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A numerical method to derive accurate temperature coefficients of material constants from high-temperature SAW measurements. Application to langasite.

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Abstract— **The design of wireless surface acoustic waves (SAW) sensors for high-temperature applications requires accurate knowledge of the constitutive materials physical properties in the desired temperature range. In particular, it is crucial to use reliable temperature coefficients of the stiffness, piezoelectric, dielectric, and expansion constants of the propagation medium to achieve correct simulations of the considered devices. Currently, the best-suited piezoelectric material for high-temperature SAW applications is langasite (LGS). Unfortunately, the available coefficients do not allow for precise prediction of the temperature dependence of LGS-based SAW devices above 300°C. A novel method, based on a simulated annealing algorithm coupled with a Rayleigh wave simulation program, was developed to find optimal LGS temperature coefficients. This approach has proven to yield accurate results up to at least 800°C.**

Keywords-simulated annealing; high-temperature; langasite; material constants; surface acoustic waves

I. INTRODUCTION

The need for passive wireless sensors able to operate at very high temperature is steadily growing. Surface acoustic wave (SAW) technology constitutes a promising way to meet this need. The best results so far have been obtained with sensors based on langasite ($La_3Ga_5SiO_{14}$; LGS). Recently, a SAW signal was recorded up to 1140°C [1] and a first commercial sensor able to operate above 800°C for long-time periods was developed [2]. Accurate simulations at high temperatures are now needed to enable the design of even better SAW sensors. Unfortunately, such simulations are currently impossible to perform

as the first and second order temperature coefficients of the material constants (stiffness, piezoelectric, dielectric, and expansion constants) of LGS are not precisely known. Several groups worldwide have spent a lot of efforts measuring the first [3] and second [4-6] order temperature coefficients of LGS. It is also possible to extract third order coefficients from the data published in [7]. However, none of the published sets of coefficients (which significantly differ from each other) allow for a precise prediction of the behavior of SAW on LGS at temperatures higher than 300°C [8-10].

To overcome this current limitation, we developed a new computer-assisted method to derive optimized temperature coefficients of LGS material constants. This method yielded excellent results up to at least 800°C and is described in the following section.

II. METHOD PRINCIPLES

The basic idea of the method is to start from the best set of available temperature coefficients and to then tune it in order to optimally fit the available experimental data (i.e. to reduce the distance or error between simulated and experimental data). For this purpose, simulated annealing (SA) was chosen as an algorithm to optimize the set of temperature coefficients because of its ability to avoid local minimums and converge efficiently towards the optimum of a given multivariable function in a large search space [11]. In our case, a SA function readily available in the Matlab environment was used [12]. The function was only slightly modified to comply with our needs. The number of variables was changed as well as the "initial guess" calculation formula. The latter was modified in order for the calculation to start from a chosen set of values. The SA function generated new sets of test-coefficients to be used by a specific calculation program (SCP) to compute the corresponding simulated data and the resulting global error. The error was fed back into the SA function, thus enabling the optimization process to run adequately. The SCP was also developed in Matlab environment (R2011b). Once provided with the stiffness, piezoelectric, dielectric, and expansion constants as well as the respective temperature coefficients, the SCP allowed for calculating the temperature coefficient of delay (TCD) and the fractional frequency change (FFC) for Rayleigh modes whatever the cut, propagation direction and temperature. The SCP was

based on the well-known Campbell and Jones method [13]. A full description of the calculation steps can also be found elsewhere [14].

To ensure good convergence towards the global minimum, it is important to use relevant experimental data. These data must be accurate and diverse. Ideally, they are measurements of various physical quantities, each of them dependent on the coefficients to be optimized. For instance, SAW velocities (or the associated FFC) can be measured on different crystal cuts. Accordingly, we used the FFC measured in a wide temperature range for five different LGS crystal cuts [8, 15-16]. The Euler angles of the cuts were (0,22,31), (0,90,0), (0,138.5,26.6), (0,144,24), and (0,22,90). The FFC was provided for Rayleigh modes on the first four cuts, and for shear horizontal (SH) mode on the fifth cut. It was decided to use the first three cuts as targets for the optimizer and the two remaining cuts to subsequently test and validate the optimized set of coefficients. Note that the selected experimental data were obtained using low-thickness transducers ($h/\lambda \sim 0.6\%$). Consequently, the electrodes had a negligible influence on the temperature behavior of the considered devices. In our case, this was an important point for proper derivation of accurate temperature coefficients of LGS material constants. Indeed, the electrodes were not simulated in the SCP.

