Supplementary Materials: A Theoretical Study of Love Wave Sensors Based on ZnO–Glass Layered Structures for Application to Liquid Environments

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1. Half-Space/Guiding Layer

A piezoelectric ZnO layer of thickness \( h_{\text{gl}} \) overlays a glass isotropic half-space, as shown in Figure S1. The space above the layer is occupied by air or vacuum which is assumed to have no mechanical contact with the layer.

\[ \begin{align*}
\begin{bmatrix}
T_1 \\
T_2 \\
T_3 \\
T_4 \\
T_5 \\
T_6 \\
D_1 \\
D_2 \\
D_3
\end{bmatrix} &=
\begin{bmatrix}
\epsilon_{11} & \epsilon_{12} & \epsilon_{13} & \epsilon_{14} & 0 & 0 & 0 & -\epsilon_{31} & -\epsilon_{31} \\
\epsilon_{12} & \epsilon_{22} & \epsilon_{23} & \epsilon_{24} & 0 & 0 & 0 & -\epsilon_{31} & -\epsilon_{31} \\
\epsilon_{13} & \epsilon_{23} & \epsilon_{33} & \epsilon_{34} & 0 & 0 & 0 & -\epsilon_{31} & -\epsilon_{31} \\
\epsilon_{14} & \epsilon_{24} & \epsilon_{34} & \epsilon_{44} & 0 & 0 & 0 & -\epsilon_{31} & -\epsilon_{31} \\
0 & 0 & 0 & 0 & \epsilon_{55} & \epsilon_{56} & -\epsilon_{31} & 0 & 0 \\
0 & 0 & 0 & 0 & \epsilon_{56} & \epsilon_{66} & -\epsilon_{31} & 0 & 0 \\
0 & 0 & 0 & 0 & \epsilon_{15} & \epsilon_{16} & \epsilon_{11} & 0 & 0 \\
\epsilon_{31} & \epsilon_{32} & \epsilon_{33} & \epsilon_{34} & 0 & 0 & 0 & \epsilon_{22} & \epsilon_{23} \\
\epsilon_{31} & \epsilon_{32} & \epsilon_{33} & \epsilon_{34} & 0 & 0 & 0 & \epsilon_{23} & \epsilon_{33}
\end{bmatrix}
\begin{bmatrix} S_1 \\ S_2 \\ S_3 \\ S_4 \\ S_5 \\ S_6 \\ E_1 \\ E_2 \\ E_3 \end{bmatrix} \end{align*} \]

The wave under consideration is assumed to travel in the \( x_1 \)-direction along a surface whose normal is in the \( x_2 \) direction, and to be polarized parallel to the \( x_3 \) direction. The only non null particle displacement component is \( U_3 \), and both \( U_3 \) and the electric potential \( \Phi \) are independent of the \( x_3 \) coordinate: since travelling wave solutions are in the form \( U_3 = U_3(x_1, x_2, t) \) and \( \Phi = \Phi(x_1, x_2, t) \), then the Equation (S1) can be rewritten as
The equations of motion for the piezoelectric finite thickness layer and for the isotropic half-space are:

\[ \rho \frac{\partial^2 u_3}{\partial x_2^2} = \frac{\partial^2 \Phi}{\partial x_2^2}, \quad 0 < x_2 < -h \]  

(S3)

\[ \rho_{\text{sub}} \frac{\partial^2 u_{3\text{sub}}}{\partial x_2^2} = c_{14} \left( \frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial x_2^2} \right) u_{3\text{sub}}, \quad x_2 > 0 \]  

(S4)

\[ \epsilon_{11\text{sub}} \left( \frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial x_2^2} \right) \Phi = 0, \quad x_2 < 0 \]  

(S5)

The assumed solutions to the propagation equation in the substrate (sub), guiding layer (gl) and in the region above the free surface of the guiding layer are the following:

\[ u_3^\alpha = [A e^{-qz_2}] \cdot e^{j(kx_1 - \omega t)} \]  

(S6)

\[ \Phi_{\text{sub}} = B e^{-qz_2} e^{j(kx_1 - \omega t)} \]  

\[ u_3^{\text{gl}} = [C_1 \cdot e^{jkx_2} + C_2 \cdot e^{-jkx_2}] \cdot e^{j(kx_1 - \omega t)} \]  

(S7)

\[ \Phi_{\text{gl}} = [C_3 \cdot e^{jkx_2} + C_4 e^{-jkx_2}] \cdot e^{j(kx_1 - \omega t)} \]  

