

**A TWO PARAMETER COUPLING-OF-MODES MODEL  
FOR SHEAR HORIZONTAL TYPE SAW PROPAGATION IN PERIODIC GRATINGS**

Victor P. Plessky

Advanced SAW Products SA, CH-2022, Bevaix, Switzerland

**ABSTRACT**

A closed form dispersion relation for shear surface acoustic waves (BGW, STW, leaky waves) propagating in periodic structures in the frequency range corresponding to the Bragg stopband is found. The consideration includes the changes in spatial structure of the waves mutually reflecting on the grating as well as bulk wave scattering. A comparison with numerically obtained dispersion curves for leaky waves on 36-LiTaO<sub>3</sub> and with experimental data on STW in quartz shows good agreement.

**1. Introduction**

Interest in shear surface acoustic waves arises due to a growing demand for high frequency, low loss, surface acoustic wave (SAW) devices. As a rule, shear surface waves have a higher velocity than that of Rayleigh waves, and additionally some crystal cuts have better temperature stability and high electromechanical coupling.

Since surface transverse waves (STW) were discovered simultaneously and independently by two groups [1,2], efforts have been made to develop a theory of STW propagation and reflection in a periodic structure in frequency ranges corresponding to the Bragg stopband [3]-[5]. These theories can also include the case of Bleustein-Gulyaev waves (BGW), since the spatial structure of the waves is basically the same. A theory, based on numerical solutions of the equations of coupled harmonics was reported some time ago [3]. For these waves the localization depth is strongly frequency dependent inside the stopband and largest at the lower edge of the stopband and smallest at the upper edge. In the case of a strong periodic perturbation, the stopband frequency region can overlap with the frequency range in which bulk wave scattering takes place. Similar behavior can be observed for leaky waves in 36-LiTaO<sub>3</sub> [6].

In this paper it is shown that by introducing non critical simplifications, as are usually used in the coupling of mode (COM) approach, we can obtain a system of equations for the coupled space harmonics of propagating waves which has an explicit analytic solution. Formulas for the reflection coefficient from the reflecting grating of finite length are obtained. The results are compared with the standard COM formulas and with the experimental data.

**2. Main equations**

Let us consider here the following geometry of the problem. The piezoelectric crystal occupies the half space  $y < 0$ , and waves, whose displacement vector is parallel to  $OZ$ , propagate along the  $OX$  axis. This geometry is applicable to BGW, surface transverse waves (STW), surface skimming bulk waves (SSBW) and in some important cases, for example, 36-LiTaO<sub>3</sub>, to leaky waves. It is also assumed, that there is some periodic perturbation, (like grooves, metal strips, dielectric strips) on the surface with period  $p$ . Let us suppose that the waves can be described by the sum of harmonics satisfying Floquet's theorem:

$$u = u_+ \exp(\kappa_+ y + j(Q/2 + \delta)x) + u_- \exp(\kappa_- y + j(-Q/2 + \delta)x) + \dots \quad (1)$$

Here, for the frequencies close to the stopband, only two of the most important harmonics, corresponding to the incident and the reflected waves, are retained. The time factor is taken in the form  $\exp(-j\omega t)$  and omitted everywhere. In formula (1)  $u_+$  and  $u_-$  are respectively the amplitudes of the waves propagating in the positive and negative  $x$ -directions. The wavenumber of the wave  $q = Q/2 + \delta$ ,  $|\delta| \ll Q/2$ , (where  $Q = 2\pi/p$ ), is supposed to be almost equal to the Bragg wavenumber  $Q/2 = \pi/p$ , the deviation  $\delta$  can be a complex value, and the frequency of the wave is close to the Bragg frequency  $\omega = \omega_b + \Delta\omega$ ,  $\Delta\omega \ll \omega_b$ .

