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ACOUSTIC SURFACE WAVES IN PIEZOELECTRIC CRYSTALS WITH THIN OVERLAYERS

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Resume - Nous étudions des cristaux piézoélectriques (symétrie 6 mm) avec des couches minces en surface de même symétrie, en utilisant une nouvelle version de la méthode "Surface Green Function Matching" (SGFM). Nous considérons les combinaisons possibles des surfaces et interfaces métallisées/non métallisées.

Abstract - Piezoelectric systems of 6 mm symmetry with thin overlayers of the same symmetry are considered by using a recent extension of the surface Green function matching (SGFM) method. The possible combinations of metallized/non metallized surfaces and interfaces are considered.

1. Introduction. The one-interface problem.

Surface waves at the surfaces or interfaces of piezoelectric materials can be studied /1/ by means of the Surface Green Function Matching (SGFM) method /2/. Here is a brief summary in a concise notation adapted for the extension to the two interface problem. Consider a medium with elastic stiffness coefficients \( C_{ijkl} \), piezoelectric coefficients \( e_{ijk} \) and dielectric coefficients \( \varepsilon_{ij} \). We define a tetravector \( V=(V_M, V_E)=(u, \phi) \) in a manifold spanned by greek symbols \( \alpha, \beta, \ldots =1, 2, 3, 4 \), in which \( u \) is the mechanical (M) part, i.e. the elastic wave amplitude with components \( u_i \) in the manifold \( M \) spanned by latin symbols \( i, j \), \( i, j =1, 2, 3 \). The fourth component of the complete manifold is the electrostatic potential \( \phi \). We define also the tetravector \( W=(W_M, W_E)=(f, q) \), where \( f=\)force/volume and \( q=\)charge/volume. The elastic wave equation and Poisson's equation can be compacted into one formal equation of motion:

\[
L_{MM}V_M + L_{ME}V_E = W_M,
\]

\[
L_{EM}V_M + L_{EE}V_E = W_E.
\]

In Fourier transform (summation over repeated indices)

\[
L_{j\alpha}(k, \omega) = -\rho \delta_{j\alpha} \omega^2 + C_{ijkl} \delta_{\alpha i} k^i k^j + e_{ikj} \delta_{\alpha 4} k^i k^k,
\]

\[
L_{4\alpha}(k, \omega) = -\delta_{\alpha 4} e_{ikl} k^i k^k + \delta_{\alpha 4} \varepsilon_{ik} k^i k^k,
\]

whence the Green function \( G(k, \omega) \), i.e. the reciprocal of \( L(k, \omega) \). We put a surface at \( x_3=0 \) and, from the constitutive relations, define

\[
A_{j\alpha} = c_{3ijkl} \nabla^l G_{\alpha} + e_{ikj} \nabla^l G_{4\alpha},
\]

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which involves normal derivatives. Let $A^{(\pm)}$ indicate the surface projection of $A$ with the sign specification corresponding to the side from which normal derivatives are taken. Then

$$ G^{-1}_s = A^{(+)}_1 \cdot G^{-1}_s \cdot A^{(-)}_2 \cdot G^{-1}_s \ . $$

The objects entering this formula are now 4x4 supermatrices in the (M,E) manifold, as indicated. Knowing $G$, one extracts from it the desired physical information in the standard way /2/. In particular, the surface mode dispersion relation (SMDR) is \( \kappa \) = projection of \( k \) parallel to the surface

$$ \det G^{-1}_s(\kappa, \omega) = 0 \ . $$

We shall consider the case of 6 mm symmetry (e.g. CdS, ZnO) with the \( \sigma \)-axis in the 0x3 direction, contained in the surface \( x_3 = 0 \) and normal to the propagation direction 0x1. For this geometry the only coefficients needed are \( \rho, \sigma_{1,2,3}, \epsilon_{1,2,3} \) and \( \sigma_{1,5} \). For a free surface, medium 1 is the vacuum, with \( \rho_1 = \sigma_1 = \sigma_3 = 0 \) and (in rationalised MKS units)

$$ \epsilon_1 = \epsilon_3 \ . $$

Whether for a free surface or for an interface, with this geometry the supermatrices are diagonalized in 2x2 blocks /1/ corresponding to a decoupling of the Rayleigh sagittal mode \((u_1, \omega)\) and the Bleustein-Gulyaev /3/ piezoelectric mode \((u_2, \phi)\). The analysis of /1/ will now be extended to the case of two interfaces a finite distance apart.

