Characterisation of a micromachined degenerate fused quartz-microbalance

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This paper presents an energy trapped resonator with degenerate modal properties for application in mass sensing. Actuation and detection of the resonant modes of circular fused quartz disc is performed electromagnetically. The highly localised displacement field of the energy trapped modes makes them attractive due to their low support loss. In addition, the displacement of some of the energy trapped modes is shown to be dominated by in-plane motion at the surface of the plate and therefore radiative energy loss into any surrounding fluid will be considerably reduced. This feature, when used in conjunction with the differential sensing made possible with a degenerate mode pair, is highly attractive for biosensing applications. A thorough theoretical and experimental characterisation of the modal properties of the fused quartz plate is presented. Fused quartz is elastically isotropic and as a result the natural frequencies and normal modeshape are determined by the device geometry and material properties. For crystalline materials the elastic anisotropy can disrupt the modal properties. A numerical analysis of the modal properties of the device fabricated in single crystalline material is presented. It is shown that specific degenerate modeshapes in a silicon (111) orientated plate remain unperturbed due to its anisotropy.
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1. Introduction

Mass sensing in a liquid environment presents a significant challenge to many conventional mechanical resonators since out-of-plane displacement causes severe damping in liquid, rendering resonant based mass detection impossible [1]. In this work, the resonator geometry is configured to support vibrations which are highly dominated by shear horizontal (SH) modes and in this regard the concept is similar to the conventional Quartz Crystal Microbalance (QCM) which has been widely used in gas sensing [2]. As the vibration at the surface is dominated by in-plane displacements, this type of device offers potential use for biological mass sensing in liquid to ultimately develop a novel form of biosensor. However, the conventional QCM uses a single mode of vibration for mass detection [2–4] and is therefore highly susceptible to temperature sensitivity [5–9]. For the alternative configuration presented herein, the vibrations possess the property of modal degeneracy which offers rejection of common mode environmental effects e.g. temperature and non-specific interactions [10–13]; whereas degeneracy is not possible in the conventional QCM, making the use of peripheral temperature control instrumentation essential for mass sensing applications. Thus, making it challenging to develop QCM technology into a portable biosensor platform which is able to operate in a diverse range of environments. In this study, the resonator geometry is configured such that the degenerate vibrations used for mass sensing are energy trapped, thereby increasing the resonant Q-factor and isolating the device from support loss mechanisms prevalent in conventional MEMS designs [14]. Modal degeneracy is described in detail in [15]. In modally degenerate systems the natural frequencies occur in distinct pairs. The natural frequencies within each pair are equal and their corresponding modeshapes are identical subject to a rotation. Measuring the frequency split between the otherwise degenerate mode pair, [15], due to added mass provides a sensing strategy which removes common mode effects [16–18]. This means that the sensor will be robust against temperature changes which severely compromises the QCM.

The history of energy trapped resonant devices extends back several decades and include successful manifestations as the ubiquitous high frequency crystal filter and the QCM [19,20]. Literature
on degenerate trapped shear mode resonators includes only two recent papers [21,22], produced by the authors of this current work. The underpinning theory for degenerate trapped shear mode resonators is described in [21], and the experimental evaluation of a magnetic-acoustic degenerate resonator is presented in [22]: which confirms trapping of the degenerate SH wave in a macromachined aluminium structure. The non-degenerate trapping of pure torsional SH modes is reported in [23–25]. The undesirable out-of-plane motion in the degenerate form of energy trapped resonators is determined by the geometry, symmetry and material homogeneity of the device design. The use of aluminium as the basic resonator is disadvantageous due to its relatively low intrinsic Q-factor and the difficulty in maintaining the required dimensional tolerance and symmetry during manufacturing to minimise parasitic out-of-plane motion. Crystalline quartz, typically AT-cut, as used in the QCM, is strongly anisotropic and does not allow modal degeneracy. Fused quartz is isotropic, which allows for degeneracy in modes of circumferential order greater than 1. The use of fused quartz instead of aluminium further permits alternative fabrication routes that enable batch fabrication and miniaturisation. Fused quartz is electrically insulating, therefore electromagnetic actuation can be efficiently performed through Lorentz interaction of deposited metal tracking alongside a permanent magnetic field acting normal to the plane of the substrate [23,24]. This excitation approach permits the tracking to be placed at a location where the forcing of the desired mode pair is maximised and, hence, improve the signal to noise performance of the device. To perform the excitation via an eddy current approach, as described in previous work [22,25], results in a force that is distributed both radially and circumferentially, which is consequently less effective at putting energy into the mode of interest.

2. Description of the system

Fig. 1(a) shows the circular fused quartz substrate of thickness 2H with the plateau formed on both sides. Ideally, the plateau will be symmetric across the thickness of the plate such that \( h_2 = h_0 = h_0 \). The fundamental geometry is similar to that reported in [22]. The tracking used to Lorentz actuation is shown in Fig. 1(b). Energy trapping of the antisymmetric SH wave is well-known [4,19,26,27]. The geometrical conditions required for energy trapping are described by the wave dispersion relations for an infinite isotropic plate [26,27]. The dispersion relation for an infinite isotropic plate can be plotted for the two thicknesses corresponding to the plate, with and without the plate aligned symmetrically between both sides. Fig. 2 shows the dispersion plots. The frequencies \( k_0 \) and \( k_2 \), define the frequencies in the plate regions of thickness \( H \) and \( H + h_0 \), respectively where the radial wave number \( \xi \) of the antisymmetric SH wave is zero [19,20]. These two frequency points demarcate the frequency range within which an energy trapped mode may reside and knowledge of their location facilitates the design of the sensor.

