ARCHIVES OF ACOUSTICS
24, 2, 161–167 (1999)

HIGHER-ORDER SINGULARITIES OF THE EFFECTIVE PERMITTIVITY FUNCTION

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A method is given of calculating second-order singularities which are related to inflection points of slowness curves. An approximated formula is derived for the effective permittivity function in the neighbourhood of its singular points. A numerical analysis is presented of several piezoelectrics, and crystal cuts are calculated for the singular points. The analysis shows that inflection points may appear for almost every crystal cut, as is the case of lithium niobate and langasite.

1. Introduction

The effective permittivity [1, 2] of a piezoelectric half-space is a complex-valued function $Y(r)$ where r is the surface wave slowness. The well known Ingebrigtsen approximation of the imaginary part of this function is valid in the neighbourhood of the Rayleigh wave slowness r_i.

The function $Z(r) = 1/Y(r)$ is infinite for $r = r_\mathrm{i}$. Such a singularity of $Z(r)$ will be called zero-order. For $r < r_\mathrm{i}$ the function $Z(r)$ has three other singular points that coincide with cutoff slownesses of the three bulk waves. At these points $Z(r)$ is finite but its first derivative may be infinite. These are first-order singularities.

The Ingebrigtsen approximation has been improved by including contributions from the first-order singularities in the special case of SH waves [3]. In the general case, an approximation of the function $Z(r)$ has been found in the neighbourhood of the cutoff slowness r_c of bulk waves [4]. The method that leads to the approximation can be applied to the remaining two first-order singularities.

A slowness curve is described by the function $s = s(r)$, where $s(r)$ is the real part of the normal component of slowness (normal to the boundary of the the piezoelectric half-space). At the cutoff point of the curve, the first derivative of the inverse function $r = r(s)$ is equal to zero. The second derivative is usually different from zero, and is related to the curvature of the slowness curve at the cutoff point.

In the paper, we examine singularities of the function $Z(r)$ at points of a slowness curve different from the cutoff point and such that both the first and second derivative of the inverse function are equal to zero. These are inflection points of the slowness curve.

Such singularities of $Z(r)$ will be called second-order. At these points $Z(r)$ is finite but its first derivative may be infinite.

2. Second-order singularities

We adopt notations and conventions of Refs. [4] and [5]. The function $Z(r)$ is given by the equality $Z(r) = -Z_{44}^{-}(r)$, where Z_{44}^{-} is the element $(4,4)$ of the 4×4 matrix

$$Z_{KL}^{\pm} = R_{KJ}^{\pm} L_{JL}^{\pm} \tag{1}$$

with the minus superscript. This matrix is determined completely by eigenvectors of the eigenvalue problem that is related to the electro-mechanical field equations as explained in Ref. [4].

Suppose we know the function $s(r)$ that describes the slowness curve corresponding to the J-th eigenvalue in the (r,s) plane near the inflection point $(r_{\mathrm{f}}, s_{\mathrm{f}})$. Regarding the eigenvector $\widetilde{F}_K^{(J)}$ as a function of the variable s we can write, in the neighbourhood of r_{f}, the Taylor expansion

$$\widetilde{F}_K^{(J)}(s) = \widetilde{F}_K^{(J)}(s_{\mathrm{f}}) + \widetilde{F}_K^{\bullet(J)}(s_{\mathrm{f}})\,\Delta s, \tag{2}$$

where the higher-order terms are neglected. The dot denotes differentiation with respect to s, and $\Delta s = s - s_{\mathrm{f}}$.

In the neighbourhood of r_{f} the slowness curve can be approximated by an algebraic curve of third order. If the tangent to the slowness curve at the inflection point is parallel to the s axis then we may use the algebraic curve given by the equation

$$(s - s_{\mathrm{f}})^3 + \alpha^3 (r^3 - r_{\mathrm{f}}^3) = 0, \tag{3}$$

where α is a constant coefficient to be calculated. Hence

$$\Delta s = \alpha\,\varrho(r), \qquad \varrho(r) = (r_{\mathrm{f}}^3 - r^3)^{1/3}. \tag{4}$$

Straightforward differentiation of Eq. (3) with respect to s shows that $\alpha^3 = -2/r_{\mathrm{f}}^2 r^{\bullet\bullet\bullet}$, where $r^{\bullet\bullet\bullet}$ denotes the value of the third derivative for $s = s_{\mathrm{f}}$.