$\omega_b = V^*(Q/2)$ , where  $V$  is the velocity of the wave in the limit of a very weak perturbation. The decay constants  $\kappa_{\pm}$  describe the localization depth of the waves near to the surface, ( $\text{Re } \kappa_{\pm} > 0$ ). It is assumed that, as for BG-waves in hexagonal crystals,

$$\kappa_{\pm} = \sqrt{(Q/2 \pm \delta)^2 - k_l^2}, \quad (2)$$

where  $k_l = \omega / V$  is the wavenumber of the bulk shear wave.

For this problem, the corresponding coupling-of-modes (coupling of harmonics) equations, including electric and mechanical perturbations of the boundary, were derived earlier [3], [5] in the following form:

$$(\kappa_+ - \eta_0(Q/2 + \delta) - 2\varepsilon_0 \frac{k_l^2}{Q})u_+ = \varepsilon_1 \frac{2k_l^2}{Q}u_+ \quad (3a)$$

$$(\kappa_- - \eta_0(Q/2 - \delta) - 2\varepsilon_0 \frac{k_l^2}{Q})u_- = \varepsilon_1^* \frac{2k_l^2}{Q}u_+ \quad (3b)$$

where  $\eta_0$  is the piezoelectric coupling constant,  $\varepsilon_0$  is a parameter determined by uniform mass loading and  $\varepsilon_1$  is a parameter of a periodic boundary perturbation. For a narrow frequency range including the Bragg stopband, the frequency and wavenumber dependence of the terms proportional to the small parameters  $\eta$  and  $\varepsilon_{0,1}$  can be neglected. This allows the equations (3) to be rewritten in a simplified form:

$$(\kappa_+ - \eta(Q/2))u_+ = \varepsilon(Q/2)u_+, \quad (4a)$$

$$(\kappa_- - \eta(Q/2))u_- = \varepsilon^*(Q/2)u_+ \quad (4b)$$

where parameter  $\eta \approx \eta_0 + 4\varepsilon_0 \frac{k_l^2}{Q^2}$  is responsible for localization depth of the wave, propagating on the uniformly loaded surface and  $\varepsilon = \varepsilon_1$  describes the interaction of counter propagating waves. Both parameters are assumed to be small ( $\eta < 1$ ,  $\varepsilon \ll 1$ ) and must be considered as phenomenological parameters of this model which can be found from numerical or experimental data. By introducing a normalized wavenumber deviation  $q$  and a normalized frequency shift  $\Delta$ ,

$$\xi = (Q/2 + \delta)/(Q/2) = 1 + q, \quad \Delta = (\Delta\omega / \omega_b) \quad (5)$$

the following is obtained:

$$(\sqrt{2(q - \Delta)} - \eta)u_+ = \varepsilon u_+, \quad (6a)$$

$$(\sqrt{2(-q - \Delta)} - \eta)u_- = \varepsilon^* u_+. \quad (6b)$$

Here, as well as in (3) and (4),  $\varepsilon^*$  is the complex conjugate of  $\varepsilon$ . As a further simplification, second order terms, proportional to  $\Delta^2$ ,  $q^2$  have been omitted. The first parameter  $\eta$  in (6) is responsible for the spatial structure (i.e. the depth of localization) of the wave and its velocity. The second parameter ( $\varepsilon$ ) describes the coupling strength of the waves propagating in opposite directions.

### 3. Dispersion equation

From the system of equations (6) the dispersion equation is obtained:

$$(\sqrt{2(q - \Delta)} - \eta)^*(\sqrt{2(-q - \Delta)} - \eta) = |\varepsilon|^2. \quad (7)$$