To define the optimization starting point, the SCP was used to test all available sets as well as combinations of them. The best results were obtained using the combination of stiffness, piezoelectric, and dielectric constants (and temperature coefficients) from Bungo *et al.* [5] with the expansion coefficients from Krausslich *et al.* [6] (see Fig. 1). As mentioned before, the SCP was used to (1) compute the FFC of the three target cuts in the [20-800°C] range for each new set of coefficients, (2) compare the simulated and experimental results, and (3) compute the error. To reduce computation time, the following special property of the TCD on LGS cuts was used: it was experimentally observed that the TCD evolution with temperature is linear on LGS cuts. As a consequence, the FFC is parabolic. It is therefore possible to compute the whole FFC plot in a desired temperature range by calculating only a very limited number of TCD values in the range of interest, then linearly fitting the results and properly integrating the obtained linear equation. In our case, one point was calculated every 100°C, from -50 to +850°C. The

computation was made on a standard commercial FUJITSU Desktop, equipped with an Intel Core i5-2500 CPU, clocked at 3.3GHz. About thirty seconds were needed per iteration (i.e. to calculate the three cuts in the whole temperature range for each new set of test-coefficients). At the end of each iteration, a mean squared error (MSE) was calculated for each of the three cuts. The total error to be minimized was simply taken as the sum of the three MSE(s). The error was steadily and quickly reduced over the first 500 iterations (see thick black line in Fig. 2). The algorithm managed to further reduce the error over the next 2000 iterations. It finally reached a plateau after 3000 iterations.

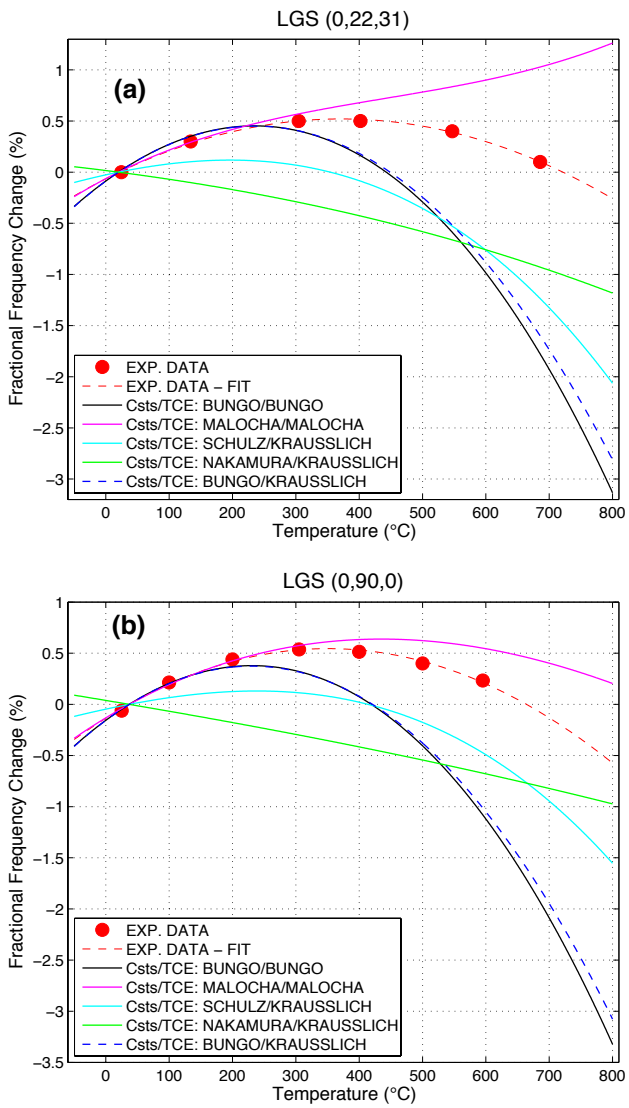

Fig. 1. Simulated results for LGS cuts, obtained with different sets of published material constants (Csts) and temperature coefficients of expansion (TCE) – (a) (0,22,31), (b) (0,90,0).

