## Thickness Shear Mode Quartz Oscillator

## Introduction

AT cut quartz crystals are widely employed in a range of applications, from oscillators to microbalances. One of the important properties of the AT cut is that the resonant frequency of the crystal is temperature independent to first order. This is desirable in both mass sensing and timing applications. AT cut crystals vibrate in the thickness shear mode-an applied voltage across the faces of the cut produces shear stresses inside the crystal. This example considers the vibration of an AT cut thickness shear oscillator, focusing on the mechanical response of the system in the frequency domain. The effect of a series capacitor on the mechanical resonance is also considered. Adding a series capacitance is a technique frequently employed to tune crystal oscillators.

## Model Definition

The model geometry is shown in Figure 1. The oscillator consists of a single quartz disc, supported so as not to impede the motion of the vibrational mode. There are two electrodes on the top and bottom surfaces of the geometry, one of which is grounded.


Figure 1: Model geometry.

In the first version of the model an AC voltage is applied to the top electrode. In the second version, the crystal is still driven by an AC voltage, but a capacitor is placed between the voltage source and the top electrode of the crystal.

## DOMAIN LEVEL EQUATIONS

Within a piezoelectric there is a coupling between the strain and the electric field, which is determined by the constitutive relation:

$$
\begin{align*}
& \mathbf{T}=c_{E} \mathbf{S}-e^{T} \mathbf{E}  \tag{1}\\
& \mathbf{D}=e \mathbf{S}+\varepsilon_{S} \mathbf{E}
\end{align*}
$$

Here, $\mathbf{S}$ is the strain, $\mathbf{T}$ is the stress, $\mathbf{E}$ is the electric field, and $\mathbf{D}$ is the electric displacement field. The material parameters $c_{E}, e$, and $\varepsilon_{S}$, correspond to the material stiffness, the coupling properties and the permittivity. These quantities are tensors of rank 4,3 , and 2 respectively, but, since the tensors are highly symmetric for physical reasons, they can be represented as matrices within an abbreviated subscript notation, which is usually more convenient. In the Piezoelectric Devices interface, the Voigt notation is used, which is standard in the literature for piezoelectricity but which differs from the defaults in the Solid Mechanics interface. In addition to Equation 1 the equations of solid mechanics and electrostatics must also be solved within the material.

## MATERIAL ORIENTATION

The orientation of a piezoelectric crystal cut is frequently defined by the system introduced by the I.R.E. standard of 1949 (Ref. 1). This standard has undergone a number of subsequent revisions, with the final revision being the IEEE standard of 1989 (Ref. 2). Unfortunately the more recent versions of the standard have not been universally adopted, and significant differences exist between the 1949 and the 1987 standards. The 1987 standard was ultimately withdrawn by the IEEE. COMSOL follows the conventions used in the book by Auld (Ref. 3) and defined by the 1987 standard. While these conventions are often used for many piezoelectric materials, unfortunately practitioners in the quartz industry frequently adhere to the older 1947 standard, which results in different definitions of crystal cuts and of material properties.

The crystal axes used to define material properties in COMSOL correspond to the 1987 IEEE standard. The stiffness, compliance, coupling, and dielectric material property matrices are defined with the crystal axes aligned with the local coordinate axes. In the absence of a user defined coordinate system, the local system corresponds to the global $X, Y$, and $Z$ coordinate axes. To define a particular crystal cut, a local set
of rotated coordinates must be defined; this local system then corresponds to the orientation of the crystal axes within the model. Note that the orientation of the local co-ordinate system should change both when the crystal cut is changed and if the plate changes orientation with respect to COMSOL's global co-ordinate system.