This equation can be solved analytically. However, prior to this, the particular frequency points at which the wavenumber is equal to the Bragg wavenumber  $Q/2$  and its imaginary part is equal to zero can be found. From equation (7), by assuming  $q = 0$ , it follows that

$$\sqrt{-2\Delta} = \eta \pm |\varepsilon|. \quad (8)$$

These frequency points look like the edges of the stopband[3], [7]:

$$\Delta_- = -\frac{1}{2}(\eta + |\varepsilon|)^2, \quad \Delta_+ = -\frac{1}{2}(\eta - |\varepsilon|)^2, \quad (9)$$

where  $\Delta_-$  stands for the lower and  $\Delta_+$  for the upper stopband edge. It can be shown that for  $\Delta_+$  the statement is valid only for  $|\varepsilon| < 0.5\eta$ . From (8) it can be seen that if  $|\varepsilon| > \eta$  the second edge of the stopband cannot be separated from the frequencies at which the bulk-wave scattering takes place. More detailed analysis shows that it occurs if  $|\varepsilon| > 0.5\eta$ . For  $|\varepsilon| < 0.5\eta$  the center frequency of the stopband

$$\omega_c = \frac{1}{2}(\Delta_- + \Delta_+) = -\frac{\eta^2 + |\varepsilon|^2}{2}, \quad (10)$$

is shifted down both due to the uniform loading (parameter  $\eta$ ) and as a result of the interaction of the waves (parameter  $\varepsilon$ ). The stopband width is determined by both the localization depth of the waves ( $\propto \eta^{-1}$ ) and

by the coupling coefficient  $\varepsilon$  and is given (for  $|\varepsilon| < 0.5\eta$ ) by

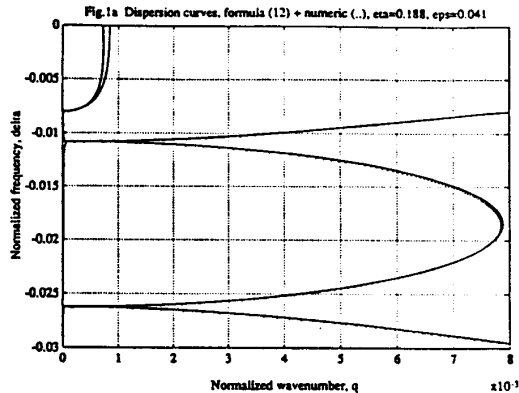
$$\Omega = (\Delta_+ - \Delta_-) = 2\eta|\varepsilon|. \quad (11)$$

The exact analytical solution of equation (7) can be written in the form [9]:

$$q = \sqrt{(\Delta)^2 - \frac{1}{4} \left( |\varepsilon|^2 \pm \eta \sqrt{2|\varepsilon|^2 - \eta^2 - 4\Delta} \right)^2}. \quad (12)$$

Analysis of the solutions (12) shows that in most cases physical solutions correspond to the sign "+". Obviously there is also a solution with the wavenumber  $-q$ . The stopband range of frequencies begins at the frequency:  $\Delta = \Delta_-$  and has the upper edge either at the frequency  $\Delta = \Delta_+ < \Delta_b$ , if  $|\varepsilon| < 0.5\eta$  (where  $\Delta_b = -\frac{\eta^2 - 2\varepsilon^2}{4}$ ) or at the frequency  $\Delta_b$  if  $|\varepsilon| > 0.5\eta$ . In the latter case the stopband is not separated from the frequency range which corresponds to the scattering of the bulk waves.

Figure 1 illustrates the dispersion curves calculated numerically [6] for shorted (Fig. 1a) and open (Fig. 1b) thin metal electrode structures on 36-LiTaO3 and the fitted analytic solutions (12). (Parameters  $\eta$  and  $\varepsilon$  are determined using least squares fitting procedure). It is seen that the agreement is quite satisfactory. The analytic formula gives a slightly smaller magnitude of the attenuation which results from bulk wave scattering. Fig. 1c shows dispersion curves for STW on 36 Y rotated cut quartz (with propagation direction perpendicular to the X-axis).



These curves correspond to experimental devices with period  $p = 2.5 \mu$  and the thickness of Al near 1100 Å, electrode to period ratio is about 0.42.

