# CUT-OFF FREQUENCY COALESCENCE OF SURFACE ACOUSTIC WAVES UNDER METALLIC GRATINGS ON PIEZOELECTRIC HOMOGENEOUS AND LAYERED SUBSTRATES

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**Abstract**
The paper discusses the effect of crystallographic symmetry on the coalescence of the cut-off frequencies confining the stop-band of SAW or leaky SAW (LSAW) spectrum for short- and open-circuited gratings. Four families of the orientation have been determined at which two of the four frequencies coalesce on the homogeneous substrate. On layered substrates, the coalescence occurs provided the orientation of both the substrate and the layers belongs to the same orientation family of the four families determined (the grating is on the outer surface of the structure). The coalescence of a pair of cut-off frequencies has been established through the analysis of the coupling-of-modes (COM) equations and a numerical algorithm conventionally used to compute cut-off frequencies and dispersion curves.

**Introduction**
The cut-off frequencies $\omega_{oc}^{(\pm)}$ and $\omega_{sc}^{(\pm)}$ at open-circuited (OC) and short-circuited (SC) electrodes, respectively, are important parameters of infinite periodic metallic gratings fabricated on piezoelectrics (the sign "+" refers to the upper edge of the stop-band) [1]. These frequencies can be estimated using the COM equations if the COM parameters are known explicitly or determined numerically by solving the appropriate dispersion equations or finding the zeros and poles of the harmonic admittance $Y_h$ [2-4]. Knowing $\omega_{oc,sc}^{(\pm)}$ allows the solution of the inverse problem: to estimate the COM parameters and, hence, the characteristics of IDT or reflectors [1].

We will be considering a simple grating formed of strips shaped symmetrically with respect to their centers. When such a grating is on the substrate oriented arbitrarily, the four $\omega_{oc,sc}^{(\pm)}$ values are distinct. However, a cut-off frequency for the OC grating coalesces with a cut-off frequency for the SC grating if the substrate assumes particular orientations.

Of interest is that once the frequency degeneracy happens, then the substrate is naturally bi- directional implying that IDTs, unless specially designed, will generate the right- and left-propagating waves with equal amplitude. Otherwise the substrate is naturally unidirectional: any IDT, even fabricated on the basis of the simple "symmetric" grating, launches the waves to the right and left with unequal amplitudes [1].

In the present paper we study the relation between the crystallographic symmetry of substrates and the occurrence of cut-off frequency degeneracy. Note that the relation between the characteristics of IDT's and the symmetry of the substrate has been discussed in [5,6]. Using a simple model of the wave propagation under gratings, the phase difference between the normal component of displacement and the potential has been estimated and some conclusions have been made regarding the position of the transduction center.

First, we shall consider the problem by analyzing a numerical model and afterwards we COM theory.

**Numerical procedure**
In this section, we outline a method commonly utilized to estimate $\omega_{oc,sc}^{(\pm)}$. According to [7], the response of the grating is studied to an external ac voltage $V(m) = V\exp[i\pi m]$ applied to the electrodes; here $m$ is the electrode number. The basic equation is

$$\mathbf{U}(x) = \int_{-a}^{a} \hat{\mathbf{G}}'(x-x')\mathbf{W}(x')\,dx', \qquad (1)$$

where $a$ is the electrode half-width, the $x$-axis is directed along the surface of the substrate, $\mathbf{U}(x) = (\mathbf{A}(x), \Phi(x))^t$ and $\mathbf{W}(x) = (\mathbf{f}(x), \sigma(x))^t$ are constructed from the displacement $\mathbf{A}(x)$, the potential $\Phi(x)$, the force $\mathbf{f}(\mathbf{x})$, and the surface charge density $\sigma(x)$, the latter two quantities being non zero only within the under-electrode interval; the symbol $()^t$ means transposition. Eq. (1) involves Green's function

$$\hat{\mathbf{G}}'(x) = (1/p)\sum_{n=-\infty}^{\infty} \hat{\mathbf{G}}(k^{(n)})e^{ik^{(n)}x}, \qquad (2)$$

where $k^{(n)} = 2\pi(n+0.5)/p$, $p$ is the period of the grating.