If the design frequency is selected to reside with the range defined by the cut-off frequencies then it is possible for the anti-symmetric SH wave to be “trapped” or localised in the region where the plate is of thickness \( H \). Outside of this plateau region,
the antisymmetric SH wave will be decaying with the decay rate determined the elastic and inertia properties of the layer. Forming the plate from a material of greater mass density than the substrate enables the thickness of the plate required for trapping to be reduced. This has important consequences when the vertical edge of the plate is incorporated into the analysis of the wave dynamics. The natural frequency $\omega_n$ is related to the frequency parameter $k_n$ by

$$k_n^2 = \omega_n^2 H^2 \frac{\rho}{\mu}$$

where $\rho$ and $\mu$ are the mass density and shear modulus of the substrate.

As described in [15] cyclically symmetric structures possess the property of degeneracy for modes of vibration with cyclic order $n = 1, 2, 3, \ldots$. In the absence of any structural imperfections the modes within each pair have an identical natural frequency $\omega_n$. Furthermore, the modeshapes are identical subject to a rotation of $\pi/2n$. Degeneracy also results in the absolute orientation of the modeshape being indeterminate. Determinacy is only established if some symmetry breaking stiffness or inertia is present either via the excitation method or by the addition of matter. This causes the degenerate frequency $\omega_n$ to split into two close frequencies $\omega_{n1}$ and $\omega_{n2}$. The trapped modes are expected to have a natural frequency $\omega_n$ with $\omega_{n1} < \omega_n < \omega_{n2}$ where $\omega_{n1}$ and $\omega_{n2}$ are the cut-off frequencies corresponding to $k_{n1}$ and $k_{n1}$, respectively. The modeshapes corresponding to the natural frequencies $\omega_{n1}$ and $\omega_{n2}$ will still be trapped. Fig. 3 also includes the dispersion relation for the lowest order symmetric P and SV waves. If the boundary conditions permit, the resonant response in the vicinity of $\omega_n$ will contain components of symmetric P and SV waves which are always propagating.

The energy trapped modes correspond to the particular modal solutions where the domain is infinite [28]. This means that while the plate radius is of finite extent, the outer boundary of the circular substrate is at infinity. The energy trapped modes predicted by the model presented in [21], corresponds to this geometrical case. When the outer boundary of the substrate is finite, the wave dynamics can then include reflections from the outer boundary. This situation is effectively modelled using finite element analysis and is discussed in Section 5. For the finite domain case, it will be shown that modes very similar to the energy trapped modes are possible. These modes will be referred to hereafter as trapped.

In the finite case, modes where the displacement field is highly localised due to the presence of the finite outer boundary, are also possible. These modes will be referred to hereafter as localised. Axisymmetric energy trapped modes exist for the device structure shown in Fig. 1. It can be shown that for the axisymmetric case corresponding to $n = 0$ that the out-of-plane displacement field totally decouples from the radial and tangential displacement. The result is that pure torsional modes with excellent energy trapping attributes exist in the structure. Axisymmetric pure torsional devices are reported in [23,24]. But axisymmetric modes do not allow for differential measurement of added mass since they are not degenerate. The $n = 1$ modes are degenerate but both modes are affected by added mass identically, thus preventing differential measurement of added mass. In this body of work, the focus is on degenerate energy trapped modes that enable differential measurement of added mass. Therefore, the family of modes with $n = 2, 3, \ldots$ will be targeted for investigation.

Fig. 3 shows the displacement components along the radial line OQ with $\theta = \varphi = \pi/8$ of an n = 2 energy trapped mode calculated by a 2D finite element model. The mode shown is one of a degenerate pair and corresponds to Mode (B) of Fig. 7. The finite element model used harmonic elements and extracted modes where the radial displacement is described by $\cos(n\psi)$. Alternatively, an identical mode described by $\sin(n\psi)$ may be extracted instead. It is this trapped mode pair which the experimental device is designed to preferentially excite.

3. Excitation and detection of the degenerate in-plane shear modes

Excitation of the SH dominated energy trapped modes is performed electromagnetically using Lorentz excitation. Fig. 4 shows a drive electrode located on the plate at radius $r_o$. The drive electrode comprises a current element aligned so that its centre is concentric with the plate. Excitation of different modes can be performed using different numbers of the drive electrodes; which was as a method to identify the resonant responses. Here, the excitation is considered from a single drive electrode with the coordinate $\theta$, shown bisecting the current element. The analysis can readily be extended to incorporate any number of electrodes. A time harmonic current $I\sin\omega t$ is provided to the drive electrode in the path shown. A permanent magnetic field of flux density $B\sin\omega t$ is directed normal to the plane containing the drive electrode.
The displacement of point $P(r_0,\theta)$ located on the drive electrode is given by [21] where:

$$
\begin{align*}
u &= u_x e_x + u_y e_y + u_z e_z \\
ur &= q_1 X(r_0, z) \cos(n\psi) + q_2 X(r_0, z) \sin(n\psi) \\
ur_0 &= q_1 Y(r_0, z) \sin(n\psi) + q_2 Y(r_0, z) \cos(n\psi) \\
u_2 &= q_1 W(r_0, z) \cos(n\psi) + q_2 W(r_0, z) \sin(n\psi)
\end{align*}
$$

The generalised coordinates $q_1$ and $q_2$ represent the contributions made to the motion by the modes defining an $n^{th}$ order degenerate pair. The functions $X(r, z)$, $Y(r, z)$ and $W(r, z)$ are the displacement components of the modeshape in the radial, tangential and out-of-plane directions of the degenerate pair. Closed form expressions for the $X(r, z)$, $Y(r, z)$ modeshapes of the energy trapped modes are described in [21]. Fig. 3 shows the modeshape functions $X(r, H + h_2)$, $Y(r, H + h_2)$ and $W(r, H + h_2)$ determined by 2D finite element analysis for the mode of vibration which the device design is primarily focused on. The differential force acting on the current element $dL_m$ is given by:

$$
dF_m = dL_m \times B(r, \psi)
$$

The generalised differential force [29] acting on the current element $dL_m$ is:

$$
dQ_{mj} = dF_m \cdot \frac{\partial u}{\partial \theta_j} j = 1, 2, m = 1, 2, 3.
$$