(S8)

where \( C_1, C_2, C_3, C_4 \), A and B are arbitrary constants, \( k = \omega / v \) is the wave-number (it is real since the ZnO and glass are lossless materials), \( v \) is the Love mode velocity (whose value is in between the shear horizontal bulk acoustic wave velocity in the layer and in the substrate, \( v_{\text{SH}} \)), \( \omega = 2\pi f \), \( f = v / \lambda \), q and \( \beta \) account the variation in depth of the wave amplitude. By substituting Equations (S6–S8) into Equations (S3–S5), two system of equations for the displacement and the potential are obtained, that involve the layer and substrate material parameters. An algebraic equation in \( \beta \) and one in q are obtained by solving the secular equations for the layer and for the substrate. From the two algebraic equations, only q and \( \beta \) values are retained that correspond to a wave displacement that decay to zero with depth below the \( x_2 = 0 \) plane, and that varies sinusoidally into the layer. By substituting the Equations (S6–S8) into the boundary and continuity conditions, a set of homogeneous equations for the \( C_i \), \( C_2, C_3, C_4 \), A and B coefficients are obtained with \( v \) as the unknown. By setting the determinant of the coefficients equal to zero, real values of \( v \) are found for fixed layer thickness and wavelength \( \lambda \). An optimized numerical procedure was used to find a real velocity value that drives the size of the determinant of the coefficients as close to zero as possible.

2. Half-Space/Guiding Layer/Liquid

The guiding layer, as well as the half-space, is assumed to be isotropic with the constant \( c_{44} \) numerically equal to the stiffened value calculated in the previous paragraph. A viscous non
conductive liquid half-space contacts the upper surface of the layer, as shown in Figure S2: \( \rho \) and \( \eta \) are the liquid mass density and viscosity.

![Figure S2](image)

**Figure S2.** The half-space/guiding layer/viscous liquid system.

The equations of motion for the three media are the following:

\[
\rho_{\text{sub}} \frac{\partial^2 u_{\text{sub}}}{\partial x_2^2} = c_{44}^{\text{sub}} \left( \frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial x_2^2} \right) u_{\text{sub}}^3, \quad x_2 > 0 \tag{S9}
\]

\[
\rho_{\text{gl}} \frac{\partial^2 u_{\text{gl}}}{\partial x_2^2} = c_{44}^{\text{gl}} \left( \frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial x_2^2} \right) u_{\text{gl}}^3, \quad 0 < x_2 < -h_{\text{gl}} \tag{S10}
\]

\[
\frac{\partial v_2}{\partial t} = \frac{\eta}{\rho_l} \left( \frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial x_2^2} \right) v_2, \quad x_2 < -h_{\text{gl}} \tag{S11}
\]

The assumed solutions to the Equations (S9–S11) are the following:

\[
u_3^3 = \left[ U_0^{\text{sub}} \cdot e^{-q x_2} \right] \cdot e^{i(k x_1 - \omega t)} \tag{S12}
\]

\[
u_3^g = \left[ U_0^{\text{gl}} \cdot \sin(b x_2) + U_0^{\text{gl}} \cos(b x_2) \right] \cdot e^{i(k x_1 - \omega t)} \tag{S13}
\]

\[
u_3^{\text{liquid}} = \left[ U_{0l} \cdot e^{k x_2} \right] \cdot e^{i(k x_1 - \omega t)} \tag{S14}
\]

where \( k = k_0 + j \cdot \alpha \), \( q^2 = k^2 - k_s^2 \), \( b^2 = k_{gl}^2 - k^2 \), \( k_s = \omega / v_{\text{SHBAW}}^z \), \( k_{gl} = \omega / v_{\text{SHBAW}}^g \), and \( v_{\text{SHBAW}}^z \) and \( v_{\text{SHBAW}}^g \) are the particle displacement and the traction components of the stress must be continuous across the \( x_2 = 0 \) and \( x_2 = -h_{\text{gl}} \) interfaces. When the Equations (S12–S14) are substituted into the boundary conditions, a set of four homogeneous algebraic equations are obtained in the four coefficients \( U_0^{\text{sub}} \), \( U_0^{\text{gl}} \), \( U_{0l} \), and \( U_{0h} \); a non trivial solution of this equations system exists if the determinant of the coefficients vanishes. The determinant is:

\[
\sqrt{\frac{c_{44}^{\text{sub}}}{\rho_{\text{sub}}}}, \quad v_{\text{SHBAW}}^g = \sqrt{\frac{c_{44}^{\text{gl}}}{\rho_{\text{gl}}}} \text{ and } \lambda_1^2 = k^2 - j \omega (\rho_1 / \eta) \]
From Equation (S15) the wave dispersion equation is obtained: the system of two equations, the real and imaginary parts of the dispersion equation, were numerically solved by using the Levenberg-Marquardt-Fletcher method implemented within a Matlab routine, and the real and imaginary parts of the Love wave velocity were then calculated, \( v^{im} \) and \( v^{real} \).