The crystal cuts are defined differently within the 1949 and 1987 standards. Both standards use a notation that defines the orientation of a virtual slice (the plate) through the crystal. The crystal axes are denoted $X, Y$, and $Z$ and the plate, which is usually rectangular, is defined as having sides $l, w$, and $t$ (length, width, and thickness). Initially the plate is aligned with respect to the crystal axes and then up to three rotations are defined, using a right-handed convention about axes embedded along the $l, w$, and $t$ sides of the plate. The 1987 standard defines the AT cut as: $(Y X l)-35.25^{\circ}$. The first two letters in the bracketed expression always refer to the initial orientation of the thickness and the length of the plate. Subsequent bracketed letters then define up to three rotational axes, which move with the plate as it is rotated. Angles of rotation about these axes are specified after the bracketed expression in the order of the letters, using a right-handed convention. For AT cut quartz only one rotation, about the $l$ axis, is required. This is illustrated in Figure 2.


Figure 2: Definition of the AT cut of quartz within the IEEE 1987 standard. The AT cut is defined as: $(Y X l)-35.25^{\circ}$. The first two bracketed letters specify the initial orientation of the plate, with the thickness direction, $t$, along the crystal $Y$ axis and the length direction, $l$, along the $X$ axis. Then up to three rotations about axes that move with the plate are specified by the corresponding bracketed letters and the subsequent angles. In this case only one rotation is required about the $l$ axis, of $-35.25^{\circ}$ (in a right-banded sense).

e)


$$
\int_{x}^{2} \rightarrow y
$$

Figure 3: Defining an AT cut crystal plate within COMSOL, with normal in the global $Z$-direction. Within the 1987 IEEE standard the AT cut is defined as $(Y X l)-35.25^{\circ}$. Begin with the plate normal in the $Z_{\text {cr }}$-direction, so the crystal and global systems are coincident. Rotate the plate so that its thickness points in the $Y_{\text {cr }}$-direction (the starting point for the IEEE definition), the global system rotates with the plate (b). Rotate the plate $-35.25^{\circ}$ about the l axis (d). Finally rotate the entire system so that the global coordinate system is orientated as it appears in COMSOL (d). The local coordinate system should be defined with the Euler angles (ZXZ: 0, $\left.-54.75^{\circ}, 0\right)$. (e) shows a coordinate system for this system in COMSOL.

Note that within the 1949 convention AT cut quartz is denoted as: $(Y X l)+35.25^{\circ}$, since the $X$-axis rotated by $180^{\circ}$ in this convention and positive angles therefore correspond to the opposite direction of rotation.

Figure 3 describes in detail how to define the AT cut in a quartz crystal, with the plate orientated with its normal pointing in the Z -axis of the global co-ordinate system. This is the orientation of the device in this model. In general for defining any crystal cut, care must be taken with defining the co-ordinate system and detailed diagrams, similar to those in Figure 3, should be drawn.

## ELECTRICAL CIRCUIT

In the first part of the model an AC voltage is applied directly to the top plate of the oscillator, which is grounded. In the second part of the model, a capacitor is added between the voltage source and the oscillator, as shown in Figure 4. In COMSOL the oscillator is coupled into the circuit using the External I Terminal feature. The terminal boundary condition within the model is set to Circuit and this feature then captures the charge generated by the circuit.


Figure 4: Top left: Electrical circuit for the first part of the model. Top right: Electrical circuit for the second part of the model. Bottom: Circuit for the second part of the model as implemented in COMSOL.

## Results and Discussion

Figure 5 shows the crystal displacement at its resonant frequency of 5.11 MHz . The form of the displacement shows clearly the shear nature of the resonance. The potential on cut slices through the plate is illustrated in Figure 6. The mechanical domain frequency response of the oscillator is shown in Figure 7. A clear anti-resonance is apparent, with a resonant frequency close to 5.11 MHz .

The addition of a series capacitance between the oscillator and the voltage source is expected to pull the resonant frequency to higher values. Figure 8 shows that this effect occurs as expected, with the resonant frequency increasing the most for smaller values of the series capacitance (in the limit of very large series capacitance the impedance of the series capacitor goes to zero and we obtain the result shown in Figure 7).