The generalised force acting on the current sector $L_m$ $m = 1, 2, 3$ is therefore:

$$
Q_{mj} = \left( \int dQ_{mj} \right)_{L_m}
$$

The total generalised force acting on the total current line $L = \sum_{m=1}^{3} L_m$ is given by:

$$
Q_j = \sum_{m=1}^{3} Q_{mj}
$$

The expressions for the generalised forces generated by an arbitrary electrode located at $\theta_0$ for the case $r_2 = r_3$ are:

$$
Q_1 = \int_{-\theta_0 - \delta}^{\theta_0 - \delta} IB(r, \phi)X(r, H + h_2) \cos(n\phi) d\phi + \int_{r_2}^{r_3} \int 2 d\phi B(r, \phi_1)Y(r, H + h_2) \sin(n\phi_1) dr - \int_{r_2}^{r_3} \int 2 d\phi B(r, \phi_3)Y(r, H + h_2) \sin(n\phi_3) dr
$$

$$
Q_2 = \int_{-\theta_0 - \delta}^{\theta_0 - \delta} IB(r, \phi)X(r, H + h_2) \sin(n\phi) d\phi + \int_{r_2}^{r_3} \int 2 d\phi B(r, \phi_1)Y(r, H + h_2) \cos(n\phi_1) dr - \int_{r_2}^{r_3} \int 2 d\phi B(r, \phi_3)Y(r, H + h_2) \cos(n\phi_3) dr
$$

The generalised forces $Q_1$ and $Q_2$ contain contributions from both the radial and tangential displacement fields when the magnetic field is not axisymmetric. This allows excitation of torsional modes through the displacement field $Y(r, z)$. For the case where the magnetic field is perfectly axisymmetric then $B(r, \phi_1) = B(r, \phi_2)$. In this case excitation through the tangential displacement $Y(r, z)$ is not possible and only modes with nonzero radial displacement $X(r, z)$ can be excited.

The angular offset $\delta$ between the modal line and the line bisecting the electrode is unknown and depends upon the distribution of mass and elasticity of the system. To gain an insight into how the forcing can be used to discriminate between the modal responses it is convenient to set $\delta = 0$. Integration of the generalised force equations for the case where excitation is performed using a system of drive electrodes located at $\theta_0 i = 1 \cdots p$ with $\delta = 0$ gives:

$$
Q_1(n) = \frac{2}{n} IBrX(r, H + h_2) \sin(n\alpha) \sum_{i=1}^{p} \cos(n\theta_0 i)
$$

$$
Q_2(n) = \frac{2}{n} IBrX(r, H + h_2) \sin(n\alpha) \sum_{i=1}^{p} \sin(n\theta_0 i)
$$

Excitation of the modes $n = 1, 2, 3, \ldots$ is possible through the force component described by Eq. (2). Note that the centre of the permanent magnet has been assumed to coincide with centre of the
plate. If the magnet is misaligned then a net circumferential forcing component will contribute to the generalised forces \( Q_1(n) \) and \( Q_2(n) \) [25]. The net generalised forces \( Q_j(n) \) can be determined for different mode order \( n \) and different drive electrodes. If one drive electrode located at \( \theta_0 = 0 \) is used then \( Q_1(0) = Q_2(0) = 0 \) since \( X(r, H + \delta_H) = 0 \) and \( Q_1(1) \), \( Q_1(2) \), \( \ldots \), \( Q_1(N) \) are all non-zero.

If two drive electrodes located at \( \theta_0 = 0 \) and \( \theta_0 = \pi \) then \( Q_1(0) = 0 \) and \( Q_1(1) = Q_1(3) = 0, Q_1(2) \neq 0 \). Similarly \( Q_2(0) \neq 0, Q_2(1) = Q_2(3) = 0, Q_2(2) \neq 0 \).

The equation of motion defining the resonant characteristics of the system can be obtained using Lagrange’s equation [29]

\[
\frac{d}{dt} \frac{\partial T}{\partial \dot{q}_j} - \frac{\partial T}{\partial q_j} + \frac{\partial V}{\partial \dot{q}_j} = Q_j \text{, } j = 1, 2. \tag{3}
\]

where \( T \) and \( V \) are the kinetic and potential energy.

The purpose of the analysis is to determine the optimal design of the electrode for the mode of vibration of greatest interest. An estimation of the resulting forced response amplitude also provides useful information for the sensing circuit. The kinetic energy of the system is described by:

\[
T = \frac{1}{2} \int_0^{2\pi} \int_0^R \frac{\rho \cdot \dot{u} \cdot \dot{u}}{\rho} dV \text{ where } dV = rH dr d\theta.
\]

Since the gold layer defining the plate is approximately 1% of the substrate thickness its contribution has been ignored in the kinetic energy calculation. The modal stiffness is described by \( \frac{\partial V}{\partial q_j} \).

The modeshape components of the energy trapped modes with displacement components \( X(r, z), Y(r, z) \) and \( W(r, z) \) are known. This allows the equation of motion to be written in the standard form [30]

\[
\ddot{q}_j + \omega_{nj}^2 - \frac{1}{\beta_j} \omega_{nj} q_j = \frac{Q_j}{m_j} \tag{4}
\]

The terms \( \beta_j, \omega_{nj}, Q_j \) and \( m_j \) correspond to the Q-factor, natural frequency, generalised force and generalised mass of the mode \( q_j \).

For harmonic excitation \( Q_j = Q_{j0} e^{i \omega t} \) the response is given by \( q_j = q_{j0} e^{i \omega t} \).

