary conditions are enforced at each interface [7] such that particle displacement (u_i), normal stress (T_{3j}) and voltage (ϕ) are continuous. Normal electric flux (D_3) is also continuous at each interface except at $x_3 = 0$ (location of IDTs), where it's discontinuity is related to the charge density [8].

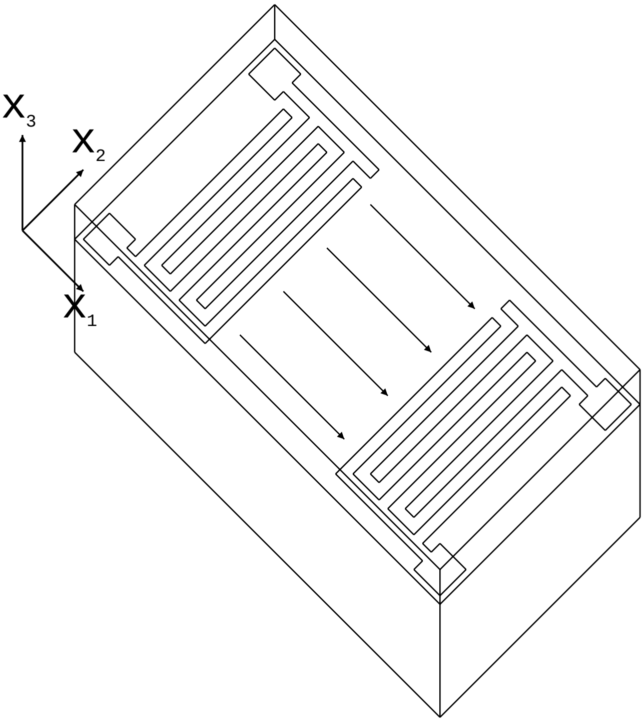

Fig. 2. Stylised representation of SAW device showing coordinate system.

The resultant Green's function is simply a reformulation of the piezoelectric constitutive equations in integral form. In the form used here it gives the voltage response due to a line source of charge located at $x_1 = 0$, $x_3 = 0$. Thus voltage and charge at the interface will satisfy the convolution relation

$$\phi(x_1) = \int_{-\infty}^{+\infty} G(x_1 - x_1')\rho(x_1')\mathrm{d}x_1' \qquad (1)$$

where G is the Green's function and ρ is the charge density. However, G is most readily calculated in the spectral domain, where spatial variable x is Fourier transformed into wave number k. This is typically expressed in normalised form as $s = k/\omega$, where ω is the angular frequency. Thus Eq. (1) becomes

$$G(s_1) = \frac{\phi(s_1)}{\rho(s_1)} \qquad (2)$$

Fig. 3 shows the quantity $k_1 G(s_1)$ for a 2 µm layer of (1 1 0) ZnO on a semi-infinite 36°-YX $LiTaO_3$ substrate, calculated at 103.86 MHz, thus giving a centre wavelength (λ_0) of 40 µm. In particular note the pole[1] at $s = s_f$. By comparison with Eq. (2), we see that this must be due to ρ approaching zero, hence this is a solution satisfying the boundary condition of no charge at the interface. This is denoted a free surface[2] mode and it's propagation velocity is given by $v_f = 1/s_f$. Conversely, the zero crossing of the function at $s_1 = s_m$ corresponds to $\phi = 0$, and thus we have a mode

---

[1] In this example the mode is a leaky SAW, and the poles and zeros are displaced slightly into the complex s plane due to energy loss. However, to first order this effect can be ignored for the low leakage cuts typically employed.

[2] As there is a layer above the substrate surface, free should be taken to mean free of charge.