The vector $\mathbf{W}(x)$ is sought for in the form

$$\mathbf{W}(x) = \sum_n \mathbf{C}^{(n)} P^{(n)}(x), \tag{3}$$

where $P^{(n)}(x)$ are orthogonal polynoms of degree $n$, $P^{(2m)}(x)$ and $P^{(2m+1)}(x)$ being x-even and x-odd, respectively; the vector $\mathbf{C}^{(n)} = (C_x^{(n)}, C_y^{(n)}, C_z^{(n)}, C_\sigma^{(n)})^t$ involves three components $C_{x,y,z}^{(n)}$ of force and the charge $C_\sigma^{(n)}$.

Within $|x| \le a$ it is required that $\Phi(x) = V$, $\mathbf{A}(x) = \mathbf{A}^{(el)}(x)$, $\mathbf{f}(x) = \mathbf{f}^{(el)}(x)$, where $\mathbf{A}^{(el)}(x)$ and $\mathbf{f}^{(el)}(x)$ are the displacement and traction produced by the vibrations in the electrode at the electrode-substrate interface. Let the electrode be isotropic and shaped symmetrically. The x-odd $A_x^{(el)}(x,z)$ is then coupled with the x-even $A_z^{(el)}(x,z)$ and the x-even $A_x^{(el)}(x,z)$ with the x-odd $A_z^{(el)}(x,z)$. As a result, we obtain that the x-even $\mathbf{U}^{(e)}(x)$ and x-odd $\mathbf{U}^{(o)}(x)$ parts of $\mathbf{U}(x)$ become at $|x| \le a$ [8]

$$\begin{array}{l} \mathbf{U}_e(x) = \hat{\mathbf{E}}^{(2n)}(x)\mathbf{C}^{(2n)} + \hat{\mathbf{E}}^{(2n+1)}(x)\mathbf{C}^{(2n+1)} \\ +\hat{\mathbf{I}}' V, \\ \mathbf{U}_o(x) = \hat{\mathbf{O}}^{(2n)}(x)\mathbf{C}^{(2n)} + \hat{\mathbf{O}}^{(2n+1)}(x)\mathbf{C}^{(2n+1)}, \end{array} \tag{4}$$

where summation over $n$ is understood. In (4) $(\hat{I}')_{ij} = \delta_{4i}\delta_{j4}$, $i,j = 1,\ldots,4$; $\hat{\mathbf{E}}^{(n)}(x)$ and $\hat{\mathbf{O}}^{(n)}(x)$ are 4x4 x-even and x-odd matrices, respectively, with non-zero elements

$$\begin{array}{l} (\hat{E}^{(2n)})_{ii},\ (\hat{E}^{(2n+1)})_{13},\ (\hat{E}^{(2n+1)})_{31}; \\ (\hat{O}^{(2n+1)})_{ii},\ (\hat{O}^{(2n)})_{13},\ (\hat{O}^{(2n)})_{31}, \end{array} \tag{5}$$

where $i = 1,2,3$. The functions $\hat{\mathbf{E}}^{(n)}(x)$ and $\hat{\mathbf{O}}^{(n)}(x)$ can be computed using, e.g., the FVM-method [9]. However, of importance for us is only how $C_{x,y,z}^{(2n)}$'s and $C_{x,y,z}^{(2n+1)}$'s enter into (4).

Let us turn to Green's function $\hat{\mathbf{G}}(k)$ entering (2). Since $\hat{\mathbf{G}}(-k) = [\hat{\mathbf{G}}(k)]^t$,

$$\begin{array}{l} \hat{\mathbf{G}}(k>0) = \hat{\mathbf{G}}^{(s)} + i\hat{\mathbf{G}}^{(a)}, \\ \hat{\mathbf{G}}(k<0) = \hat{\mathbf{G}}^{(s)} - i\hat{\mathbf{G}}^{(a)}, \end{array} \tag{6}$$

where $\hat{\mathbf{G}}^{(s)}$ and $\hat{\mathbf{G}}^{(a)}$ are symmetric and anti symmetric parts of $\hat{\mathbf{G}}(k)$, respectively. In view of $k^{(n)} = -k^{(-n-1)}$ one has

$$\hat{\mathbf{G}}'(x) = \hat{\mathbf{G}}_e^{(s)}(x) + \hat{\mathbf{G}}_o^{(a)}(x), \tag{7}$$

where $\hat{\mathbf{G}}_e^{(s)}(x)$ is a symmetric x-even matrix and $\hat{\mathbf{G}}_o^{(a)}(x)$ is an anti symmetric x-odd matrix.