2. The two-interface problem.

This is of practical interest, as it includes the case of a layer of finite thickness \( h \) deposited on a substrate of a different material. Formally we consider medium 1 in \( x_3 < 0 \), 2 in \( 0 < x_3 < h \) and 3 in \( x_3 > h \). For the film problem medium 1 is the vacuum. The formula for the general case (three different media) can be written down /4/ in terms of projectors \( I^L \) (for left, surface at \( x_3 = 0 \)) and \( I^R \) (for right, surface at \( x_3 = h \)) with cross terms describing the coupling between the two surfaces. The formula can be readily used, as given in /4/, for computational purposes. When the problem can be solved analytically, as is the case for the Bleustein-Gulyaev mode with the 6 mm symmetry, then it may be more practical to use an alternative procedure. First consider 1 and 2 matched at \( x_3 = 0 \). This yields (4) from which, when both \( r \) and \( r' \) are on the side \( x_3 > 0 \) we have /2/

$$ < r | G_s | r' > = < r | G_2 | r' > + < r | G_2 | 0 > \cdot G_2^{-1} \cdot (G_1 - G_2) \cdot G_2^{-1} \cdot < 0 | G_2 | r' > \ . $$

The idea is to match the medium 1/2, described by (6), with medium 3 and to effect this matching at \( x_3 = h \).

Let \( G \) etc indicate projections at \( x_3 = 0 \) and \( g \), etc indicate projections at \( x_3 = h \). Since \( G_2 \) and \( G_3 \) describe homogeneous media, these Green functions and their normal derivatives have the same projections at \( x_3 = 0 \) and at \( x_3 = h \). Now, from (4) and (6) we can obtain \( g_3 \), hence \( g_3^{-1} \), and \( a^+ \). (All the information needed about \( G_2 \) and its derivative is given in /1/). Let \( G \) indicate the Green function of the one-surface system which results when (4) is matched with \( G_3 \) at \( x_3 = h \). The same analysis yields

$$ g_3^{-1} = a_3^{(+)} \cdot G_3^{-1} = a_3^{(-)} \cdot G_3^{-1} \ , $$

(7)
whence we can obtain the normal modes of the film on a substrate, for arbitrary film thickness.

The matrix \( a_{(+)} \) is obtained by applying the general prescription (3) to \( G_s \), given by (6). As indicated, we shall concentrate on the piezoelectric mode which is the Bleustein-Gulyaev mode for the free surfaces. In our notation the block corresponding to this mode is labeled with \( \alpha, \beta = 2, 4 \). For media 2 (film) and 3 (substrate) we define

\[
\theta = \epsilon_2^2/\epsilon_c, \quad d = c + \theta, \quad d = d/\epsilon
\]

\[
\beta = (\kappa^2 - \rho d^2/\bar{d})^{1/2}
\]

The result for (7) is of the form

\[
g_{ss}^{-1} = fm
\]

where \( f \) is a scalar factor given by

\[
f = \frac{1}{4} \, \frac{d_2^2 \epsilon_3^2}{\epsilon_2} \left[ \left( \epsilon + \epsilon E_3 + \epsilon E_4 + \epsilon E_5 \right) \kappa^2 + \frac{\theta_2 \epsilon_3}{2 \epsilon_2} \left[ -\epsilon - \epsilon E_4 + \epsilon E_6 \right] \kappa^2 + \frac{\theta_2 \epsilon_3^2}{d_2^2 \epsilon_2} \left[ -1 - E_6 + E_4 \right] \kappa^3 \right]
\]