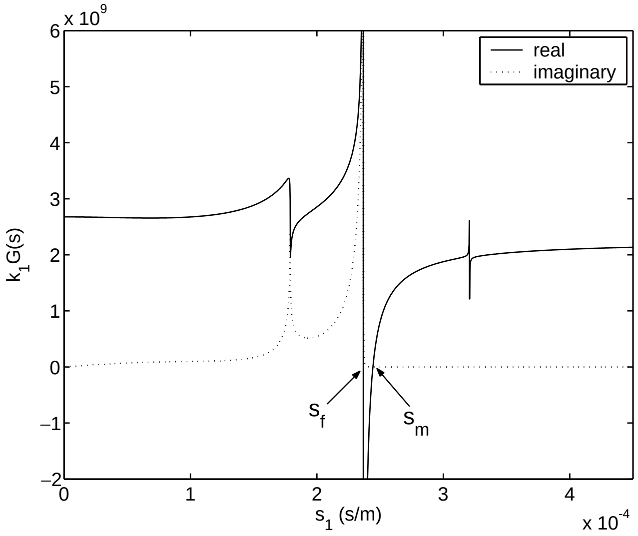

Fig. 3. Green's function for (1 1 0) ZnO layer on a 36°-YX $LiTaO_3$ substrate.

with zero voltage at the interface. This condition corresponds to an infinitely conductive, zero thickness layer at the interface, and $v_m = 1/s_m$ is termed the metallised surface velocity.

In a layered device the Green's function is frequency (and hence wavelength) dependant, and in subsequent sections it will be most useful to consider parameters as a function of normalised layer thickness h/λ_0. Note that a particular subtlety occurring in the case of a ZnO layer on a $LiTaO_3$ substrate is the differing orientation of ZnO on the metal layer substrate. Thus a separate Green's function is required for the (0 0 1) and (1 1 0) ZnO orientations.

4. Phase velocity

For a fixed IDT geometry, the phase velocity of the acoustic waves determines the operating frequency of the device (since $v_P = f_0\lambda_0$). The operating frequency is an important parameter, as higher frequency yields higher sensitivity, but also increases wave attenuation in the presence of viscous losses. Additionally, the most common way of reading sensor response is through frequency change.

Fig. 4 shows the theoretically derived phase velocity for ZnO layers on $LiTaO_3$. Experimental velocities were determined by measuring the frequency of peak radiation conductance (G_a), which is the real part of the input admittance of the device. It was found that the propagation velocity was almost identical to the predicted surface velocity in metallised regions. The slight discrepancy can be attributed to the mechanical loading by the electrodes of the IDT, which is not accounted for in this Green's function.

5. Electromechanical coupling coefficient

The electromechanical coupling coefficient (k^2) is a measure of the interaction between electrical and mechanical fields in a piezoelectric material. In the case of SAW sensors, it is particularly important to have high coupling for conductivity-based measurements [9]. The theoretical values presented in Fig. 5 were estimated from the difference between the pole and zero (s_f and s_m) of the spectral Green's function for both the (0 0 1) and (1 1 0) ZnO orientations:

$$k^2 \approx 2\frac{\Delta v}{v} = 2\frac{v_f - v_m}{v_f} \tag{3}$$

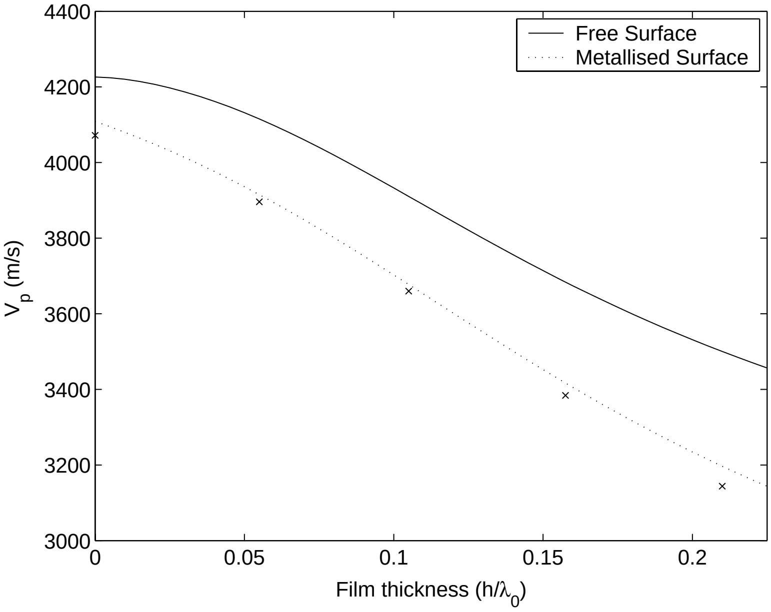

Fig. 4. Measured phase velocity and calculated free and metallised surface velocities.