Besides, a first useful step before running the optimization was to slightly change the different coefficients and then use the SCP to evaluate the effect on the simulated results. This helped selecting the most impacting coefficients to be optimized and thus further reducing the computing effort. If needed, the less impacting coefficients might be optimized in a second step, to fine-tune the results. Practically, the optimization was performed on the first and second order temperature coefficients of the independent stiffness constants (TCS) only – c_{11}, c_{13}, c_{14}, c_{33}, c_{44} and c_{66} in the case of LGS. Indeed, it was observed that the temperature coefficients of the piezoelectric and dielectric constants do not significantly alter the FFC in the [20 – 800°C] temperature range. It was also observed that an optimization conducted on both the stiffness constants and expansion coefficients do not yield significantly better results than the ones conducted on the stiffness coefficients alone, although the convergence is a bit faster (see thin red line in Fig. 2). Since it is not necessary to modify the expansion coefficients to obtain a good reduction of the error, it was decided not to alter these coefficients at all.

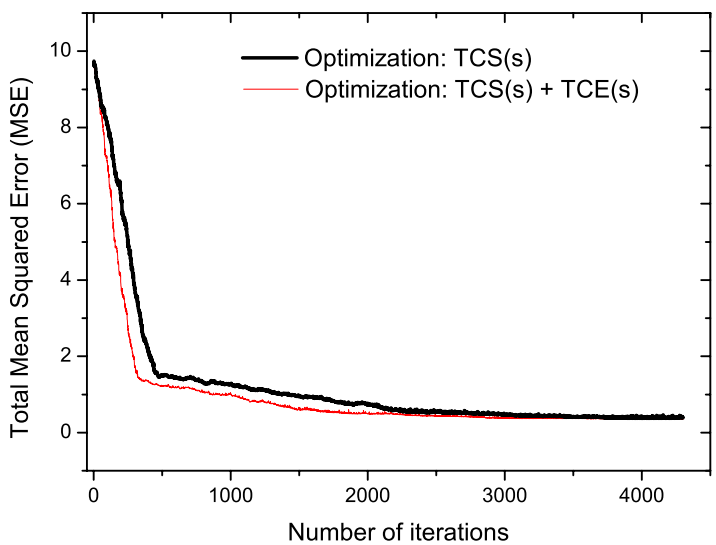

Fig. 2. Error reduction vs. number of iterations – thick black line: optimization of the TCS(s) only; thin red line: simultaneous optimization of the TCS(s) and TCE(s).

III. RESULTS AND DISCUSSION

The obtained coefficients are presented in Table I. They are optimized temperature coefficients of the Bungo *et al*. stiffness constants. They must be used in conjunction with the Bungo *et al*. values for the piezoelectric and permittivity parameters (constants and temperature coefficients), as well as the Krausslich *et al*. values for the temperature coefficients of expansion. All of these coefficients are also presented in Table I.

Tab. I. Optimized set of LGS material constants. Stiffness, piezoelectric, permittivity and density constants are from Bungo *et al.* [5], as well as temperature coefficients for piezoelectric and permittivity parameters. TCS were determined within this study. Temperature coefficients of expansion are from Krausslich *et al.* [6].

Units: **c → 10^{10} [N/m^2]** **e → [C/m^2]** **ρ → [kg/m^3]**	Material constants @ 20°C	1st order (ppm/°C)		2nd order (ppb/°C^2)	
		This study	Bungo *et al.*	**This study**	Bungo *et al.*
c_{11}	18.89	**- 65**	- 57.54	**- 39**	- 82.65
c_{13}	10.15	**- 84**	- 81.61	**- 86**	- 68.1
c_{14}	1.442	**- 304**	- 307.5	**88**	95.34
c_{33}	26.83	**- 105**	- 104.0	**- 55**	- 89.61
c_{44}	5.33	**- 63**	- 57.39	**- 80**	- 130.5
c_{66}	4.237	**- 29**	- 7.576	**- 23**	- 119.4
e_{11}	- 0.4371	469.8		- 428.5	
e_{14}	0.1039	- 713.8		1594	
$\varepsilon_{11}/\varepsilon_0$	19.05	134.5		118	
$\varepsilon_{33}/\varepsilon_0$	51.81	- 787.0		658.6	
α_{11}	-	5.20		6.7	
α_{33}	-	3.72		1.1	
ρ	5764				

Note that the only significant discrepancy between the optimized first order coefficients and the original ones from Bungo *et al.* is for c_{66}. However, for the second-order coefficients, the difference is much higher. As the constants and higher-order coefficients constitute a coherent whole, it is possible that in Bungo *et al.,* a significant measurement error on c_{66} has generated a cascade of errors in the second order coefficients. This will be analyzed further in future work.

