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Comparative Analysis of the Search Procedures for Surface Acoustic Wave Solutions in Piezoelectric Crystals

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Abstract—Various search procedures for finding the global extremum of a multivariate target function (TF) necessary for calculating the characteristics of surface acoustic waves (SAW) and leaky surface acoustic waves (LSAW) in crystals are analyzed. The search procedures aimed at determining the optimal orientations for SAW in crystals are considered. A comparative analysis of the promising methods for finding the global extremum of the TF is performed. © *2001 MAIK "Nauka/Interperiodica".*

One of the specific features of the SAW technology is that, prior to designing any SAW device (a generator, delay line, filter, etc.), it is necessary to determine the orientation in the piezocrystal space for the wave propagation with optimal characteristics. The optimal characteristics of SAW and leaky SAW (LSAW) are known to be as follows [1]: thermal stability in a wide range of temperatures (expressed by the temperature coefficient of frequency TCF), a high electromechanical coupling factor K^2, a small angle between the directions of the group and phase velocities pfa, and a small diffraction loss characterized by the anisotropy factor ($\gamma = -1$). In the case of LSAW, it is also necessary to have a low damping factor δ along the direction of wave propagation. It is well known that, to find the wave parameters K^2, pfa, γ, and TCF, one should first determine the phase velocity of the wave V and the damping factor δ.

To determine V and δ, and also the optimal orientation for SAW and LSAW in the piezocrystal space, various search procedures for finding the global extremum of a multidimensional target function (TF) can be used [2–7]. The value of TF depends on the three Euler angles, f1, f2, and f3; [8] describing the crystal cut and the direction of wave propagation; and also on the values of material constants of the piezocrystal. The parameters of the TF are the wave velocity V and the damping factor δ. In its turn, finding the extremum of the TF in terms of the optimal characteristics of SAW and LSAW is a separate complicated computational problem of a multiparameter search for the extremum of the TF [2, 9].

The object of this work is to perform a comparative analysis of several search methods for finding the global extremum of a multivariate function with the aim to solve the above-mentioned problems.

We use the equations describing the propagation of an acoustic wave in a piezocrystal [1]:

$$\rho\frac{\partial^2 u_j}{\partial t^2} - C_{ijkl}\frac{\partial^2 u_k}{\partial x_i \partial x_l} - e_{klj}\frac{\partial^2 \varphi}{\partial x_i \partial x_k} = 0,$$
$$e_{ikl}\frac{\partial^2 u_k}{\partial x_i \partial x_l} - \varepsilon_{ik}\frac{\partial^2 \varphi}{\partial x_i \partial x_k} = 0. \quad (1)$$

Here, C_{ijkl}, e_{ikl}, and ε_{ik} are the material constants of the piezocrystal, u_i are the mechanical displacements, φ is the potential, ρ is the substrate density, t is time, and x_j are the spatial coordinates. The indices are i, j, k, l = 1, 2, 3.

To calculate the characteristics of SAW and LSAW propagating at the free surface of a piezocrystal, we should solve the system of equations (1) formulated for an anisotropic piezoelectric medium. If a layer of finite thickness covers the surface of the piezocrystal, a problem of the propagation of SAW in the layer–piezoelectric substrate structure should be solved. In this case, we have two systems of equations (1) relating respectively to the layer material and the substrate material. In both cases, the equations that describe the wave propagation cannot be solved analytically and require the utilization of numerical methods.

Directing the x_1 axis along the wave propagation at the surface (the x_3 axis is normal to the surface), we can write the required solutions for the displacement amplitudes and for the potential in the piezocrystal space as follows:

$$u_j = \alpha_i \exp(jk\beta x_3)\exp\{jk[(1+i\delta)x_1 - Vt]\},$$
$$\varphi = \alpha_4 \exp(jk\beta x_3)\exp\{jk[(1+i\delta)x_1 - Vt]\}. \quad (2)$$

Here, $k = \omega/V$ is the wave number, and ω is the circular frequency. The first exponents in Eqs. (2) describe the decrease in amplitude along the x_3 direction with the damping factors β determined by their imaginary parts, and α_1 and α_4 are the unknown amplitude factors.