To calculate the coefficient α in terms of the derivatives with respect to r we choose another approach. Inflection points are located on slowness curves so that the tangent at an inflection point is usually not parallel to the s axis. In other words, the derivative s' (the prime denotes differentiation with respect to r) is finite for $r = r_{\mathrm{f}}$. The system of coordinates (x,y,z) should be rotated about the y axis by the angle $\zeta = -\mathrm{atan}(1/s'(r_{\mathrm{f}}))$ in order to make the tangent parallel to the s axis. This means that second-order singularities of $Z(r)$ appear only for particular crystal cuts. Now, the coefficient α can be calculated for an arbitrary inflection point, and then used in Eq. (3) after a suitable rotation of the system of coordinates. We have

$$\alpha^3 = 2(1 + (s')^2)^3 / s'''(r_{\mathrm{f}} s' - s_{\mathrm{f}})^2, \tag{5}$$

where s' and s''' denote the values of the derivatives for $r = r_{\mathrm{f}}$.

The value of s is changing fast for $r \to r_{\mathrm{f}}$ (the first derivative of s tends to infinity in the rotated system of coordinates), and so do the corresponding eigenvalue $q^{(J)}$ and eigenvector $\widetilde{F}_K^{(J)}$. Other eigenvalues and eigenvectors may be considered constant in the neighbourhood of r_{f}. Thus, it suffices to take into account only the eigenvector $\widetilde{F}_K^{(J)}$, to find its approximation given by Eq. (2), and to calculate the function $Z(r)$ with the use of Eq. (1).

Since $s(r) = q(r)\, r$, then

$$s' = q'r + q, \qquad s'' = q''r + 2q', \qquad s''' = q'''r + 3q'' \tag{6}$$

(here $s(r)$ denotes a complex-valued function). The derivatives q', q'', q''', and $\widetilde{F}_K^{\bullet(J)}$ can be found as follows.

Denote by $\mathcal{H}_{KL}^{(J)}$ the difference $H_{KL} - q^{(J)} I_{KL}$ where I_{IJ} is the identity matrix. The equality

$$\mathcal{H}_{KL}^{(J)} \widetilde{F}_L^{(J)} = 0 \tag{7}$$

is satisfied for every r. Differentiating the both sides of Eq. (7) with respect to r gives the recurrence of equalities

$$\begin{aligned}
\mathcal{H}_{KL}^{\prime(J)} \widetilde{F}_L^{(J)} + \mathcal{H}_{KL}^{(J)} \widetilde{F}_L^{\prime(J)} &= 0, &(8)\\
\mathcal{H}_{KL}^{\prime\prime(J)} \widetilde{F}_L^{(J)} + 2\mathcal{H}_{KL}^{\prime(J)} \widetilde{F}_L^{\prime(J)} + \mathcal{H}_{KL}^{(J)} \widetilde{F}_L^{\prime\prime(J)} &= 0, &(9)\\
\mathcal{H}_{KL}^{\prime\prime\prime(J)} \widetilde{F}_L^{(J)} + 3\mathcal{H}_{KL}^{\prime\prime(J)} \widetilde{F}_L^{\prime(J)} + 3\mathcal{H}_{KL}^{\prime(J)} \widetilde{F}_L^{\prime\prime(J)} + \mathcal{H}_{KL}^{(J)} \widetilde{F}_L^{\prime\prime\prime(J)} &= 0. &(10)
\end{aligned}$$