As can be seen in Fig. 3, there is an excellent agreement between the experimental data and the simulated results obtained with the new set of coefficients for the cuts (0,22,31) and (0,138.5,26.6). This certainly can be seen as a direct consequence of the optimization procedure. Indeed, both presented cuts were used as targets for the optimizer.

The results presented in Fig. 4 for the cuts (0,144,24) and (0,22,90) definitely confirm the quality of the obtained constants. Both plots were indeed calculated *a posteriori* for cuts that were not considered in the optimization process.

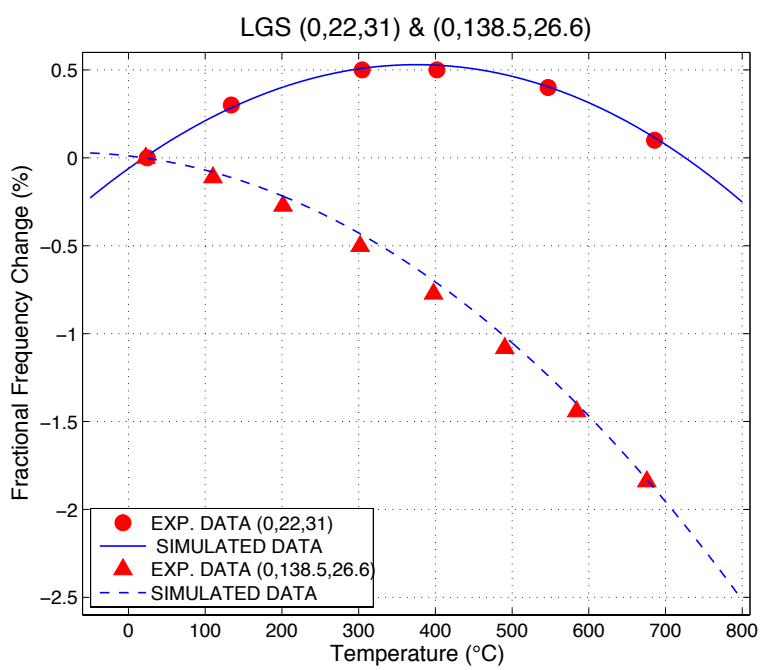

Fig. 3. Experimental results vs. simulated results obtained with the optimized set of TCS(s), for the cuts (0,22,31) and (0,138.5,26.6). Both cuts were used as targets for the optimizer.

As no Rayleigh wave can propagate along the (0,22,90) direction, another software (COM/FEMSDA) developed by K. Hashimoto [17] was slightly modified and used to compute the SH-SAW characteristics in the desired temperature range. Again, simulations fitted almost perfectly the experimental results.