Figure 5: Displacement of the crystal at resonance.


Figure 6: Electric potential inside the crystal at resonance.


Figure 7: Mechanical response of the structure with no series capacitance.


Figure 8: Mechanical response of the structure with different series capacitances.

## References

1. Standards on Piezoelectric Crystals, 1949", Proceedings of the I. R. E.,vol. 37, no.12, pp. 1378-1395, 1949.
2. IEEE Standard on Piezoelectricity, ANSI/IEEE Standard 176-1987, 1987.
3. B. A. Auld, Acoustic Fields and Waves in Solids, Krieger Publishing Company, 1990.

Model Library path: MEMS_Module/Piezoelectric_Devices/
thickness_shear_quartz_oscillator

## Modeling Instructions

## MODEL WIZARD

I Go to the Model Wizard window.
2 Click Next.
3 In the Add physics tree, select Structural Mechanics>Piezoelectric Devices (pzd).
4 Click Add Selected.
5 Click Next.
6 Find the Studies subsection. In the tree, select Preset Studies>Frequency Domain.
7 Click Finish.

## GLOBAL DEFINITIONS

Add parameters for the model geometry and series capacitance.

## Parameters

I In the Model Builder window, right-click Global Definitions and choose Parameters.
2 In the Parameters settings window, locate the Parameters section.

3 In the table, enter the following settings:

| Name | Expression | Description |
| :--- | :--- | :--- |
| Cs | $1[\mathrm{pF}]$ | Series Capacitance |
| R0 | $0.835[\mathrm{~mm}]$ | Oscillator Radius |
| H0 | $334[\mathrm{um}]$ | Oscillator Thickness |

Create the geometry.

## GEOMETRY I

## Cylinder I

I In the Model Builder window, under Model I right-click Geometry I and choose Cylinder.

2 In the Cylinder settings window, locate the Size and Shape section.
3 In the Radius edit field, type RO.
4 In the Height edit field, type HO.

## Cylinder 2

I In the Model Builder window, right-click Geometry I and choose Cylinder.
2 In the Cylinder settings window, locate the Size and Shape section.
3 In the Radius edit field, type Ro.
4 In the Height edit field, type $\mathrm{HO} / 2$.
5 Click the Build All button.
Set up a rotated system appropriate for AT cut Quartz.

## DEFINITIONS

## Rotated System 2

I In the Model Builder window, under Model I right-click Definitions and choose Coordinate Systems>Rotated System.

2 In the Rotated System settings window, locate the Settings section.
3 Find the Euler angles (Z-X-Z) subsection. In the $\beta$ edit field, type -54.75 [deg].

## materials

## Material Browser

I In the Model Builder window, under Model I right-click Materials and choose Open Material Browser.

2 In the Material Browser settings window, In the tree, select Piezoelectric>Quartz.

## 3 Click Add Material to Model.

## Quartz

Use the rotated system to define the orientation of the crystal.

## PIEZOELECTRIC DEVICES

## Piezoelectric Material I

I In the Model Builder window, expand the Model I>Piezoelectric Devices node, then click Piezoelectric Material I.

2 In the Piezoelectric Material settings window, locate the Coordinate System Selection section.

3 From the Coordinate system list, choose Rotated System 2. Add damping to the model.

## Damping and Loss I

I Right-click Model I>Piezoelectric Devices>Piezoelectric Material I and choose Damping and Loss.

2 In the Damping and Loss settings window, locate the Damping Settings section.
3 From the Damping type list, choose Isotropic loss factor.
4 From the $\eta_{\mathrm{s}}$ list, choose User defined. In the associated edit field, type 1e-3.
Set up point constraints to prevent rotational and translational modes.

## Fixed Constraint I

I In the Model Builder window, right-click Piezoelectric Devices and choose Points>Fixed Constraint.