As the damping ratio \( \frac{1}{\beta_j} \) is 1 then resonance may be approximated by the condition \( \omega_{nj} = \omega \). In this case the response amplitude is given by:

\[
q_{j0} = \frac{\beta_j Q_{j0}}{m_j \omega_{nj}^2} j = 1, 2
\]

The approximate response can be obtained by using the approximation \( \beta_1 \cong \beta_2 = \beta \), \( m_1 \cong m_2 = m, \omega_{j1} \cong \omega_{j2} = \omega_n \) where \( \beta, m, \) and \( \omega_n \) are the average Q-factor, average modal mass and average natural frequency, respectively:

\[
q_{j0} = \frac{\beta \omega_{j0} Q_{j0}}{m \omega_n^2} j = 1, 2
\]

The magnitude of the response amplitude is given by:

\[
|q_{j0}| = \frac{\beta \omega_{j0} Q_{j0}}{m \omega_n^2} \text{, } j = 1, 2
\tag{5}
\]

The natural frequency \( \omega_n \) of the layered plate is described in [21] and is also available from the finite element model. For the general case, where the modal diameter corresponding to the mode \( q_j \) is rotated by \( \delta \) relative to the datum defining the electrode, the generalised force amplitudes \( Q_{j0} \) and \( Q_{j0} \) are then both non-zero. Optimisation of the electrode geometry can be performed by considering the case \( \delta = 0 \). Clearly \( Q_{j0}(n) \) and \( Q_{j0}(n) \) are maximised when \( \alpha \epsilon = \frac{\pi}{2} \). Fig. 5 shows the variation in the generalised forcing amplitudes \( |Q_{j0}| \) and \( |Q_{j0}| \) as the radial location \( r \) of the current track is increased from the centre of the plate, 0, towards the edge. In this plot, the modeshapes used correspond to modes B and C of Fig. 7. Table 1 summarises the parameters used in the calculation. Recall that the \( Q_{j0} \) and \( Q_{j0} \) depends upon the product \( rX(r, z) \). In the experimental design the electrode radius was set \( r = r_0 = 2.5 \) mm. With reference to Fig. 5, with \( r = r_0 = 2.5 \) mm the generalised forces \( |Q_{j0}| \) and \( |Q_{j0}| \) corresponding to modes B and C are approximately equal. This should enable forcing of these modes. Note that \( |Q_{j0}| \cong 10 |Q_{j0}| \), therefore it is expected that Mode B will be more readily excited for the general case where \( \delta \neq 0 \).

4. Detection of the degenerate in-plane shear modes

The detection arrangement is shown in Fig. 6. A planar sense coil grounded midpoint forms a pair of sense coils, labelled S1 and S2. The vibration of the conducting layer of the plate in the magnetic field of the permanent magnet produces the EMF \( V \) described by:

\[
V(z) = \int_0^z \left( v(z) x B(z) \right) dl
\]

With reference to Fig. 1, the motional EMF generated in the top and bottom conducting plates is:

\[
V_1 = V(H) \quad \text{and} \quad V_2 = V(-H)
\tag{6}
\]
Fig. 7. Localised and trapped modes $n = 2, n = 3$ in fused quartz.
The magnetic field from the permanent magnet is directed along the Z axis and

\[ B_1 = B(H) \quad \text{and} \quad B_2 = B(-H) \]

with:

\[ B_2 = B_1 + \Delta B, \quad B_2 > B_1 \]

The velocity in the top and bottom conducting plates are defined:

\[ v = \nu(H) \quad \text{and} \quad v = \nu(-H). \]

The energy trapped modes are skew symmetric through the thickness of the plate:

\[ v = -\nu \]

The interaction of the conducting plate and the sense coils can be represented as a transformer with:

\[ V_{s1} = -\alpha_1 v_1 - \beta_1 v_2 \]
\[ V_{s2} = \alpha_2 v_1 + \beta_2 v_2 \]

where \( V_{s1} \) and \( V_{s2} \) are the transformed EMFs in S1 and S2, respectively.

In differential sensing the EMF from the pair of sense coils is given by:

\[ V_{s2} - V_{s1} = (\alpha_1 + \alpha_2) V_1 + (\beta_1 + \beta_2) V_2 \]

Differential sensing from the sense coils in the configuration shown in Fig. 6 is advantageous since it removes noise common to both S1 and S2. Whilst \( B_2 > B_1 \) and consequently \( |V_2| > |V_1| \), the transformer parameters corresponding to the electromagnetic interaction between the sense coil and the two conductive layers are related:

\[ \beta_1, \beta_2 < \alpha_1, \alpha_2 \]

As a result, the differential signal can be approximated to:

\[ V_{s2} - V_{s1} \approx (\alpha_1 + \alpha_2) V_1 \]

In order to maximise the signal \( V_{s2} - V_{s1} \) it is important to maximise the electromagnetic interaction defined by \( \alpha_1, \alpha_2 \). The distance \( s_0 \), between the sense coils and the top conductive plate, should be minimised to avoid electrical contact.

5. **Finite element based modal analysis**

5.1. **Energy trapped modes and localised modes for \( n = 2, 3 \)**

An elastic model of the experimental device was developed using ANSYS finite element software. The step height of the plate was optically profiled using a ZYGO New-View 500 profilometer to determine the exact dimensions. The measured dimensions were then imported into ANSYS for modal analysis. Ideally, the step heights on both sides of the substrate should be equal. Since it is skew symmetric modes, that permit energy trapping [26,27], any through thickness asymmetry results in a contribution to the motion from symmetric modes. The symmetric modes are always propagating and hence their presence will provide a route for energy leakage and hence lower the Q-factor. Table 2 summarises the dimensions of the experimental fused quartz device used in the finite element modal analysis.