The substitution of Eqs. (2) into Eqs. (1) leads to a system of dispersion equations, which is a homogeneous system of algebraic equations in the unknown variables β for the predetermined values of V and δ. Further, it is necessary to use the boundary conditions at the mechanically and electrically free surface of the crystal [1]: the zero values of the normal components of the stress tensor T_{3i} and the continuity of the normal component of the electric displacement D_3. As a result, we obtain a system of homogeneous complex equations, which has a nontrivial solution only when its determinant, depending on the velocity V and the coefficient δ, is zero:

$$F(V, \delta) = 0. \qquad (3)$$

Here, $F(V, \delta)$ is the determinant or the function of the boundary conditions. Generally, $F(V, \delta)$ is a complex function of two real variables, V and δ. According to Eq. (3), the values of V and δ should be found for which both real and imaginary parts of the function $F(V, \delta)$ become zero. The function of the boundary conditions $F(V, \delta)$ is taken as the TF. To solve the Eq. (3), we use a variety of techniques to search for the global extremum of the multivariate target function. We seek the global extremum (the zero minimum) of the TF that is the square of the magnitude of the complex function $F(V, \delta)$. Note that, in the case of the SAW solution ($\delta = 0$), one should minimize the function of one variable $|F(V)|^2$, and in the LSAW case, the function of two variables $|F(V, \delta)|^2$ should be minimized.

The most used search procedures for finding the global extremum of the TF can be classified as follows [5]:

(1) methods of transition from one local minimum to another;

(2) random search methods;

(3) methods based on statistical models of the TF;

(4) covering methods; and

(5) methods of an incomplete directed scanning of the search area.

The main problem in the development of efficient procedures for global search is related to the necessity of assessing a great number of variants. It is generally recognized [5] that none of the search methods possesses such advantages over the other ones to be considered a universal means for solving any problems. Besides, the total number of the TF calculations required to determine the coordinates of the extremum point grows as a power function of the dimensionality of the search area for the majority of the global search procedures.

For the solution of complex optimization problems, such search procedures are required that possess the following set of necessary features:

(1) a high reliability of the extremum search;

(2) the minimal sensitivity to the details of the TF relief, including the ravine situations, the small-slope regions, and the local-extremum regions;

(3) the ability to work in a space of high dimensionality;

(4) the minimal number of adjustable parameters; and

(5) low cost of the search.

This combination of features of the search procedures is contradictory to a considerable extent and, hence, difficult to realize.

The LSAW, contrary to SAW, attenuate along the direction of wave propagation x_1 at the surface ($\delta > 0$). Two types of LSAW are known [9]: the pseudosurface acoustic waves (PSAW) and the high-velocity pseudosurface acoustic waves (HVPSAW). In the SAW and LSAW search area, the TF is almost always a multiextremal function. Furthermore, a complex behavior of the TF for some orientations is attributable to the fact that, for these orientations, the system of dispersion equations becomes ill-conditioned, the corresponding matrix is almost singular, and the problem as a whole becomes ill-posed.

The complications arising in the search for the LSAW solutions in piezocrystals can be illustrated by a specific example. Figures 1 and 2 demonstrate the reliefs of the TF, $F(V, \delta) = 0$, calculated for a $LiNbO_3$ crystal cut with the (0°, –49°, 0°) orientation and covered with an aluminium layer ($h = 0.01\lambda$, where λ is the wavelength) in the velocity V and damping factor δ domain. Figures 1 and 2 relate to the PSAW and to the HVPSAW cases, respectively. It is seen from the figures that the TF reliefs have a rather intricate shape (with many deep and narrow local extremums). This fact limits the possibility of the application of many currently known procedures of global search [5, 6]. The methods of transition from one local minimum to another use in most cases the derivatives of the TF, which is inefficient in the flat-plateau situations. The methods based on statistical models of the TF and the random search methods too strongly depend on the adjustable parameters in the situations with a large number of narrow deep extremums, which makes them inoperative in the absence of *a priori* information on the TF behavior. It only remains to rely on some specific versions of the covering methods and on the methods of an incomplete directed scanning of the search area. In deciding on a particular search procedure, one should also take into account one more specific criterion of efficiency, the computational speed. The search procedures should quickly process their specific information. The high speed requirement for a search procedure is reduced to its software implementation possessing such operating speed that allows the absolutely predominant share of computation time to be allocated to the fulfilment of the model procedure of the user.