We can put (2)) and (3) into (1) and integrate to obtain, accounting for (7),

$$\begin{array}{l} \mathbf{U}_e(x) = \hat{\mathbf{G}}_e^{(s)(2n)}(x)\mathbf{C}^{(2n)} + \hat{\mathbf{G}}_e^{(a)(2n+1)}(x)\mathbf{C}^{(2n+1)}, \\ \mathbf{U}_o(x) = \hat{\mathbf{G}}_o^{(a)(2n)}(x)\mathbf{C}^{(2n)} + \hat{\mathbf{G}}_o^{(s)(2n+1)}(x)\mathbf{C}^{(2n+1)}. \end{array} \tag{8}$$

In (8) the sign of summation over $n$ is omitted and, with understanding that "$*$" means convolution,

$$\begin{array}{l} \hat{\mathbf{G}}_e^{(s)(2n)}(x) = \hat{\mathbf{G}}_e^{(s)}(x) * P^{(2n)}(x), \\ \hat{\mathbf{G}}_o^{(s)(2n+1)}(x) = \hat{\mathbf{G}}_e^{(s)}(x) * P^{(2n+1)}(x), \\ \hat{\mathbf{G}}_o^{(a)(2n)}(x) = \hat{\mathbf{G}}_o^{(a)}(x) * P^{(2n)}(x), \\ \hat{\mathbf{G}}_e^{(a)(2n+1)}(x) = \hat{\mathbf{G}}_o^{(a)}(x) * P^{(2n+1)}(x); \end{array} \tag{9}$$

$\hat{\mathbf{G}}_e^{(s)(2n)}$ and $\hat{\mathbf{G}}_e^{(a)(2n+1)}$ are x-even while $\hat{\mathbf{G}}_o^{(s)(2n+1)}$ and $\hat{\mathbf{G}}_o^{(a)(2n)}$ are x-odd.

Equating now (4) to (8) we arrive at a set of equations. From the condition for its solubility with respect to $\mathbf{C}^{(n)}$ at $V = 0$ (SC-grating) and $I \propto C_\sigma^{(0)} = 0$ (OC-grating, $I$ is current per electrode) the $\omega_{sc,oc}^{(\pm)}$-values are found.

Note for further use that $\hat{\mathbf{G}}(k>0)$ can be written in terms of the admittance $\hat{\mathbf{Y}}$ connecting the vectors $\mathbf{U} = (\mathbf{A}, \Phi)^t$ and $\mathbf{V} = ik^{-1}(\mathbf{f}, D)^t$ constructed from the characteristics of the wave field $\propto \exp[i(kx - \omega t)]$ involving right-propagating (rp) either non- uniform decaying or uniform reflected partial plane modes; $D$ is normal projection (i.e. $z$- component) of the electric displacement. Specifically, $\mathbf{U} = i\hat{\mathbf{Y}}\mathbf{V}$ and $\hat{\mathbf{G}} = [k(\varepsilon_0(\hat{Y})_{44} - 1)]^{-1}\hat{\mathbf{G}}''$, where $(\hat{G}'')_{ij} = (1 - \varepsilon_0(\hat{Y})_{44})(\hat{Y})_{ij} + \varepsilon_0(\hat{Y})_{i4}(\hat{Y})_{4j}$, $i,j = 1,2,3$, $(\hat{G}')_{i4} = (\hat{Y})_{i4}$, $(\hat{G}')_{4j} = (\hat{Y})_{4j}$, $i = 1,\ldots,4$; $\varepsilon_0$ is the dielectric constant.