<table>
<thead>
<tr>
<th>Table 2</th>
<th>Dimensions of device used in the 2D finite element modal analysis.</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>10.0 mm</td>
</tr>
<tr>
<td>R</td>
<td>25.5 mm</td>
</tr>
<tr>
<td>H</td>
<td>2.0 mm</td>
</tr>
<tr>
<td>h₁</td>
<td>22.0 µm</td>
</tr>
<tr>
<td>h₂</td>
<td>18.6 µm</td>
</tr>
<tr>
<td>s₁</td>
<td>≥250 µm</td>
</tr>
<tr>
<td>s₂</td>
<td>≥250 µm</td>
</tr>
</tbody>
</table>

The axisymmetric structure of the mechanical device lends itself to a reduced finite element model whereby the modal properties can be extracted using the 2D harmonic element PLANE83. This greatly reduces the size of the model. The modes were determined over a frequency range determined by the Bechmann numbers defining the stop band in the dispersion curve [19,27]. The circumferential mode order \( n \) used in the finite element model can be specified to be any positive integer within the element properties of the finite element code.

True energy trapped modes can exist when the domain defined by the outer radius of the substrate is infinite [28]. The energy trapped degenerate modes for the infinite domain case are reported in [21]. When the domain is finite, the presence of the outer boundary can result in reflections which result in localised modes. The localised and energy trapped modes were recorded for each value of the circumferential mode order \( n = 0, 1, 2, 3 \). Other modes of vibration were calculated by the finite element model but are of no interest in this application and are not described. The FE determined trapped and localised modes corresponding to \( n = 2, 3 \) are shown in Fig. 7. The frequency range of the extracted modes was defined by the pair of Bechmann numbers defining the cut-off frequencies. The energy trapped modes corresponding to circumferential order \( n = 2 \) are labelled as A, C. Localised modes for the \( n = 2 \) case are labelled as A, D. The energy trapped modes for the \( n = 2 \) case have all three displacement components highly localised to the stepped region. In contrast, the localised modes do not demonstrate the same level of localisation as exhibited by the true trapped modes. For the \( n = 3 \) case, energy trapped mode labelled as F is very similar to its \( n = 2 \) counterpart, B. However, the energy trapped mode labelled G is not as localised as it \( n = 2 \) counterpart, C. It is shown in [21] that the displacement components of the modeshapes depend upon the circumferential order \( n \). Therefore, the slight change in modeshape between the \( n = 2 \) and \( n = 3 \) cases is expected. The mode frequencies corresponding to trapped and localised modes extracted using the 2D finite element model are listed in Table 3 alongside the experimental values. The frequency range was defined by the Bechmann numbers of the dispersion plot.

5.2. **Energy trapped modes and localised modes for \( n = 0, 1 \)**

The modes of vibration with \( n = 0, 1 \) do not enable differential mass sensing. The mode shapes of the \( n = 0 \) modes are shown in Fig. 8. Purely torsional axisymmetric modes with excellent energy trapping attributes are labelled as modes (a) and (c). A localised asymmetric radial mode was also determined by the FE modal analysis and is shown as mode (b). The pure torsional axisymmetric modes \((a,c)\) are devoid of any out-of-plane displacement as expected. However, the radial mode \((b)\) exhibits significant out-of-plane motion Fig. 8. Fig. 9 shows the \( n = 0 \) modes.

6. **Experimental results from frequency response analysis**

The complete experimental setup is shown in Fig. 10. Note the reference signal for the lock-in amplifier was selected using the user software interface and the connection made internally by the amplifier. Frequency response tests were performed using a Zurich Instruments HF2LI Lock-in Amplifier, sense coils and permanent magnet configuration as shown in Fig. 6.

The field strength of the permanent magnet supplied from Arnold Magnetic Technologies was 200 mT measured at a distance
Fig. 8. Localised and trapped modes $n=0$ in fused quartz.

Fig. 9. Localised and trapped modes $n=1$ in fused quartz.
Table 3
FEA determined natural frequencies and the experimental resonant frequencies for \( n = 0, 1, 2, 3 \).

<table>
<thead>
<tr>
<th>Mode Reference</th>
<th>Type</th>
<th>Circumferential order</th>
<th>FEA Natural Frequency (kHz)</th>
<th>Measured Resonant Frequencies</th>
<th>Measured Q-Factor</th>
</tr>
</thead>
<tbody>
<tr>
<td>a</td>
<td>trapped</td>
<td>0</td>
<td>814.4</td>
<td>820.375</td>
<td>23,636</td>
</tr>
<tr>
<td>b</td>
<td>localised</td>
<td>0</td>
<td>846.7</td>
<td>849.433</td>
<td>1566</td>
</tr>
<tr>
<td>c</td>
<td>trapped</td>
<td>0</td>
<td>856.8</td>
<td>802.479</td>
<td>43,612</td>
</tr>
<tr>
<td>a</td>
<td>trapped</td>
<td>1</td>
<td>809.2</td>
<td>802.488</td>
<td>53,858</td>
</tr>
<tr>
<td>b</td>
<td>trapped</td>
<td>1</td>
<td>823.3</td>
<td>849.433</td>
<td>23,636</td>
</tr>
<tr>
<td>c</td>
<td>localised</td>
<td>2</td>
<td>827.4</td>
<td>840.067</td>
<td>19,998</td>
</tr>
<tr>
<td>A</td>
<td>localised</td>
<td>2</td>
<td>855.3</td>
<td>840.087</td>
<td>46,708</td>
</tr>
<tr>
<td>B</td>
<td>trapped</td>
<td>2</td>
<td>912.7</td>
<td>877.140, 877.355</td>
<td>21,765</td>
</tr>
<tr>
<td>C</td>
<td>localised</td>
<td>3</td>
<td>930.6</td>
<td>877.140, 877.355</td>
<td>20,215</td>
</tr>
<tr>
<td>D</td>
<td>localised</td>
<td>3</td>
<td>846.7</td>
<td>877.140, 877.355</td>
<td>20,215</td>
</tr>
<tr>
<td>E</td>
<td>localised</td>
<td>3</td>
<td>882.3</td>
<td>877.140, 877.355</td>
<td>20,215</td>
</tr>
<tr>
<td>F</td>
<td>trapped</td>
<td>3</td>
<td>943.4</td>
<td>877.140, 877.355</td>
<td>20,215</td>
</tr>
<tr>
<td>G</td>
<td>localised</td>
<td>3</td>
<td>1190</td>
<td></td>
<td></td>
</tr>
<tr>
<td>H</td>
<td>localised</td>
<td>3</td>
<td></td>
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</table>

Fig. 10. Experimental configuration used to electromagnetically measure the modal responses. The detection coils were fabricated onto two separate PCBs. Frequency responses were extracted using the Zurich Instruments HF2 lock-in amplifier.