Below, we briefly describe three search procedures for finding the global extremum of the TF given

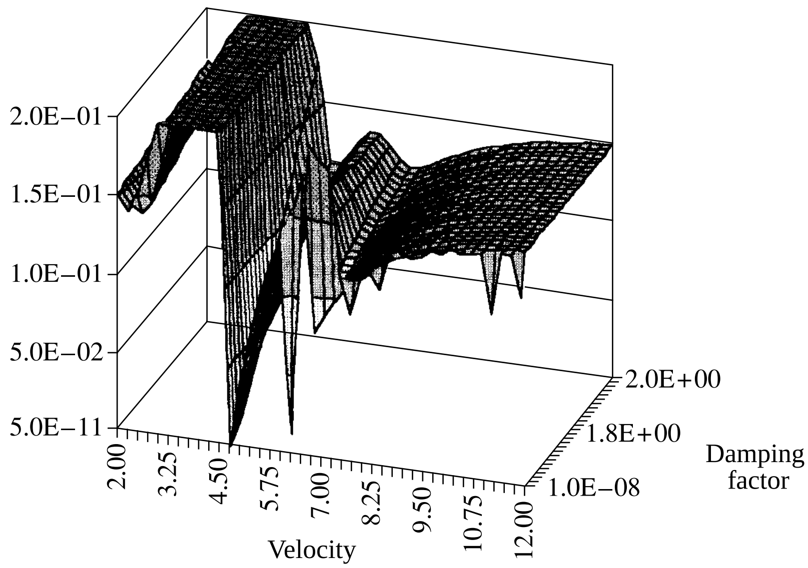

Fig. 1. Relief of the target function $F(V, \delta)$ used in the search for an LSAW solution in a $LiNbO_3$ crystal with the (0°, –49°, 0°) orientation.

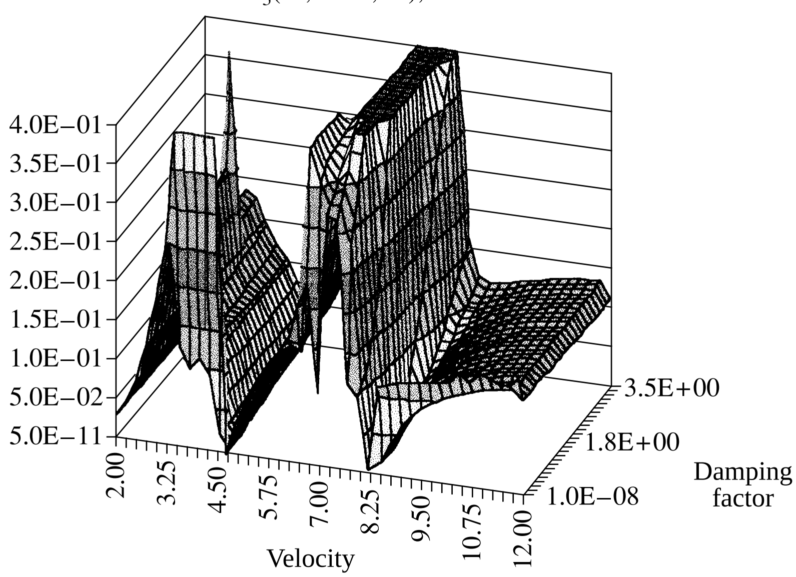

Fig. 2. Relief of the target function $F(V, \delta)$ used in the search for an HVPSAW solution in a $LiNbO_3$ crystal with the (0°, –49°, 0°) orientation.

by Eq. (3) in the calculation of the main characteristics of LSAW.