If the substrate is homogeneous, then

$$\hat{\mathbf{Y}} = \hat{\mathbf{B}}^{-1}(\hat{\mathbf{I}} + i\hat{\mathbf{S}}^t); \tag{10}$$

$\hat{\mathbf{B}}^{-1}$ is the inverse and $\hat{\mathbf{S}}^t$ is the transpose of

$$\begin{array}{l} \hat{\mathbf{B}} = i\sum_{\alpha=1}^4 [\mathbf{V}_\alpha \otimes \mathbf{V}_\alpha - \mathbf{V}_{\alpha+4} \otimes \mathbf{V}_{\alpha+4}], \\ \hat{\mathbf{S}} = i\sum_{\alpha=1}^4 [\mathbf{U}_\alpha \otimes \mathbf{V}_\alpha - \mathbf{U}_{\alpha+4} \otimes \mathbf{V}_{\alpha+4}]. \end{array} \tag{11}$$

The symbol "$\otimes$" denotes diadic multiplication. The 4-component vectors $\mathbf{U}_\alpha = (\mathbf{A}_\alpha, \Phi_\alpha)^t$ and $\mathbf{V}_\alpha = ik^{-1}(\mathbf{f}_\alpha, D_\alpha)^t$ are associated with the partial modes labelled by the index $\alpha$ and together with decay factors $p_\alpha$ are found from an eigenvalue problem $\hat{\mathbf{N}}\xi_\alpha = p_\alpha\xi_\alpha$, where $\xi_\alpha = (\mathbf{U}_\alpha, \mathbf{V}_\alpha)^t$ and

$$\hat{\mathbf{N}} = -\left\{ \begin{array}{cc} \hat{\mathbf{N}}_{11} & \hat{\mathbf{N}}_{12} \\ \hat{\mathbf{N}}_{21} & \hat{\mathbf{N}}_{11}^t \end{array} \right\}, \tag{12}$$

$\hat{\mathbf{N}}_{IJ}$ are $4 \times 4$ matrices, $\hat{\mathbf{N}}_{12}$ and $\hat{\mathbf{N}}_{21}$ being symmetric. The matrices $\hat{\mathbf{N}}_{IJ}$ involve material constants and velocity $v = \omega/k$ (see [10] for more details). Eq. (10) follows from

$$\mathbf{U}_\alpha \cdot \mathbf{V}_\beta + \mathbf{V}_\alpha \cdot \mathbf{U}_\beta = \delta_{\alpha\beta} \tag{13}$$

under assumption that $\alpha = 1, \ldots, 4$ label the modes from which rp-wave fields are constructed.

For layered substrates we use the equation

$$i\frac{d\hat{\mathbf{Y}}}{dz} = -\hat{\mathbf{Y}}\hat{\mathbf{N}}_{21}\hat{\mathbf{Y}} + i[\hat{\mathbf{Y}}\hat{\mathbf{N}}_{11}^t - \hat{\mathbf{N}}_{11}\hat{\mathbf{Y}}] - \hat{\mathbf{N}}_{12}, \quad (14)$$

where $\hat{\mathbf{N}}_{IJ}$ are z-dependent. Eq. (14) is an analogue of the equation derived in [11] for the impedance of layered substrates.

**Symmetry and frequency degeneracy**

Consider four orientation families.

$$\begin{array}{l} \text{1) x-axis is perpendicular to a plane} \\ \text{of symmetry;} \\ \text{2) x-axis is along an even-fold} \\ \text{symmetry axis;} \\ \text{3) the surface is a plane of symmetry;} \\ \text{4) the surface is perpendicular} \\ \text{to an even-fold symmetry axis.} \end{array} \quad (15)$$

We want to prove that in the case of homogeneous substrate one of the frequencies $\omega_{oc}^{(\pm)}$ becomes equal to one of $\omega_{sc}^{(\pm)}$ at orientations (15).