Let $\widetilde{E}_L^{(I)}$ be the left eigenvector corresponding to the eigenvalue $q^{(I)}$. We assume the normalization

$$\widetilde{F}_L^{(J)} \widetilde{F}_L^{(J)} = 1, \qquad \widetilde{E}_L^{(I)} \widetilde{F}_L^{(J)} = I_{IJ} \tag{11}$$

for every r, and introduce the symbols

$$Q_1^{(IJ)} = \widetilde{E}_K^{(I)} H'_{KL} \widetilde{F}_L^{(J)}, \qquad Q_2^{(IJ)} = \widetilde{E}_K^{(I)} H''_{KL} \widetilde{F}_L^{(J)}, \qquad Q_3^{(IJ)} = \widetilde{E}_K^{(I)} H'''_{KL} \widetilde{F}_L^{(J)}. \tag{12}$$

Multiplying each of Eqs. (8) – (10) by $\widetilde{E}_K^{(J)}$ we obtain

$$\begin{aligned}
q^{\prime(J)} &= Q_1^{(JJ)}, &(13)\\
q^{\prime\prime(J)} &= Q_2^{(JJ)} + 2\widetilde{E}_K^{(J)} \mathcal{H}_{KL}^{\prime(J)} \widetilde{F}_L^{\prime(J)}, &(14)\\
q^{\prime\prime\prime(J)} &= Q_3^{(JJ)} + 3\widetilde{E}_K^{(J)} \mathcal{H}_{KL}^{\prime\prime(J)} \widetilde{F}_L^{\prime(J)} + 3\widetilde{E}_K^{(J)} \mathcal{H}_{KL}^{\prime(J)} \widetilde{F}_L^{\prime\prime(J)}. &(15)
\end{aligned}$$

The derivatives $\widetilde{F}_L^{\prime(J)}$ and $\widetilde{F}_L^{\prime\prime(J)}$ can be represented as linear combinations of eigenvectors, i.e.

$$\widetilde{F}_L^{\prime(J)} = \sum_I C_{IJ}^1 \widetilde{F}_L^{(I)}, \qquad \widetilde{F}_L^{\prime\prime(J)} = \sum_I C_{IJ}^2 \widetilde{F}_L^{(I)}, \tag{16}$$

where the constants C_{IJ}^1 and C_{IJ}^2 are to be calculated.

Inserting $\widetilde{F}_L^{\prime(J)}$ from Eq. (16) into Eq. (14) and taking into account Eq. (8) we obtain

$$q^{\prime\prime(J)} = Q_2^{(JJ)} + 2\sum_{I \neq J} C_{IJ}^1 Q_1^{(JI)}, \tag{17}$$

where $C^1_{IJ} = -(q^{(I)} - q^{(J)})^{-1} Q^{(IJ)}_1$ for $I \neq J$, and

$$\widetilde{F}'^{(J)}_L = C^1_{JJ} \widetilde{F}^{(J)}_L + \widetilde{D}^{1(J)}_L, \tag{18}$$

where $C^1_{JJ} = -\widetilde{D}^{1(J)}_L \widetilde{F}^{(J)}_L$, and $\widetilde{D}^{1(J)}_L = \sum\limits_{I \neq J} C^1_{IJ} \widetilde{F}^{(I)}_L$.

Similarly, inserting $\widetilde{F}''^{(J)}_L$ from Eq. (16) into Eq. (15), and taking into account Eq. (9) and the last results, we obtain the derivative $q'''^{(J)}$ given by Eq. (15) with

$$\widetilde{F}''^{(J)}_L = C^2_{JJ} \widetilde{F}^{(J)}_L + \widetilde{D}^{2(J)}_L, \tag{19}$$

where $C^2_{JJ} = -\widetilde{D}^{2(J)}_L \widetilde{F}^{(J)}_L - \widetilde{F}'^{(J)}_L \widetilde{F}'^{(J)}_L$; $\widetilde{D}^{2(J)}_L = \sum\limits_{I \neq J} C^2_{IJ} \widetilde{F}^{(I)}_L$, and

$$C^2_{IJ} = \left(q^{(I)} - q^{(J)}\right)^{-1} \left(-Q^{(IJ)}_2 + 2\left(q'^{(I)} - q'^{(J)}\right)^{-1} Q^{(IJ)}_1 \right.$$
$$\left. + 2 \sum_{K \neq I} (q^{(K)} - q^{(J)})^{-1} Q^{(KJ)}_1 Q^{(IK)}_1 \right) \tag{20}$$

for $I \neq J$ and $K \neq J$.