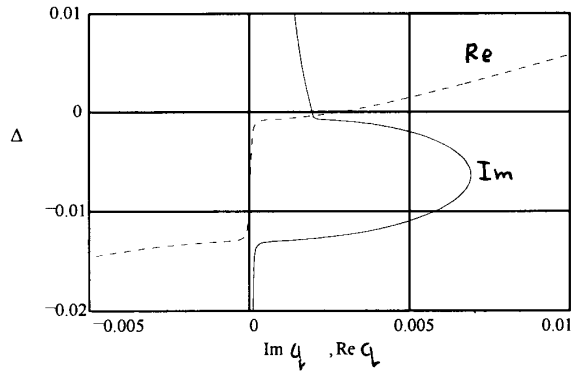
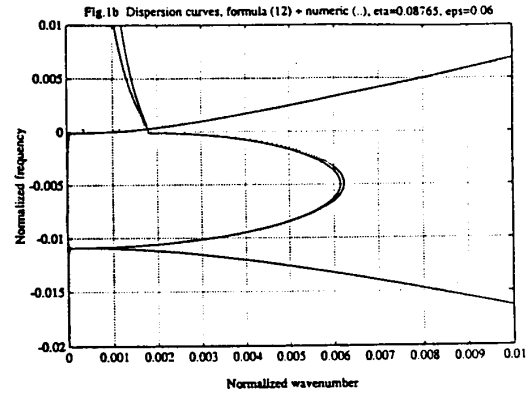


Fig. 1c Dispersion curve for STW, eta=0.1, eps=0.06

#### 4. Reflection coefficient

Each of the solutions  $\pm q$  corresponds to the eigenmode of the system and comprises two harmonics propagating in opposite directions. Therefore, we can write the waves propagating along 0X-axis in the form:

$$u^{(\rightarrow)} = h_1 \exp(\kappa_+ y + j \frac{Q}{2} (1+q)x) + h_2 H_0 \exp(\kappa_- y + j \frac{Q}{2} (1-q)x) \quad (13a)$$

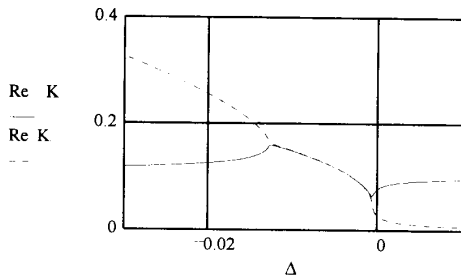
and for "-1" harmonic, describing the waves, propagating in an opposite direction we get:

$$u^{(\leftarrow)} = h_1 H_0 \exp(\kappa_- y + j \frac{Q}{2} (-1+q)x) + h_2 \exp(\kappa_+ y + j \frac{Q}{2} (-1-q)x) \quad (13b)$$

where

$$H_0 = \frac{\varepsilon}{\sqrt{2(-q - \Delta) - \eta}} \quad (14)$$

is the ratio of the amplitudes of harmonics in each of eigenmodes and  $h_1, h_2$  are the amplitude factors. The localization depth of each spatial harmonic is determined by the real part of  $\kappa_{\pm}$  (see Fig. 2) and is the same for the opposite propagating harmonics only inside the stopband. Outside the stopband the "-1" harmonic is either strongly localized near the surface (at the frequencies lower than the stopband) or becomes non-localized bulk scattered wave, at higher frequencies.



the ends of the grating. Thus we get for reflection and transmission coefficient the following formulas:

$$R = H_0 * \sqrt{\frac{|\kappa_+|}{|\kappa_-|}} * \frac{1 - \exp(2jqL)}{1 - H_0^2 * \frac{|\kappa_+|}{|\kappa_-|} * \exp(2jqL)} \quad (15)$$

$$T = \frac{1 - H_0^2 * \frac{|\kappa_+|}{|\kappa_-|}}{1 - H_0^2 * \frac{|\kappa_+|}{|\kappa_-|} * \exp(2jqL)} * \exp(jqL) \quad (16)$$