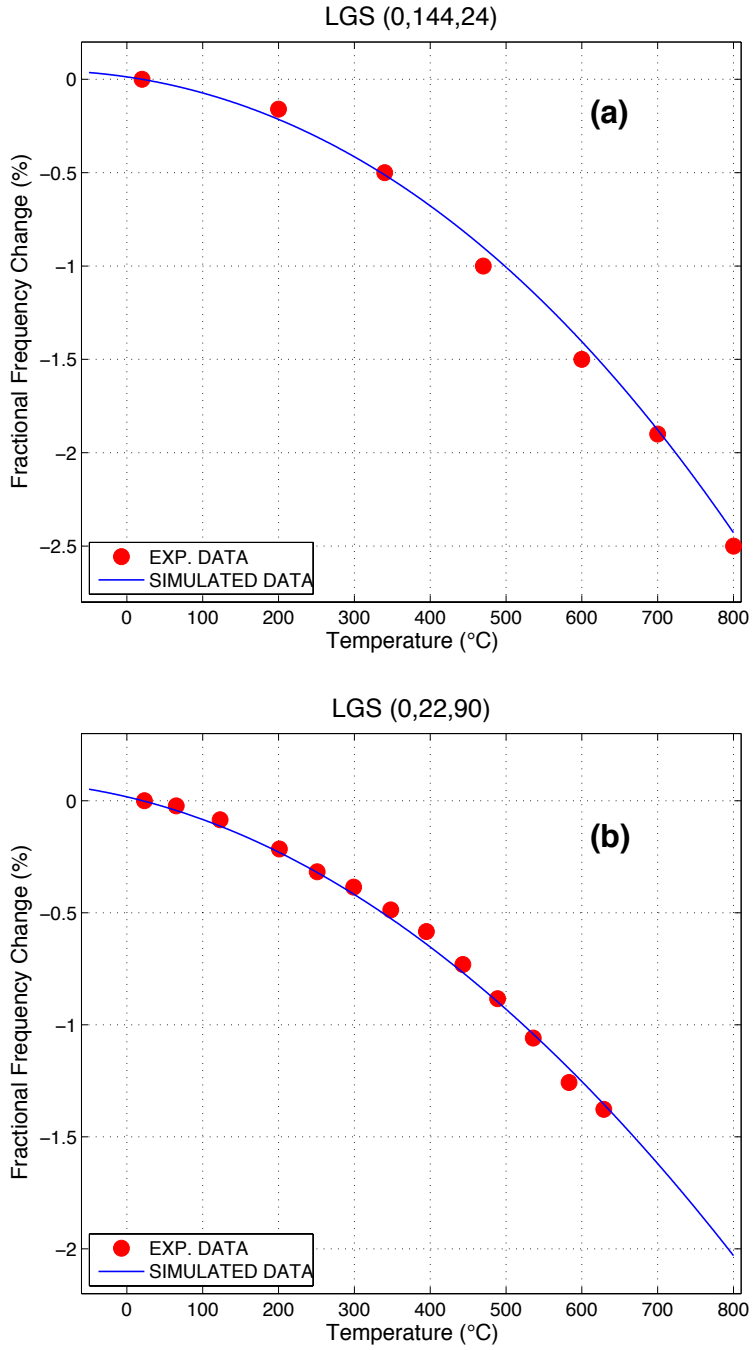

Fig. 4. Experimental results vs. simulated results obtained *a posteriori* with the optimized set of TCS(s), for the cuts (0,144,24) (a) and (0,22,90) (b).

However, the agreement between experimental and simulated results is not as good in the (0,90,0) case, although this cut was also taken as an optimization target (see Fig. 5). This cut actually was the limiting factor that prevented the optimizer to further reduce the error towards zero. It is suggested that the lack of perfect convergence might be linked to the imperfection of the experimental data themselves. This will be verified in future work. A confirmation of the latter hypothesis would indicate that the optimization procedure could also be used to check *a posteriori* the quality of experimental data obtained for new cuts.

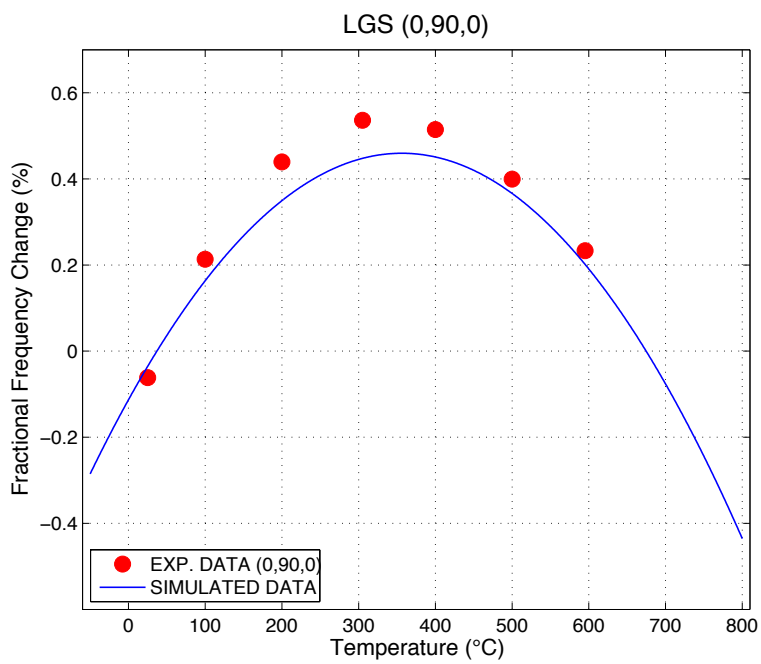

Fig. 5. Experimental results vs. simulated results obtained with the optimized set of TCS(s) for the cut (0,90,0).

IV. CONCLUSION

A new set of temperature coefficients of LGS material constants was numerically derived. To do so, a SA function, generating new sets of test-coefficients, was coupled to a SCP that enables the calculation of Rayleigh modes characteristics throughout any temperature range. The final set resulting from the SA optimization procedure yielded excellent results. Accurate simulations of the temperature dependence of various Rayleigh and SH-SAW LGS cuts were performed between the ambient and 800°C.