The above formulae are true for all eigenvalues and eigenvectors (for r different from the cutoff values). In this way, we find the coefficient α from Eq. (5), and the derivative $\widetilde{F}^{\bullet(J)}_K(s) = \widetilde{F}'^{(J)}_K(r)/s'(r)$.

Inserting the eigenvector given by Eq. (2) into Eq. (1) we get the approximated matrix

$$Z^{\pm}_{KL}(r) = Z^{\pm(0)}_{KL} \pm Z^{\pm(1)}_{KL} \alpha \varrho(r) \tag{21}$$

(the higher-order terms are neglected) where the constant matrices $Z^{\pm(0)}_{KL}$ and $Z^{\pm(1)}_{KL}$ can be easily expressed in terms of $\widetilde{F}^{(J)}_K$, $\widetilde{F}^{\bullet(J)}_K$, and the remaining seven eigenvectors for $r = r_{\mathrm{f}}$ (see Appendix of Ref. [4]). In particular,

$$Z(r) = Z_0 - Z_1 \alpha \varrho(r), \tag{22}$$

where the coefficients Z_0 and Z_1 are the elements (4,4) of the corresponding matrices in Eq. (21).

3. Numerical search of inflection points

The location of inflection points on slowness curves is calculated with the use of numerical procedures similar to those described in Ref. [5]. The main procedure solves the eigenvalue problem associated with the field equations. A scanning is performed over crystal cuts (triplets of Euler angles) for several piezoelectric media. The calculations shows that for some crystal cuts there is more than 10 inflection points, and that inflection points may appear for almost every cut (the case of lithium niobate and langasite) or for only a minority of crystal cuts (the case of bismuth germanium oxide).

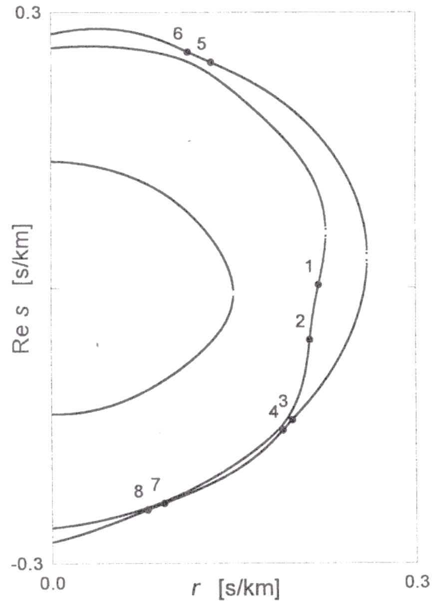

Fig. 1. Inflection points for lithium niobate (Euler angles: 20°, 160°, 120°).

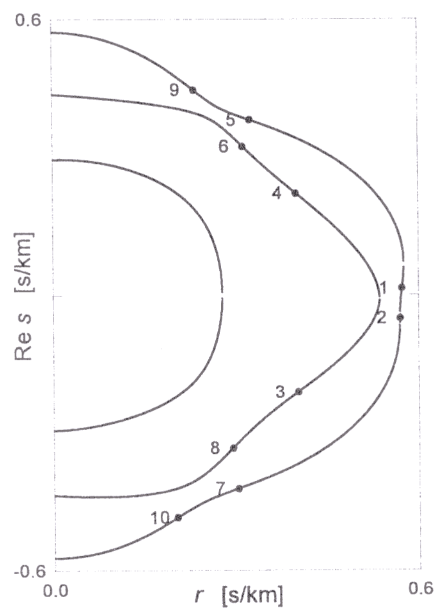

Fig. 2. Inflection points for bismuth germanium oxide (Euler angles: 0°, 40°, 20°).