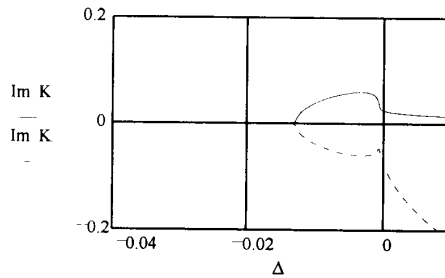


Fig.2 Inverse localization depth

This change of the localization depth creates major difficulties when these eigenmodes are used for description of wave propagation in finite grating. We suppose here that the wave is incident from the left side on the finite length grating occupying the area  $x \in (0, L)$ . Obviously at the ends of the grating the spatial structure of the waves can change abruptly, if the surface is free or metallized outside of the grating region. In this case there must be scattering and transformation of the wave. Equally, "reflected" waves harmonics (13b) also have different localization depth. In standard COM model this difficulty is absent, because all waves are supposed to have exactly the same parameters except amplitudes.

The following solution is proposed. The energy flow in the waves is determined by the amplitudes and by the localization depth:  $\frac{|u^{\leftrightarrow}|^2}{|\kappa_{\pm}|}$ . We can introduce "effective

amplitudes"  $\frac{|u^{\leftrightarrow}|}{\sqrt{|\kappa_{\pm}|}}$  and consider these values as the amplitudes of the waves which must be matched with the amplitudes of the incident and the reflected waves at

These formulas are analogous to the ones obtained in standard variant of COM model briefly summarized in the Appendix. Figure 3 shows a reflection coefficient frequency dependence for STW (the same case as in Fig. 1c) calculated using formulas (15), (16) and the corresponding formulas from the Appendix. One can see that the high attenuation at the frequencies higher than the stopband results in an asymmetric form of the curve. The phase of reflection coefficient is not equal to  $-\pi/2$  in the center of the stopband and tends to  $-\pi/4$  for STW if  $\eta \approx \varepsilon$ , [3], [8].

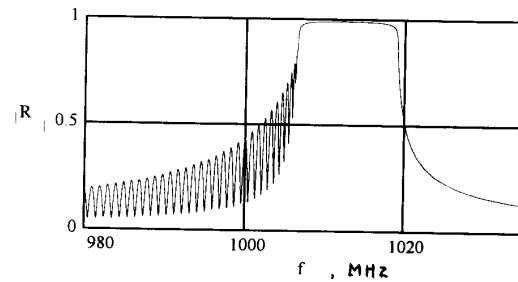


Fig. 3a The absolute value of reflection coefficient (15), Nr=1000

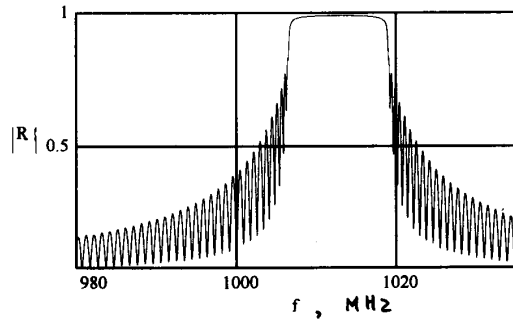


Fig.3b Standard COM theory,  $|R|$  for the same grating as on Fig.3a

Finally Figure 4 shows the comparison of the measured admittance curve of a one port synchronous resonator ( $p=2.5$ , number of electrodes in reflectors  $Nr=1000$ , in IDT  $Nr=75$  pairs of electrodes). Formulas (15), (16) were used for the reflectors, but the transducer was described by standard COM formulas. The agreement between the measured and simulated curves is satisfactory.