(1) One of the possible implementations of the covering method is the Hooke–Jeeves Search (HJS) [2–4]. The HJS is a version of the local extremum search by the method of configurations in space. However, this technique can also be adapted for seeking the global extremum of the TF by performing a global exhaustive search over a determinate searching mesh in combination with the local search over the promising points. The local search can be performed by the HJS with the automatic inclusion of the Mudgel procedure in the case of the configuration method failure in ravine situations [4]. The investigated area is covered by a uniform searching mesh. Then, a local search is performed, beginning from an arbitrary point in the area and leading to a local extremum. The values of the TF at the mesh nodes are compared with the values at the

local extremum found. If a point is found that is better than the previous one, the local search is continued from this point on, leading to a new better local extremum, and so on. As a result, after the exhaustive search over the whole mesh is completed, the last of the extremums found will be the global one. A distinctive feature of this procedure is its simplicity, which makes it possible to create a short program implementing this algorithm. In the HJS procedure, the search is performed over a large number of points, but only once and without any additional processing.

(2) Another global-search implementation of the covering method is the Nelder–Meed Search (NMS). This procedure implies the definition of a mesh of starting points followed by the search for a local extremum on the basis of the deformed-polyhedron technique [6]. The local search consists in the determination of the TF values at sampling points belonging to the search area and being the vertices of a polyhedron. The special operations that deform the polyhedron in the space of variables and shift it to the region of the most probable location of an extremum finally result in an exact determination of the coordinates of this extremum. A distinctive feature of the procedure is its low sensitivity to the details of the TF relief: the ravines and the small-slope regions are successfully overcome. The procedure is reliable for the space dimensionality up to ten, the cost of the search being very low. In terms of the global search organization, the competition of starting points is realized.

(3) One of the possible implementations of the method of incomplete directed scanning of the search area is the determinate procedure of seeking the global extremum over the discrete mesh defined by the Grey binary code, the Global Discrete Search (GDS) [7]. A characteristic feature of this procedure is the discretization of variables. In this case, the whole space is covered with the regular mesh whose nodes characterize definite states of the described object. The discretization step in each variable represents the accuracy of the extremum determination. Any discrete state of the object can be unambiguously represented by the binary numbers of the discrete states of each variable, these numbers being recorded in series. In the search procedure under consideration, the state of the object is recorded in terms of the Grey reflexive binary code [7]. Thus, the problem of finding the minimum is reduced to the combinatorial problem of finding a binary word of predetermined length, which satisfies the condition of the minimal value of the TF. The operation of the search procedure consists in the creation of a set of sampling points with an adjustable density of positions relative to the point that is the best at the moment. The specific processing of the information about the values of the TF at the sampling points provides the advance into the region of the most probable location of the global extremum. The advance towards the extremum takes place not along the relief of the TF, but within a cloud that moves with all its points in the direction of the expected position of the extremum. The program implementing this algorithm provides an effective operation in the space of high dimensionality (about ten) and is characterized by a nearly linear growth of the search cost with the number of dimensions of the problem being solved. The only adjustable parameter is the discreteness of the search space.

The comparison of the search procedures for finding the global extremum of the TF was performed by the example of the search of LSAW solutions at the open surface of a $LiNbO_3$ piezocrystal with the (0°, –49°, 0°) orientation. For the LSAW problem, the search for the global minimum was carried out in a two-parameter region formed by the velocity V (km/s) and the damping factor δ (dB/λ, where λ is the wavelength). The coordinates of the initial starting point were chosen at random. The required accuracy of calculating the extremum coordinates corresponded to the accuracy of real data provided by the IBM PC.

In the course of the HJS search procedure for the LSAW problem, after performing 281 calculations of the TF, the parameters $V = 4.7515$ km/s and $\delta = 2.4 \times 10^{-4}$ dB/λ were found with the TF value about 1.2×10^{-18}. For the HVPSAW problem, after performing 4263 calculations of the TF, the parameters $V = 8.314$ km/s and $\delta = 0.531$ dB/λ were found with the TF value of 1.2×10^{-18}. In both cases, the values obtained correspond to the global optimal solutions for the respective types of waves. The considerable search cost in the HJS procedure is explained by the small spacing of the initial searching mesh used for starting the procedure of the local search.