Three examples of location of inflection points are given in Figs. 1 to 3 for lithium niobate, bismuth germanium oxide, and langasite. The crystal cuts have been chosen from those with a large number of inflection points. It should be noted that some inflec-

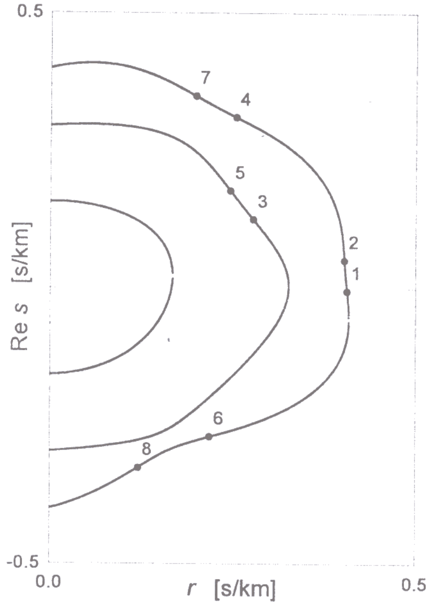

Fig. 3. Inflection points for langasite (Euler angles: 10°, 40°, 40°).

tion points may be missing due to finite precision of calculations. The appendices of the slowness curves above the cutoff points (cf. Fig. 1 of Ref. [4]) have been omitted. The angle ζ for each inflection point is given in Table 1. The inflection points are numbered in the order of decreasing values of the variable r.

Table 1. The angle ζ corresponding to the inflection points shown in the figures for lithium niobate (LNO), bismuth germanium oxide (BGO), and langasite (LGS).

Inflection Point No.	LNO 20 160 120 ζ [deg]	BGO 0 40 20 ζ [deg]	LGS 10 40 40 ζ [deg]
1	−9.2	−5.3	4.5
2	−4.9	−0.6	2.9
3	−34.9	−45.8	31.5
4	−34.4	42.7	56.6
5	59.6	65.4	30.3
6	58.3	38.2	−69.9
7	−62.9	−65.2	54.1
8	−62.7	−36.9	−50.4
9	–	43.6	–
10	–	−50.7	–

It is obvious that inflection points appear in pairs. A pair of inflection points is related to a concave portion of a slowness curve, which is delimited by the two points of the pair.

4. Conclusion

In contrast to first-order singularities of the effective permittivity function, which appear for every crystal cut, second-order singularities appear only for particular crystal cuts. These crystal cuts correspond to isolated points in the three-dimensional space of Euler angles. Nevertheless, for a crystal cut that is close to one of those points the first derivative of the function $Z(r)$ is very great for $r \approx r_{\mathrm{f}}$, where r_{f} is the singular point corresponding to the isolated point in the angle space. Numerical calculation of values of the function $Z(r)$ cannot reveal this feature.

The method presented in Sec. 2 can be applied in the case of N-th-order singularities of the effective permittivity function with $N > 2$. Such singularities are related to points of slowness curves where all derivatives of $r(s)$ up to the N-th-order are zero.

Acknowledgement

The author would like to thank Prof. E. Danicki for suggesting the investigation of singularities of the effective permittivity function and for discussions helpful in calculating the approximation.

This work was supported by Committee of Scientific Research (Poland) under Grant No. 7 T07A 049 13.

References

[1] K.A. Ingebrigtsen, *Surface waves in piezoelectrics*, J. Appl. Phys., **40**, 2681–2686 (1969).

[2] K. Bløtekjaer, K.A. Ingebrigtsen, and H. Skeie, *A method for analyzing waves in structures consisting of metal strips on dispersive media*, IEEE Trans. Electron Devices, **ED-20**, 1133–1138 (1973).

[3] E. Danicki, *New theory of SSBW devices*, [in:] 1980 IEEE Ultrasonics Symposium Proceedings, B.R. McAvoy [Ed.], IEEE, New York, 1980, pp. 235–239.

[4] W. Laprus and E. Danicki, *Singularities of the planar Green function in the spectral domain*, Archives of Acoustics, **22**, 169–177 (1997).

[5] W. Laprus and E. Danicki, *Piezoelectric interfacial waves in lithium niobate and other crystals*, J. Appl. Phys., **81**, 855–861 (1997).