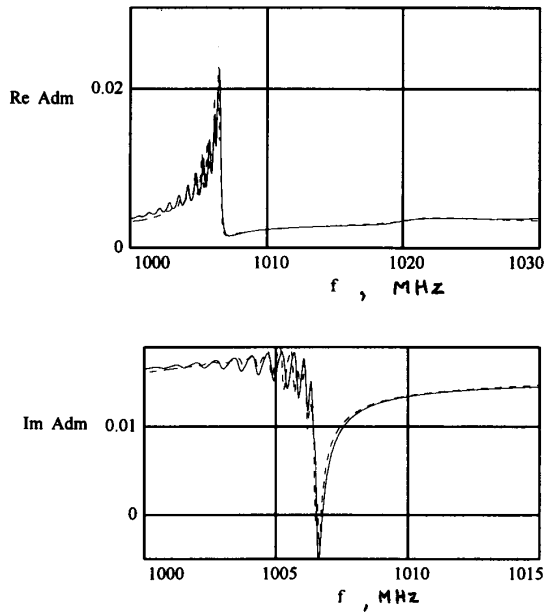


Fig.4 Admittance of STW synch. resonator, — measured

## 5. Conclusions

A closed form dispersion equation for shear types of surface acoustic waves propagating in a periodic system of reflecting elements is introduced. The equation shows that the bulk wave scattering at frequencies higher than the stopband results in strong attenuation of the waves. The upper edge of the stopband cannot be at a frequency higher than the bulk wave generation frequency. A comparison with the numerically obtained dispersion curves for leaky waves on 36-LiTaO<sub>3</sub> shows good agreement. An experimental curve for admittance of one port test STW resonator could be fitted using obtained formulas.

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### Appendix

Here the formulas of the COM model are summed up briefly. The numeration of the formulas corresponds to the text, so only an absolute minimum of comment is made. (Note that the time factor is in the complex conjugated form  $\exp(j\omega t)$ , so final results must be taken complex conjugated, if compared):

$$u^{(\rightarrow)} = h_1 * \exp(-jqx) \quad (A1a)$$

$$u^{(\leftarrow)} = h_2 * \exp(jqx) \quad (A1b)$$

Localization depth is not a parameter in COM model:

$$\kappa_{\pm} = const \quad (A2)$$

$$\frac{du^{(\rightarrow)}}{dx} = -j * \Delta * u^{(\rightarrow)} - j * K * u^{(\leftarrow)} \quad (A3a)$$

$$\frac{du^{(\leftarrow)}}{dx} = j * \Delta * u^{(\leftarrow)} + j * K * u^{(\rightarrow)} \quad (A3b)$$

( $q, \Delta = q - Q/2$  and  $K$  are not normalized here,  $K \approx \pi * \eta * \varepsilon / p$ )

After substitution of (Ap\_1a,b) we get:

$$\begin{aligned} (q - \Delta) * h_1 &= K * h_2 \\ (q + \Delta) * h_2 &= -K * h_1 \end{aligned} \quad (A4)$$

From where follows the main formula of COM:

$$q = \pm \sqrt{\Delta^2 - K^2} \quad (A12)$$

with the relative width of the stopband equal to

$$\frac{\Delta\Omega}{\omega_0} = \frac{2p}{\pi} * K \quad (A11)$$

For a finite grating the solutions are written in the form:

$$u^{(\rightarrow)} = h_1 * \exp(-jqx) + H_0 * h_2 * \exp(jqx)$$

$$u^{(\leftarrow)} = h_1 * H_0 * \exp(-jqx) + h_2 * \exp(jqx)$$

(A13a,b)

with

$$H_0 = -\frac{K}{\Delta + q} \quad (A14)$$

reflection and transmission coefficient being given by formulas:

$$R = H_0 * \frac{1 - \exp(-2jqL)}{1 - H_0^2 * \exp(-2jqL)} \quad (A15)$$

$$T = \frac{1 - H_0^2}{1 - H_0^2 * \exp(-2jqL)} * \exp(-jqL) \quad (A16)$$