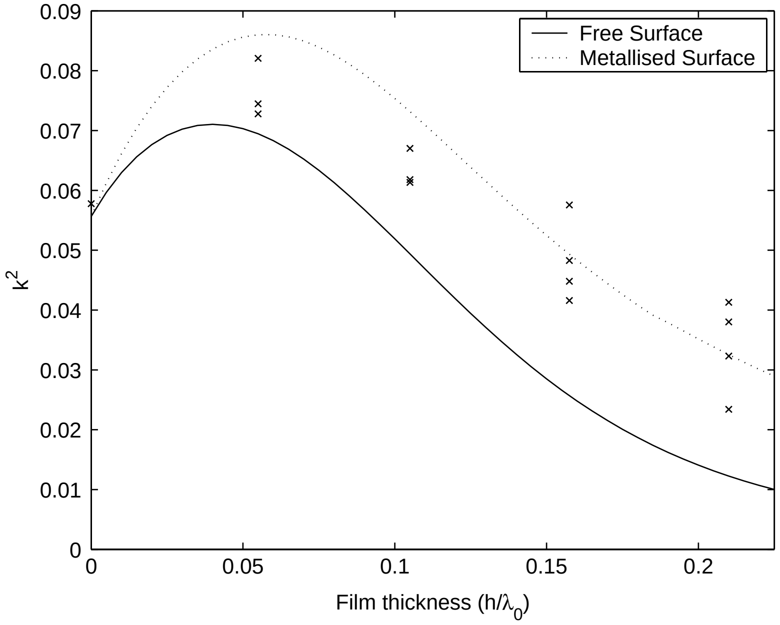

Fig. 5. Calculated and measured electromechanical coupling coefficient.

The electromechanical coupling coefficient was measured via the radiation conductance. According to the crossed-field model, the radiation conductance G_a, at centre frequency f_0, can be expressed as [10]:

$$G_a(f_0) = 8k^2 f_0 C N \tag{4}$$

where N is the number of electrode pairs in the IDT, and C is the input capacitance, which was measured using a 1 MHz capacitance meter. Fig. 5 shows the measured coupling coefficient, which achieves a maximum of ∼7.5% for $h/\lambda_0 = 0.05$. As with propagation velocity, the predicted effect of the (0 0 1) ZnO on the metallised surface shows best agreement with experimental results. This suggests that the properties of the IDTs can be easily predicted by analysing metallised surface case.

The electromechanical coupling is an important parameter in determining the sensitivity of a SAW to a change in conductivity. However, it is necessary to define the interface plane at which the electromechanical coupling is calculated. For modelling the device frequency response the interface of interest is that where the IDTs reside. For conductivity sensitivity applications it is necessary to calculate the Green's function at the upper surface of the device, and calculate the corresponding value of k^2.

6. Mass sensitivity

Layered SAW devices with SH polarisation are typically used for gravimetric measurement, often within liquid media. Mass change is typically due to additional mass attached to or absorbed into the selective layer (not considered in this paper). The resultant change in acoustic wave velocity causes a change in the operating frequency of an oscillator incorporating the SAW device. Other methods of read-out are possible, but typically require more complicated electronics or expensive equipment. For devices operating in oscillation mode, the definition of mass sensitivity is [11]:

$$S_m^f = \lim_{\Delta m \to 0} \frac{\Delta f / f_0}{\Delta m / a} \tag{5}$$

where f_0 is operating frequency and Δf is frequency change due to mass change Δm per area a. In practice, it can be regarded as the fractional frequency change due to a small mass loading per unit area, and is most commonly expressed in units cm^2/g.