The NMS search procedure was performed with ten starting points. Their coordinates corresponded to a uniform mesh superimposed on the search area. In the course of the LSAW search, a total of 1510 calculations of the TF were made, which corresponds to an average of 151 calculations of the TF at each local descent. All ten descents were completed in the accuracy-tolerable vicinity of the global optimal point with the final values of the TF being of the order of 10^{-17}–10^{-19}. For the HVPSAW problem, 1700 calculations of the TF were made, which corresponds to an average of 170 calculations of the TF at each local descent. As a result, a high probability of hitting the basin of the global extremum was demonstrated: nine out of ten descents were completed in the accuracy-tolerable vicinity of the global optimal point with the final values of the TF being of the order of 10^{-14}–10^{-18}, and only one led to the point of a false local minimum.

In the case of the GDS procedure, the discretization of variables corresponded to the required accuracy of calculating the coordinates of the global extremum. The search was performed with ten starting points, which were generated by the program on the basis of a predetermined initial point and scattered approximately uniformly over the search area. In the course of the LSAW search, a total of 2770 calculations of the TF

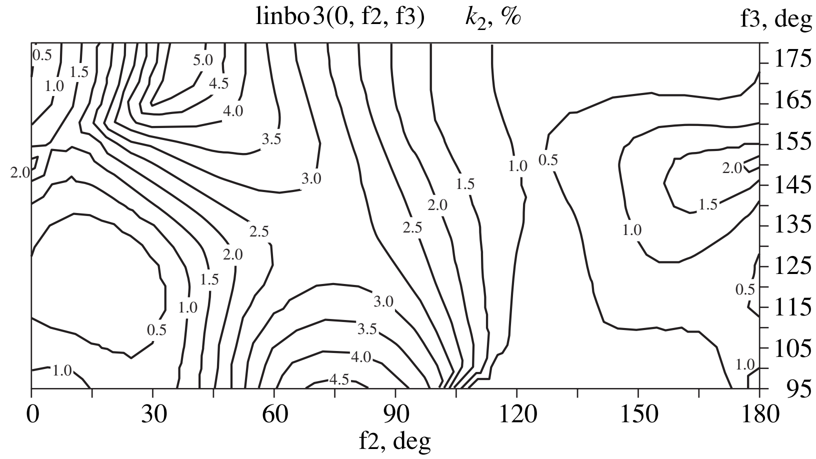

Fig. 3. Lines of equal value for K^2 in the $LiNbO_3$ crystal (f1 = 0°, f2 = 0°–180°, and f3 = 95°–180°).

were made. In this case, the search of one extremum (or the confirmation of one already found) took on average about 214 calculations of the TF, and the check of the width of a newly-found one took about 630 calculations. As a result of the search beginning from all ten starting points, the global extremum was found. In the course of the HVPSAW search, a total of 4915 calculations of the TF were made with the search of an extremum taking on average about 304 calculations of the TF and the check of its width taking about 625 calculations. The search using seven starting points resulted in finding the global extremum with three of them leading to the points of false local minimums. This allows us to assess the reliability of the GDS procedure of seeking the global extremum in the problems under consideration at about 85%, which is a rather high value at a relatively low cost of the search. The results presented above confirmed once more that the GDS search procedure provides a fast advance towards the extremum just after the start from the initial point and a rather slow refinement of its position. The refinement cost can be several times higher than the cost of the approximate determination of the extremum position.