3. Half-Space/Guiding Layer/Mass Layer/Liquid

An added mass layer (am) of thickness \( h_{am} \) is supposed to cover the guiding layer surface as shown in Figure S3. The guiding layer, the mass layer and the half-space are assumed to be isotropic.

![Figure S3. The half-space/guiding layer/mass layer/viscous liquid system.](image)

The equations of motion for the four media are the following:

\[
\rho_{sub} \frac{\partial^2 u_{sub}^{3}}{\partial x^2} = c_{sub}^{44} \left( \frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial x_2^2} \right) u_{sub}^{3}, \quad x_2 > 0 \quad \text{(S16)}
\]

\[
\rho_{gl} \frac{\partial^2 u_{gl}^{3}}{\partial z^2} = c_{gl}^{44} \left( \frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial x_2^2} \right) u_{gl}^{3}, \quad 0 < x_2 < -h_{gl} \quad \text{(S17)}
\]

\[
\rho_{am} \frac{\partial^2 u_{am}^{3}}{\partial z^2} = c_{am}^{44} \left( \frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial x_2^2} \right) u_{am}^{3}, \quad -h_{gl} < x_2 < -h_{am} \quad \text{(S18)}
\]

\[
\frac{\partial v_{3}}{\partial t} = \frac{\rho_{fl}}{\rho_{gl}} \left( \frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial x_2^2} \right) v_{3}, \quad \text{for } x_2 < -H \quad \text{(S19)}
\]

The assumed solutions to the Equations (S16–S19) are the following:

\[
u_{3}^{substrate} = \left[ u_{sub}^{3} e^{-aq_{2}x} \right] e^{j(kx_1 - \omega t)} \quad \text{(S20)}
\]
The particle displacement and the traction components of stress must be continuous across the substrate/guiding layer, guiding layer/mass layer, and mass layer/liquid interfaces. When the Equation (S20–S23) are substituted into the boundary and continuity conditions, a set of six homogeneous algebraic equations are obtained in the six coefficients $\xi_{g1}$, $\xi_{g2}$, $\xi_{am}$, $\xi_{am}$, and $\xi_{liq}$: a non trivial solution of this equations system exists if the determinant of the coefficients vanishes. The determinant is:

$$
\begin{vmatrix}
1 & -1 & 0 & 0 & 0 & 0 \\
-q\xi_{g1} & 0 & -b\xi_{g1} & 0 & 0 & 0 \\
0 & \cos(b\xi_{g1}) & -\sin(b\xi_{g1}) & -\cos(p\xi_{g1}) & \sin(p\xi_{g1}) & 0 \\
0 & c_{4g}^{bl} \sin(b\xi_{g1}) & c_{4g}^{bl} \cos(b\xi_{g1}) & -c_{44}^{ml} \sin(p\xi_{g1}) & -c_{44}^{ml} \cos(p\xi_{g1}) & 0 \\
0 & 0 & 0 & -j\omega \cos(p\xi_{g1}) & j\omega \sin(p\xi_{g1}) & -e^{-\lambda_{lt} H} \\
0 & 0 & 0 & c_{44}^{ml} \sin(p\xi_{g1}) & c_{44}^{ml} \cos(p\xi_{g1}) & -\eta_{44} e^{-\lambda_{lt} H}
\end{vmatrix} = 0 \quad (S24)
$$

where $q^2 = k^2 - k_z^2$, $b^2 = k_z^2 - k^2$, $p^2 = k_{am}^2 - k^2$, $\lambda_{lt}^2 = k^2 - j\omega (\rho_{1}/\eta)$, $k_{am} = \omega / \sqrt{\nu_{am}^{aw}}$, and $H = h_{gl} + h_{am}$. From Equation (S24) the wave dispersion equation is obtained: the system of two equations, the real and imaginary parts of the dispersion equation, were numerically solved by using the Levenberg-Marquardt-Fletcher method implemented within a Matlab routine, and the real and imaginary parts of the Love wave velocity were then calculated, $v^{im}$ and $v^{real}$.

Reference

1. Auld, B.A. *Acoustic Fields and Waves in Solids*; 2nd ed., R.E. Krieger Publishing: Malabar, FL, USA, 1990; Volume 1.