Fig. 11. Frequency response (magnitude) plot of Mode (a) measured electromagnetically.

A single resonant response in the vicinity of the modelled natural frequency of Mode (a) for \( n = 0 \) was also detected experimentally and its magnitude frequency response is shown in Fig. 11. Recall from Section 3 that excitation of this \( n = 0 \) mode is expected when

of 250 \( \mu \)m. A current of 200 mA was supplied to the excitation tracking to provide Lorentz forcing.

6.1. Experimental frequency response

Table 3 summarises the experimentally determined resonant frequencies alongside the natural frequencies of the purely elastic structure calculated via the 2D finite element model for comparison. Using the Nyquist plot enabled the Quality factor of the detected resonant responses to be calculated. A combination of single and double drive electrode, as described in Section 3, led to the detection and identification of Mode (B) and its \( n = 3 \) counterpart Mode (F). In the absence of structural imperfections, Mode (B) forms a degenerate pair. Similarly for Mode (F). For Mode (B), the natural frequencies are split by 0.002%. The measured average of the resonances for Mode (B) differ from the predicted value by 1.75%. In the case of Mode (F), the natural frequencies are split by 0.02% and the measured average of the resonances differ by 0.56% of the predicted value. The degree of frequency split between the responses of Mode (B) is sufficiently small for use in mass sensing.
the B-field is not perfectly axisymmetric. If the permanent magnet is positioned off-centre with respect to the centre of the plate then the circumferential force is non-zero. In this case excitation of the pure torsional mode $n=0$ is possible [25]. Whilst Mode (a) is predicted by the FE model to be purely torsional mode and so devoid of any out-of-plane motion, its measured Q-factor of 23,636 is comparable with the measured Q-factors of 19,998 and 46,708 of the Mode (B) pair. Therefore, the dominant mechanism for energy loss in air may not be due to out-of-plane motion. Recall that the purely torsional mode does not offer rejection of environmental effects e.g. temperature.

Fig. 12 shows the measured frequency response data of the two modes comprising Mode (B). The magnitude plot of Fig. 12(a) exhibits clear resonance behaviour. Electromagnetic feedthrough is evident on the magnitude plot. The Nyquist plot, of Fig. 12(b), which removes the effect of feedthrough, demonstrates behaviour indicative of classical resonance of two closely separated modes and was used to calculate the quality factors. The frequency response data of the two modes comprising Mode (F), are shown in Fig. 13, which exhibit similar behaviour. The quality factor of the two modes comprising Mode (F) differ by only 8%. This is significantly closer than the quality factors measured for Mode (B). This suggests that the structural damping is distributed circumferentially such that a Fourier series representation of the damping will have dominant 40 harmonics.

The resonances reported in Table 3 all demonstrate classical resonant behaviour and for the trapped modes the qualities factors are all comparable. However, an additional pair of resonant responses was detected. The quality factors of these responses are an order of magnitude greater than any of the classical trapped resonances determined. The detected resonances are 853.1, 853.4 kHz, respectively which are in the vicinity of the natural frequency determined using the purely elastic model for the $n=2$ mode pair [21]. Fig. 14 shows the frequency response for this mode pair. Similar high Q-factor resonant pairs have been obtained on other prototype electromagnetic devices of similar dimensions. As the system is electro-magnetic-elastic there is a possibility that the detected resonant response is not mechanical in origin. The Nyquist plot (not shown) of this response offers inconclusive evidence as to the nature of the “resonance” as its shape deviated from the ideal circular shape indicative of classical resonance. The question is whether these responses are purely elastic in nature or not and will be the subject of future investigation.
7. Issues associated with fabricating the device in single crystalline material

The use of isotropic material for the device guarantees that degenerate modes can exist in the absence of other structural imperfections. Fused quartz, whilst isotropic, has a relatively low tensile strength which hinders miniaturisation of the device concept in this substrate material. The possibility of fracturing the brittle fused quartz substrate during microfabrication makes it impractical for thicknesses less than approximately 200 μm. Single crystalline silicon has a tensile strength of the order of 100 times that of fused quartz, thus making it more attractive from a miniaturisation perspective. Ultra-thin single crystal substrates with thicknesses as low as 10 μm are readily commercially available. It is well-known that silicon substrates with surface normal directed along the (111) direction are transversely isotropic under the assumption of generalised plane stress. This has led to silicon (111) being the most common substrate material for MEMS ring gyroscopes, where degeneracy is exploited to maximise Coriolis coupling. However, the stress and strain fields of the device are fully 3D. Furthermore, energy trapping requires that the through thickness variation of the displacement field be skew symmetric [21,27]. As a result, the full compliance matrix must be included when assessing the effect of the material anisotropy on the trapped modes. Most importantly, it is the effect that anisotropy has on the out-of-plane displacement that must be assessed.