with \( \epsilon = \epsilon_2 + \epsilon', \epsilon' = \epsilon_2 - \epsilon, E_1 = \exp(-\beta_2 h), E_2 = \exp(-\kappa h), E_3 = E_1^2, E_4 = E_2^2, E_5 = E_1 E_2, E_6 = E_2^2, \) and the matrix elements of \( m \) are

\[
m_{22} = \frac{1}{4} \, \frac{d_2 \epsilon_3^2}{\epsilon_2} \left[ \left( \frac{d_2 \epsilon_3}{\epsilon_2} + d_3 \epsilon_3 - d_2 \epsilon_2 \right) \left( \epsilon + \epsilon E_4 + \epsilon E_5 \right) \kappa^2 + \left[ -\frac{1}{4} \epsilon \left( \frac{d_2 \epsilon_3}{\epsilon_2} + d_3 \epsilon_3 - d_2 \epsilon_2 \right) \left( \theta_2 + \frac{\theta_3}{2} \right) E_3 \right. \right.
\]

\[
+ \left. \frac{1}{4} \epsilon \left( \frac{d_2 \epsilon_3}{\epsilon_2} + d_3 \epsilon_3 - d_2 \epsilon_2 \right) \left( \theta_2 - \frac{\theta_3}{2} \right) E_4 \right. \right. \]

\[
+ \left[ \frac{1}{4} \left( \frac{\epsilon_2}{\epsilon_3} \left( \theta_2 + \frac{\theta_3}{2} \right) E_2 \right. \right. \]

\[
+ \frac{1}{4} \epsilon \left( \frac{d_2 \epsilon_3}{\epsilon_2} + d_3 \epsilon_3 - d_2 \epsilon_2 \right) \left( \theta_2 - \frac{\theta_3}{2} \right) E_4 \right. \right. \]

\[
+ \left[ \frac{1}{4} \left( \frac{\epsilon_2}{\epsilon_3} \left( \theta_2 + \frac{\theta_3}{2} \right) E_2 \right. \right. \]

\[
+ \frac{1}{4} \epsilon \left( \frac{d_2 \epsilon_3}{\epsilon_2} + d_3 \epsilon_3 - d_2 \epsilon_2 \right) \left( \theta_2 - \frac{\theta_3}{2} \right) E_4 \right. \right. \]

\[
+ \left. \left. \frac{1}{4} \left( \frac{\epsilon_2}{\epsilon_3} \left( \theta_2 + \frac{\theta_3}{2} \right) E_2 \right. \right. \]

\[
+ \frac{1}{4} \epsilon \left( \frac{d_2 \epsilon_3}{\epsilon_2} + d_3 \epsilon_3 - d_2 \epsilon_2 \right) \left( \theta_2 - \frac{\theta_3}{2} \right) E_4 \right. \right. \]

\[
+ \left. \left. \frac{1}{4} \left( \frac{\epsilon_2}{\epsilon_3} \left( \theta_2 + \frac{\theta_3}{2} \right) E_2 \right. \right. \]

\[
+ \frac{1}{4} \epsilon \left( \frac{d_2 \epsilon_3}{\epsilon_2} + d_3 \epsilon_3 - d_2 \epsilon_2 \right) \left( \theta_2 - \frac{\theta_3}{2} \right) E_4 \right. \right. \]

\[
+ \left. \left. \frac{1}{4} \left( \frac{\epsilon_2}{\epsilon_3} \left( \theta_2 + \frac{\theta_3}{2} \right) E_2 \right. \right. \]

\[
+ \frac{1}{4} \epsilon \left( \frac{d_2 \epsilon_3}{\epsilon_2} + d_3 \epsilon_3 - d_2 \epsilon_2 \right) \left( \theta_2 - \frac{\theta_3}{2} \right) E_4 \right. \right. \]
Using (11) and (10) in (9) we obtain the secular equation
\[ \det g_{ss} = 0 \]
which yields the normal modes of the film system. The case of short-circuited surfaces or interfaces /5/ can be likewise studied by modifying the electrical boundary conditions and doing the same matching analysis. Work on these problems is in progress.

References