The analysis of the costs of the global search by the procedures chosen for solving the problems of acoustoelectronics confirms their effectiveness in solving practical problems. At the same time, the HJS procedure, which uses a fine mesh of starting points, may well prove to be insufficiently economical for the problems of higher dimensionality. If the search space has four to eight dimensions, the NMS procedure with a sparse mesh of starting points is preferable. Its ability to move towards the extremum with the set of sampling points of a polyhedron appears to be better than any search strategy of the configuration method. In the problems of even higher dimensionality, the GDS procedure proves to be the most effective one. However, by virtue of the discrete nature of the search space, the user has to select this discreteness rather carefully. A too minute representation leads to unjustified search costs, whereas a too rough representation can reduce the reliability of the global search (i.e, increase the probability of missing the extremum).

The search for the spacial orientations corresponding to the optimal value of some parameter of SAW or their linear combination can also be efficiently performed by the above-mentioned procedures of seeking the global extremum of the TF. In this case, the global search should be carried out over all three Euler angles. The TF can be formed as a linear combination of the main parameters of the wave with individual weighting (expert) factors, which provide the variations of individual contributions to the TF. It is hard to expect that there exist orientations for which the values of all SAW parameters become optimal at the same time. It is more realistic to search for the optimal value of the parameter that is most important for a given specific application [2]. It is also possible to search for a compromise between several TF-forming parameters of the wave. An example of the solution of such a problem is the result of the search for the maximal value of the electromechanical coupling factor K^2 for SAW in a $LiNbO_3$ piezoelectric crystal. Using the above-mentioned procedures for the TF extremum search, we calculated the lines of equal value for K^2 in the region of the Euler angles f1 = 0°, f2 = 0°–180°, and f3 = 95°–180°. It is seen from Fig. 3 that, in this case, the region of the maximal value of K^2 (which is within 4–5%) lies in the intervals of the Euler angles f2 = 60°–95°, f3 = 95° and f2 = 30°–45°, f3 = 160°–180°.

The results presented allow us to conclude that the procedures described above are suitable for seeking the SAW and LSAW solutions in piezocrystals. A method for the numerical calculation of the characteristics of SAW and LSAW is proposed on the basis of different search procedures for finding the global extremum of a multivariate function. The procedures for seeking the global extremum of the TF were used for the minimization of the function $F(V, \delta)$ of the boundary conditions and for finding the spatial orientations that corresponded to the optimal values of the SAW and LSAW parameters.

The characteristic features of different methods used for seeking the global extremum of the TF were considered. It was shown that none of the search procedures possesses such advantages over the other ones as to be considered the universal means for solving problems. The calculations performed allow us to conclude that, in the search for the LSAW solutions and also for the optimal orientations of SAW in crystals, it is expedient to use a diversity of global-search procedures. In this case, the probability of finding the true solutions will be drastically increased.

A promising idea is to increase the efficiency of solving the search problems by using the dialog mode of interaction with a computer. Then, choosing the optimal search procedures at individual stages of the problem solution and possessing a wide variety of means, one can quickly obtain the required results.

REFERENCES

1. Farnell, J., in *Acoustic Surface Waves*, Ed. by A. A. Oliner (Springer, New York, 1978; Mir, Moscow, 1981).
2. M. Yu. Dvoesherstov, V. I. Cherednick, A. P. Chirimanov, and S. G. Petrov, Proc. SPIE **3900**, 283 (1999).
3. D. J. Wilde, *Optimum Seeking Methods* (Prentice-Hall, Englewood Cliffs, N.J., 1964; Nauka, Moscow, 1967).
4. I. D. Hill, IEEE Trans. Syst. Sci. Cybern. **SSC-S** (1), 2 (1969).
5. A. Zhilinskas, *Global Optimization* (Mokslas, Vilnius, 1986).
6. D. M. Himmelblau, *Applied Nonlinear Programming* (McGraw-Hill, New York, 1972; Mir, Moscow, 1975).
7. A. M. Botenkov, V. A. Vazin, B. S. Voinov, *et al.*, Preprint No. 8711, RTI AN SSSR (Radiotechnical Inst., USSR Academy of Sciences, Moscow, 1988).
8. M. P. Shaskol'skaya, *Acoustic Crystals* (Nauka, Moscow, 1982).
9. M. P. Cunha, in *Proceedings of IEEE Ultrasonics Symposium* (1997), p. 97.

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