The compliance matrix \( [S] \) in Voigt notation for silicon as a function of angular position \( \theta \) in the (111) plane is of the form [31]:

\[
[S] = \begin{bmatrix}
S_{11} & S_{12} & S_{13} & -S_{24}(\theta) & S_{15}(\theta) & 0 \\
S_{12} & S_{11} & S_{13} & S_{24}(\theta) & -S_{15}(\theta) & 0 \\
S_{13} & S_{13} & S_{33} & 0 & 0 & 0 \\
-S_{24}(\theta) & S_{24}(\theta) & 0 & S_{44} & 0 & -S_{15}(\theta) \\
S_{15}(\theta) & -S_{15}(\theta) & 0 & 0 & S_{44} & -S_{24}(\theta) \\
0 & 0 & 0 & -S_{15}(\theta) & -S_{24}(\theta) & S_{66}
\end{bmatrix}
\]

The elastic anisotropy is due to the \( S_{24}(\theta) \) and \( S_{15}(\theta) \) terms which are of the form:

\[
S_{24}(\theta) = F \sin(3\theta)
\]

\[
S_{15}(\theta) = F \cos(3\theta)
\]

The angular coordinate \( \theta \) is measured with respect to the X-crystal axis of the (111) oriented silicon substrate. The \( S_{24}(\theta) \) and \( S_{15}(\theta) \) compliances correspond to coupling between the components \( (\varepsilon_{xy}, \sigma_{xz}) \) and \( (\varepsilon_{xz}, \sigma_{yz}) \), respectively. The angular dependence of the \( S_{24}(\theta) \) and \( S_{15}(\theta) \) compliances of silicon (111) breaks the perfect axial symmetry of the ideal device structure and results in a through thickness dependence. The overall structure still possesses a cyclic symmetry as defined by the 3D harmonic dependency in the compliance. The modal properties of cyclically symmetric structures is a well-developed subject [15]. The eigenvectors or mode shapes still must be 2π periodic and form a complete orthogonal set. In the most general case the eigenvectors are described by full Fourier series in the spatial coordinate \( \theta \). In the absence of elastic anisotropy, the axially symmetric structure possesses degenerate eigenvalues. In this ideal case, the eigenvectors of the degenerate pair are represented by one harmonic of the general Fourier series. However, the inclusion of general elastic anisotropy means that the eigenvectors and eigenvalues can be perturbed from that pertaining to the axially symmetric case. In general, the mode shapes will require the inclusion of several spatial harmonics of \( \theta \).

The coupling defined by the \( S_{24}(\theta) \) and \( S_{15}(\theta) \) will also modify the effect of the vertical edge of step defining the layer and as result the displacement field may be perturbed in a more general way. In the case of isotropic elastic materials Mode (B) and Mode (C) are both degenerate with circumferential order \( n = 2 \) and differ in the radial and tangential distributions of displacement. Mode (F) and Mode (G) are both degenerate with circumferential order \( n = 3 \) and differ in the radial and tangential distributions of displacement. The purpose of the 3D finite element modelling is to assess the perturbations from elastic anisotropy for the modes that offer potential use in mass sensing i.e. Mode (B), Mode (C), Mode (F) and Mode (G). In the case of the mass sensor application, perfect degeneracy is not essential and some degree of frequency splitting between the modes within each pair can be tolerated.

7.1. 3D finite element modal analysis of the design realised in silicon (111)

ANSYS Workbench was used to develop the full 3D model. The step height defining the layer was set to \( h_l = h_b = 25 \mu m \). All other dimensions were set equal to the fused quartz case. In this case the step is symmetric. The layer is approximately 1% relative of the substrate thickness. In addition, the spatial scales necessary to capture the dynamic properties extend over three orders of magnitude. Consequently, if a conventional meshing approach was used in the 3D case, adopting elements of equal size on both the mesa and plate, then the number of elements necessary would exceed 20 million. This is outside the computational capabilities of desktop computing. To circumvent this issue an alternative modelling approach was used. Meshing of the silicon substrate and thin gold layer was performed separately using 10 node quadratic tetrahedral (SOLID187) and 20 node quadratic hexahedral (SOLID186) solid elastic elements respectively. A kinematic constraint was applied at the interface between the layer and the substrate such that the translational degrees of freedom were made equal. This constraint was implemented using the Bonded Contact method. In contrast with the 2D model using harmonic elements, the 3D model allows for the full compliance or stiffness matrix to be used within the modal extraction. In addition, an isotropic version of silicon (111) was included in a separate model using the elastic modulus and Poisson ratio corresponding to the stiffness components \( C_{11} \) and \( C_{12} \) of silicon (111). The 3D FE isotropic model of the silicon (111) device can be compared with the 2D harmonic element FE model to confirm its validity. After which the 3D FE isotropic model of the silicon (111) will be used to assess the perturbation of the modes due to inclusion of the elastic anisotropy in the full 3D FE model.

7.2. 2D harmonic element FE modal analysis of the device in Silicon (111)

Fig. 15 shows the displacements field measured along a radial line from the centre of the device to the outer boundary for the case \( n = 2, 3 \). The radial line was orientated at an angle of \( \frac{\pi}{3} \) with respect to the datum defined within the harmonic element. The value of \( p \) used in the plots was set equal to 3. Equivalent plots, subject to a phase offset, can be obtained using \( p = 1, 3, 5 \ldots \). This ensures that the radial, tangential and out-of-plane components could be plotted simultaneously. The displacement amplitudes being \( \frac{1}{2} \) of their maximum values.

Following the labelling used for the fused quartz device, the energy trapped modes calculated by the 2D finite element model for case \( n = 2 \) using the isotropic approximation of silicon (111) are labelled as B and C. The mode shapes for the \( n = 3 \) case are labelled as F and G, and exhibit very similar radial and tangential displacement distributions. Mode (G), corresponding to the \( n = 3 \) case, does
exhibit more out-of-plane motion than its \( n = 2 \) counterpart, Mode (C). The FE model has an outer boundary that can cause reflection of the displacement components. As the frequency of the \( n = 3 \) modes is higher than the corresponding \( n = 2 \) modes then the effect of reflection is expected to be different as the relative phase of the incoming and outgoing waves will differ in the two cases. In addition, the modes are shown in [21] to depend upon the circumferential order.