Fig. 6 shows both the theoretically derived and experimentally measured mass sensitivity of the devices. Calculation was based on the metallised surface velocity shift determined by the Green's function analysis. The additional mass was modelled as a very thin layer of material upon the surface of the device, with a known density, negligible stiffness, no conductivity and a dielectric constant of unity.

According to perturbation theory [11], the additional mass effect will dominate over the elastic effect of the layer if the velocity of the perturbing layer is much less than that of the material supporting it. Thus, the simulated perturbing layer was chosen to have low stiffness and high density. To verify these results experimentally, a 150 nm SiO_2 layer was sputter-deposited onto the surface of the devices. The frequency shift in the maximum radiation conductance was measured and from this the mass sensitivity shown in Fig. 6 was derived.

The calculated mass sensitivity is greater than that reported for $LiTaO_3/SiO_2$ [4] for h/λ_0 up to 0.2, which is the range more amenable to practical fabrication. It can be

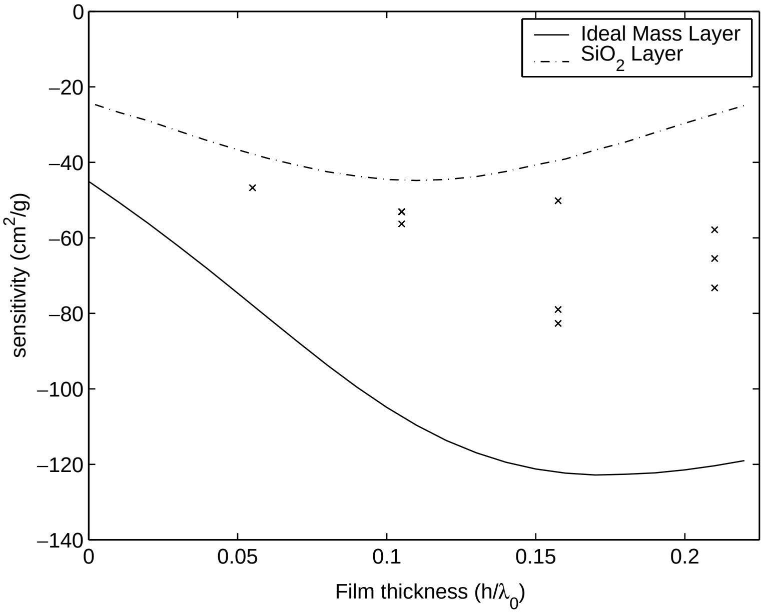

Fig. 6. Calculated and measured mass sensitivity.

seen that the measured sensitivity is much less than that predicted. This is due to the relatively high shear velocity of the deposited layer (2800 m/s), causing an additional elasticity effect.

On the other hand, the dotted curve in Fig. 6, a comparison of the measurements with a simulation including the elastic constants [1] of thin film SiO_2, it can be seen that sensitivity is somewhat higher than predicted. Better agreement could be achieved by assuming a reduced shear stiffness of the deposited SiO_2 layer, however this would need to be independently verified. Some discrepancy may also be attributed to the effect of the measurement probes, as well as the approximation of modelling poly-crystalline ZnO as a homogeneous layer with a flat surface.

It should be noted that the calculated sensitivity was only weakly dependent of the thickness of the material being sensed, up to thicknesses of 0.2 μm. The effect of the elasticity of the sputtered SiO_2 layers is similar to that due to viscosity occurring in practical bio-sensing measurements [12]. This suggests that mass sensitivity does not necessarily correspond to the response observed in an experimental situation. Ogilvy [2] also describes difficulties in reconciling the theoretically derived mass sensitivity of SiO_2/quartz devices with that obtained by deposition of Au thin films.

7. Conclusion

A layered Green's function was used to analyse the performance of SAW sensors, and generally achieved good agreement with experimental results. It was found that the ZnO/$LiTaO_3$ devices had higher mass sensitivity than previously reported SiO_2/$LiTaO_3$ devices for low h/λ_0. As a result, this configuration is a good candidate for a gravimetric sensor operating in liquid media. They also show high electro-mechanical coupling, which is advantageous for many gas sensing applications which operate via a change in the conductivity of the selective layer

Acknowledgements

The authors would like to thank the CRC for Microtechnology, Australia, for their support for this work.