For cuts (15) $p_\alpha$'s appear in pairs $\pm p_\alpha$. The eight quantities - $\mathbf{A}_\alpha$, $\Phi_\alpha$, $\mathbf{f}_\alpha$, $D_\alpha$ - become split into two four-element groups, depending on their evenness with respect to $p_\alpha$ [8, 12]. It can be checked out that some of the components of matrices (11) vanish identically [8], namely,

$$\begin{array}{l} 1)\ (\hat{B})_{ij} = (\hat{S})_{ql} = 0,\ i = 1,\ j = 2,3,4, \\ q = l = 1, q, l = 2,3,4; \\ 2)\ (\hat{B})_{12} = (\hat{B})_{13} = (\hat{B})_{24} = (\hat{B})_{34} = \\ (\hat{S})_{ii} = 0,\ i = 1,\ldots,4,\ (\hat{S})_{23} = \\ (\hat{S})_{32} = (\hat{S})_{41} = (\hat{S})_{14} = 0; \\ 3)\ (\hat{B})_{13} = (\hat{B})_{23} = (\hat{B})_{34} = (\hat{S})_{ii} = 0, \\ i = 1,\ldots,4,\ (\hat{S})_{12} = (\hat{S})_{21} = \\ (\hat{S})_{41} = (\hat{S})_{14} = (\hat{S})_{42} = (\hat{S})_{24} = 0; \\ 4)\ (\hat{B})_{13} = (\hat{B})_{14} = (\hat{B})_{23} = (\hat{B})_{24} = \\ (\hat{S})_{ij} = 0,\ i,j = 1,2,\ i,j = 3,4. \end{array} \quad (16)$$

Note that $(\hat{S})_{ij} = 0$ when $(\hat{B})_{ij} \neq 0$ and vice versa.

Let the notation $\hat{\mathbf{X}} \longmapsto \hat{\mathbf{Z}}$ indicate that the position of zero elements in a matrix $\hat{\mathbf{Z}}$ is the same as in $\hat{\mathbf{X}}$, i.e. $(\hat{Z})_{ij} = 0$ when $(\hat{X})_{ij} = 0$. By direct calculations one obtains that $\hat{\mathbf{B}} \longmapsto \hat{\mathbf{B}}^{-1}$ while $\hat{\mathbf{S}} \longmapsto \hat{\mathbf{B}}^{-1}\hat{\mathbf{S}}^t$ and, hence,

$$\begin{array}{l} \hat{\mathbf{B}} \longmapsto \hat{\mathbf{Y}}^s \longmapsto \hat{\mathbf{G}}_e^s(x), \\ \hat{\mathbf{S}} \longmapsto \hat{\mathbf{Y}}^a \longmapsto \hat{\mathbf{G}}_o^a(x) \end{array} \quad (17)$$

for each of the cases (15), where $\hat{\mathbf{Y}}^s \equiv \hat{\mathbf{B}}^{-1}$ and $\hat{\mathbf{Y}}^a \equiv \hat{\mathbf{B}}^{-1}\hat{\mathbf{S}}^t$ are symmetric and anti symmetric parts of $\hat{\mathbf{Y}}$, respectively.

With due regard for (16) and (17) we find out that the set of equations in $C^{(n)}$ becomes split into two independent subsets. One of them corresponds to $V = 0$ and in addition its solution has $C_\sigma^{(0)} = 0$. Hence, the cut-off frequency to be determined from this subset is independent of the electrode connection so that the degeneracy takes place which completes the proof.

Consider layered substrates. Let the orientation of both the substrate and the layers pertain to the same family of the four families listed in (15). Using the relation $\hat{\mathbf{N}} = \sum_{\alpha=1}^{8} p_\alpha \xi_\alpha \otimes \hat{\mathbf{T}}\xi_\alpha$, where $\hat{\mathbf{T}}$ is an $8 \times 8$ matrix with elements $(\hat{T})_{ij} = (\hat{T})_{i+4,j+4} = 0$, $(\hat{T})_{i+4,j} = (\hat{T})_{i,j+4} = \delta_{ij}$, $i, j = 1, \ldots, 4$, one can show that $\hat{\mathbf{B}} \longmapsto \hat{\mathbf{N}}_{21}, \hat{\mathbf{N}}_{12}$ and $\hat{\mathbf{S}} \longmapsto \hat{\mathbf{N}}_{11}$. From (14) it then follows that (17) holds true for layered substrates, yielding the split of the set of equations as in the case of homogeneous substrates. As a result, the cut-off frequency degeneracy occurs.