7.3. 3D Modal Analysis of the device in isotropic approximation of Silicon (111)

Fig. 15 shows the displacement components for the 3D FE isotropic approximation of silicon (111) for the case \( n = 2 \). The line plot shows the three displacements components measured along a radial line from the centre of the device to the outer boundary. The radial line was orientated at an angle of 30° with respect to the datum defined within the harmonic element with \( p \) set equal to 1. Excellent agreement between the \( n = 2 \) mode shape shown in Fig. 16 for the 2D harmonic element model and the modes shape for 3D isotropic case validates the 3D modelling approach. The phase shift between the plots is due to the index \( p \) being 1 in the 3D model and 3 in the 2D model. In this case Mode (C) was used for the comparison.

The \( n = 3 \) case for the 3D model, isotropic case is shown in Fig. 17. Again excellent agreement with the 2D Harmonic Element model is observed. As expected due to the material isotropy to the \( n = 2, 3 \) modes being degenerate. The natural frequencies for the \( n = 2, 3 \) modes are 1273.2 and 1318.2 kHz, respectively. Mode (G) was used in the comparison in this case.

7.4. Modal analysis of the device in full anisotropic silicon (111)

With the 3D modelling approach validated, the 3D full anisotropic elastic model can be used to investigate the effect of elastic anisotropy on the energy trapped modes. Fig. 18 shows the displacements components of the one mode of a perturbed pair. In isotropic silicon, this mode is characterised as a \( n = 2 \) pair with a displacement profile shown in Fig. 16. The dominant spatial harmonic in the mode shape is still \( n = 2 \), but the presence of other harmonics is apparent. This mode will be subsequently referred to as \( \tilde{n} = 2 \). The out-of-plane displacement is also significantly different from the 3D isotropic case.

Recall that for perfect axial symmetry the eigenvalues are degenerate. The inclusion of elastic anisotropy of silicon (111) breaks the axial symmetry and as a result, the eigenvalues comprising each pair will in general be split. Degeneracy can be maintained in specific cases. For the \( \tilde{n} = 2 \) pair in anisotropic silicon (111) the mode shapes are perturbed compared to their \( n=2 \) counterpart, Mode (C).

The natural frequencies of the \( \tilde{n} = 2 \) pair are shifted to 1233.7 kHz, but degeneracy is maintained. However, material anisotropy has resulted in perturbation of the mode shapes. Although the \( \tilde{n} = 2 \) modes are spatially orthogonal the demarcation of the regions of where to add mass or provide excitation are less distinct.
Fig. 16. (a) Displacement components of the FE determined 2n mode in isotropic silicon (111): Radial (i), tangential (ii) and vertical (iii) displacements. The natural frequencies of the mode pair are 1273.2, 1273.2 kHz indicating degeneracy. (b) The displacement components of the mode plotted along the radial line OQ.

Fig. 17. Displacement components of the FE determined 3n mode in isotropic silicon (111): The natural frequencies of the mode pair are 1318.2, 1318.2 kHz indicating degeneracy. Radial (i), tangential (ii) and vertical (iii) displacements.

Fig. 19 shows the displacements components of a mode pair of different circumferential order. In isotropic silicon this mode pair is characterised as a $\bar{n} = 3$ pair with a displacement profile shown in Fig. 13 and previously labelled as Mode (G). In the anisotropic case this mode pair will be referred to $\bar{n} = 3$ to distinguish it from the isotropic case.

In contrast with the $\bar{n} = 2$ case the $\bar{n} = 3$ mode shape is less perturbed due to the anisotropy of silicon (111). The eigenvalues of the $\bar{n} = 3$ modes are split. The frequency split is 0.5% of the average of the pair of natural frequencies.

7.5. Kinetic energy contributions of the displacement components in full anisotropic silicon (111)

When operating the mass sensor in liquid, an environment which biosensors typically operate, the out-of-plane displacement
Fig. 18. Displacement components of the FE determined 2n dominant modes in anisotropic silicon (111): Radial (i), tangential (ii) and vertical (iii) displacements. The natural frequencies of the mode pair are 1318.2, 1318.2 kHz.

Fig. 19. Displacement components of the FE determined 3n dominant modes in anisotropic silicon (111): (a) 1277.3 kHz, Radial (i), tangential (ii) and vertical (iii). (b) 1283.5 kHz, Radial (i), tangential (ii) and vertical (iii). (c) The displacement components of the mode plotted along the radial line OQ.
component associated with the resonant motion provide a means of losing energy to the surrounding liquid. Zero out-of-plane displacement would be ideal, but it is unnecessary and unrealistic. If the energy partitioned into the out-of-plane motion is small enough compared to the energy partitioned into the total in-plane motion, then the energy lost to the liquid environment can be small enough such that the vibration persists with sufficiently high quality factor for mass detection. Here an assessment of the kinetic energy associated with the out-of-plane motion as a proportion of the total in-plane kinetic energy is made for the isotropic and anisotropic elastic cases. The 3D finite element modal analysis was used to extract the surface displacement components $t_4, t_3, t_2$.

The kinetic energy associated with the out-of-plane resonant motion at the surface with frequency $\omega$ is given by:

$$ KE_{\text{out}} = \alpha \sum_i r_i t_{z,i}^2 $$

where $r_i$ is the radial location of the point on the surface.

The kinetic energy associated with the in-plane resonant motion at the surface with frequency $\omega$ is given by:

$$ KE_{\text{in}} = \alpha \sum_i \left( u^2 + v^2 \right) $$

To quantify the contribution made by the out-of-plane motion define the ratio

$$ R(\text{elasticity \ mode order}) = \frac{KE_{\text{out}}}{KE_{\text{in}}} $$

The ratio $R$ was then calculated for the isotropic and anisotropic elastic cases. Table 4 summarises the results.

| $R$ | 0.0015 |
| $R(100)$ | 0.20 |
| $R(111)$ | 0.010 |
| $R(311)$ | 0.0050 |

Table 4: Assessment of the energy contribution made by the out-of-plane motion.

This does not adversely affect the partitioning of energy into the out-of-plane motion and that the mode with circumferential distribution 30 are the best candidate for use in mass sensing in this case.

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References

Biographies

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