References

[1] G. Kovacs, G.W. Lubking, M.J. Vellekoop, A. Venema, Love waves for (bio)chemical sensing in liquids, Proc. IEEE Ultrason. Symp. (1992) 281–285.

[2] J.A. Ogilvy, The mass-loading sensitivity of acoustic love wave biosensors in air, J. Phys. D: Appl. Phys. 30 (1997) 2497–2501.

[3] K. Kalantar-zadeh, A. Trinchi, W. Wlodarski, A. Holland, A novel love-mode device based on a ZnO/ST-cut quartz crystal structure for sensing applications, Sens. Actuators A: Phys. 100 (2002) 135–143.

[4] F. Herrmann, M. Weihnacht, S. Biittgenbach, Properties of sensors based on shear-horizontal surface acoustic waves in $LiTaO_3$/SiO_2 and quartz/SiO_2 structures, IEEE Trans. Ultrason. Ferroelect. Freq. Contr. 48 (1) (2001) 268–273.

[5] D.A. Powell, K. Kalantar-zadeh, S. Ippolito, W. Wlodarski, A layered SAW device based on ZnO/$LiTaO_3$ for liquid media sensing applications, Proc. IEEE Ultrason. Symp. (2002) 493–496.

[6] R.C. Peach, A general Green function analysis for SAW devices, Proc. IEEE Ultrason. Symp. (1995) 221–225.

[7] T. Pasturead, V. Laude, S. Ballandras, Stable scattering-matrix method for surface acoustic waves in piezoelectric multilayers, Appl. Phys. Lett. 80 (14) (2002) 2544–2546.

[8] V.Y. Zhang, J.-E. Lefebvre, C. Bruneel, T. Gryba, A unified formalism using effective surface permittivity to study acoustic waves in

various anisotropic and piezoelectric multilayers, IEEE Trans. Ultrason. Ferroelect. Freq. Contr. 48 (5) (2001) 1449–1461.

[9] S.J. Ippolito, K. Kalantar-zadeh, A. Trinchi, W. Wlodarski, Layered SAW nitrogen dioxide sensor with WO_3 selective layer, Proc. SPIE 5116 (2003) 904–911.

[10] C.K. Campbell, Surface Acoustic Wave Devices for Mobile and Wireless Communications, Academic Press, San Diego, 1998.

[11] Z. Wang, J.D.N. Cheeke, C.K. Jen, Perturbation method for analyzing mass sensitivity of planar multilayer acoustic sensors, IEEE Trans. Ultrason. Ferroelect. Freq. Contr. 43 (5) (1996) 844–851.

[12] L. Tessier, F. Patat, N. Schmitt, M. Lethiecq, Y.F.D. Guilloteau, Significance of mass and viscous loads discrimination for an AT-quartz blood group immunosensor, Sens. Actuators B: Chem. 18 (1994) 698–703.

Biographies

David A. Powell received his bachelor of computer science and engineering from Monash University in 2001. He is currently working towards a PhD at RMIT University, modelling SAW sensors in liquid media for bio-sensing applications. His research interests include modelling of acoustic wave propagation, SAW device technology and biosensing.

Kourosh Kalantar-zadeh received his bachelor of science and master of science from Tehran University, Tehran, Iran and Sharif University of Technology, Tehran, Iran, respectively. He received his PhD from RMIT University, Melbourne Australia in 2002. Kourosh is a lecturer at RMIT University, Melbourne, Australia. He is currently undertaking a research on surface acoustic wave (SAW) biosensors under the CRC for micro-technology findings. His previous research and development involvements include: SONAR systems, MRI signal processing and ionospheric surveillance systems. He has published more than 30 scientific papers in refereed journals and in the proceedings of international conferences and hold two patents.

Wojtek Wlodarski has worked in the areas of sensor technology and instrumentation for over 30 years. He has published four books and monographs, over 250 papers and holds 28 patents. He is a professor at RMIT University, Melbourne, Australia, and heads the Sensor Technology Laboratory located at the School of Electrical and Computer Engineering.