**COM-theory**

Consider again homogeneous substrates. The mechanical part of the reflection coefficients from a single electrode $R^{(+)}$ and $R^{(-)}$ of the rp- and left-propagating (lp) waves, respectively, has the form (see, e.g., [2])

$$R^{(\pm)} = (H/p) \sum_{\alpha=x,y,z} a_\alpha e_\alpha^{(\pm)2}. \quad (18)$$

In (18) $e_\alpha^{(\pm)}$ are the components of the vectors $\mathbf{e}^{(\pm)} = \mathbf{u}^{(\pm)}/\varphi^{(\pm)}$, where $\mathbf{u}^{(+)}$ and $\mathbf{u}^{(-)}$ are the polarization vectors of the rp- and lp-SAW (LSAW), $\varphi^{(+)}$ and $\varphi^{(-)}$ are the potential these waves produce on the surface, $H$ is the electrode thickness. The coefficients $a_\alpha$ depend on the material constants and metallization ratio.

Two cut-off frequencies merge when $R^{(+)} = R^{(-)}$. This equality is satisfied for orientations (15). Indeed, it can be derived that $e_\alpha^{(+)} = \varepsilon_0(\hat{Y})_{4\alpha}$ and $e_\alpha^{(-)} = \varepsilon_0(\hat{Y})_{\alpha 4}$, where the correspondence $x, y, z \Leftrightarrow 1, 2, 3$ is meant. Due to (16) $e_\alpha^{(+)2} = e_\alpha^{(-)2}$, $\alpha = x, y, z$, wherefrom $R^{(+)} = R^{(-)}$ stems.

Note that $R^{(+)}$ as given by (18) can also be equal to $R^{(-)}$ for other orientations. In particular, when the SAW problem is being considered, $R^{(+)} = R^{(-)*} = R$ and it is required that $\mathrm{Im}[R] = 0$. The reflection coefficient is a function of three angles specifying the geometry of propagation. Since these angles are subject to one relation, two of them can be viewed as free parameters while the third angle is found from $\mathrm{Im}[R] = 0$. Hence, the set of orientations at which $\mathrm{Im}[R] = 0$ is a surface in the 3-D space of orientation angles. If one of the angles is steadily has the same value, then only two angles are changeable and one obtains a line where the frequencies are degenerate.

We have calculated such a line for the cut family $(\varphi, 38^o, \psi)$ of $LiNbO_3$ (Fig. 1); the Euler $\theta$-angle is fixed and equal to $\theta = 38^o$ and two other angles are changed. The periodicity of the line with the period $\Delta\varphi = 120^o$ is due to the crystallographic symmetry of $LiNbO_3$.

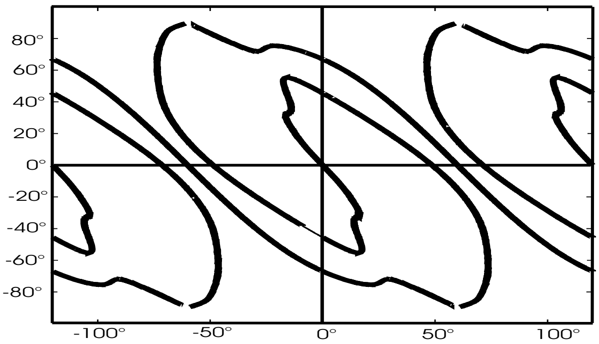


Figure 1: Line where $R^{(\pm)}$ become real.

However, in any of the above cases, except (15), the degeneracy occurs only approximately with the accuracy to $H/P$ and is lifted off if the higher- order terms are taken into account.

**Conclusion**

We have indicated four families of substrate orientations at which two cut-off frequencies of simple OC and SC gratings merge. The frequencies fall into equality not only to the lowest approximation with respect to the electrode thickness but also when they are determined via numerical computations that are believed to completely account for the "mechanical" effect of the electrode of finite thickness. The degeneracy occurs irrespective of the material constants of the substrate and the electrode and of the electrode shape. It does not depend on the metallization ratio and the thickness of layers coating the substrate.

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