Besides, the scope of the method used to derive this new set of temperature coefficients can be much larger. It basically makes it possible to easily derive accurate temperature coefficients from imperfect measurements, once the measurements are numerous and diverse enough. This might be of great interest for other scientific communities having to deal with high-temperature materials and applications.

Future work will include the search of optimized parameters for other SAW crystal materials as well as multilayered SAW substrates. The convergence process will also be thoroughly studied. Amongst others, it will be checked whether the optimizer converges towards the same global minimum when starting from another set of initial parameters.

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REFERENCES

[1] T. Aubert, J. Bardong, O. Elmazria, G. Bruckner and B. Assouar, "Iridium interdigital transducers for high-temperature surface acoustic wave applications," *IEEE Trans. Ultrason. Ferroelectr. Freq. Control*, vol. 59, no. 2, pp. 194-197, Feb. 2012.

[2] http://www.environetix.com

[3] N. Nakamura, M. Sakamoto, H. Ogi and M. Hirao, "Elastic constants of langasite and alpha quartz at high temperatures measured by antenna transmission acoustic resonance," *Rev. Sci. Instrum.*, vol. 83, art. no. 073901, 2012.

[4] D.C. Malocha, M.P. Da Cunha, E. Adler, R.C. Smythe, S. Frederick, M. Chou, R. Helmbold and Y.S. Zhou, "Recent measurements of material constants versus temperature for langatate, langanite and langasite," in *Proc. IEEE Int. Frequency Control Symp.*, 2000, pp. 200-205.

[5] A. Bungo, C. Jian, K. Yamaguchi, Y. Sawada, R. Kimura and S. Uda, "Experimental and theoretical analysis of SAW properties of the langasite substrate with Euler angle (0°,140°,θ)," in *Proc. IEEE Ultrason. Symp.*, 1999, pp. 231-234.

[6] J. Kräusslich, S. Höfer, U. Zastrau, N. Jeutter and C. Baehtz, "Temperature dependence of lattice parameters of langasite single crystals," *Cryst. Res. Technol.*, vol. 45, no. 5, pp. 490-492, 2010.

[7] M. Schulz and H. Fritze, "Electromechanical properties of langasite resonators at elevated temperatures," *Renewable Energy*, vol. 33, pp. 336-341, 2008.

[8] T. Aubert, F. Sarry, O. Elmazria, L. Bouvot, B. Assouar, P. Nicolay and M. Hehn, "Extraction of COM parameters on Pt/LGS for high-temperature SAW sensor," in *Proc. IEEE Ultrason. Symp.*, 2008, pp. 820-823.

[9] S. Sakharov, N. Naumenko, A. Zabelin and S. Zhgoon, "Characterization of langasite for application in high temperature SAW sensors," in *Proc. IEEE Ultrason. Symp.*, 2011, pp. 2289-2292.

[10] M.Weihnacht, A. Sotnikov, H. Schmidt, B. Wall and R. Grünwald, "Langasite: high temperature properties and SAW simulations," in *Proc. IEEE Ultrason. Symp.*, 2012, in press.

[11] D. Bertsimas and J. Tsitsiklis, "Simulated annealing," *Statistical Science*, vol. 8, pp. 10-15, 1993.

[12] X.S. Yang, *Simulated Annealing for Constrained Optimization*, http://www.mathworks.de/

[13] J.J. Campbell and W.R. Jones, "A method for estimating optimal crystal cuts and propagation directions for excitation of piezoelectric surface waves," *IEEE Trans. Sonics Ultrason.,* vol. SU-15, pp. 209-217, 1968.

[14] D. Royer and E. Dieulesaint, *Elastic Waves in Solids, Tome 1*, Berlin Heidelberg: Springer, 2010.

[15] J. Bardong, T. Aubert, N. Naumenko, G. Bruckner, S. Salzmann and L. M. Reindl, "Experimental and theoretical investigations of some useful langasite cuts for high-temperature SAW applications," *IEEE Trans. Ultrason. Ferroelectr. Freq. Control*, vol. 60, no. 5, in press, Apr. 2013.

[16] M. Pereira da Cunha, R. J. Lad, T. Moonlight, S. Moulzolf, A. Canabal, R. Behanan, P. M. Davulis, D. Frankel, G. Bernhardt, T. Pollard and D. F. McCann, "Recent advances in harsh environment acoustic wave sensors for contemporary applications," in *Proc. IEEE Sensors*, 2011, pp. 614-617.

[17] K. Hashimoto, *Surface Acoustic Wave Devices in Telecommunications*, Berlin Heidelberg: Springer, 2000.