2 Select Point 5 only.

## Prescribed Displacement I

I Right-click Piezoelectric Devices and choose Points>Prescribed Displacement.
2 Select Point 8 only.
3 In the Prescribed Displacement settings window, locate the Prescribed Displacement section.

4 Select the Prescribed in $\mathbf{x}$ direction check box.
5 Select the Prescribed in z direction check box.

## Prescribed Displacement 2

I Right-click Piezoelectric Devices and choose Points>Prescribed Displacement.
2 Select Point 2 only.
3 In the Prescribed Displacement settings window, locate the Prescribed Displacement section.

4 Select the Prescribed in z direction check box.
Add electrical boundary conditions to the model.

## Terminal I

I Right-click Piezoelectric Devices and choose the boundary condition Electrical>Terminal.

2 Select Boundary 7 only.
3 In the Terminal settings window, locate the Terminal section.
4 From the Terminal type list, choose Voltage.
5 In the $V_{0}$ edit field, type 10.

## Ground I

I Right-click Piezoelectric Devices and choose the boundary condition Electrical>Ground.

2 Select Boundary 3 only.
Create a swept triangular mesh.

## MESH I

## Free Triangular I

I In the Model Builder window, under Model I right-click Mesh I and choose More Operations>Free Triangular.

2 Select Boundary 7 only.

## Swept I

In the Model Builder window, right-click Mesh I and choose Swept.

## Distribution I

I In the Model Builder window, under Model I>Mesh I right-click Swept I and choose Distribution.

2 In the Distribution settings window, locate the Distribution section.
3 In the Number of elements edit field, type 2.

## 4 Click the Build All button.

Set up and solve a frequency dependent study.

## STUDY I

Step I: Frequency Domain
I In the Model Builder window, expand the Study I node, then click Step I: Frequency Domain.

2 In the Frequency Domain settings window, locate the Study Settings section.
3 Click the Range button.
4 Go to the Range dialog box.
5 In the Start edit field, type 5.09e6.
6 In the Step edit field, type 1 e 3.
7 In the Stop edit field, type 5.125e6.
8 Click the Replace button.
9 In the Model Builder window, right-click Study I and choose Compute.
Visualize the mode shape of the device at resonance.

## RESULTS

Displacement (pzd)
I In the 3D Plot Group settings window, locate the Data section.
2 From the Parameter value (freq) list, choose 5.I le6.
3 Click the Plot button.
The second default plot shows the electric potential within the device.

## Potential (pzd)

I In the Model Builder window, under Results click Potential (pzd).
2 In the 3D Plot Group settings window, locate the Data section.
3 From the Parameter value (freq) list, choose 5.1 le6.
4 Click the Plot button.
Add a plot to show the mechanical response of the device.

## ID Plot Group 3

I In the Model Builder window, right-click Results and choose ID Plot Group.
2 Right-click ID Plot Group 3 and choose Point Graph.

3 Select Point 12 only.
4 In the Point Graph settings window, click Replace Expression in the upper-right corner of the $\boldsymbol{y}$-Axis Data section. From the menu, choose Piezoelectric Devices $>$ Displacement field (Material) $>$ Displacement field, $X$ component (u).
5 In the Model Builder window, right-click ID Plot Group 3 and choose Rename.
6 Go to the Rename ID Plot Group dialog box and type Mechanical Response in the New name edit field.

## 7 Click OK.

8 Right-click ID Plot Group 3 and choose Plot.
Now add a capacitor in series with the device.

## MODEL I

In the Model Builder window, right-click Model I and choose Add Physics.

## MODEL WIZARD

I Go to the Model Wizard window.
2 In the Add physics tree, select AC/DC>Electrical Circuit (cir).
3 Click Add Selected.
4 Click Next.
5 Find the Studies subsection. In the tree, select Preset Studies for Selected Physics>Frequency Domain.

6 Click Finish.

## ELECTRICAL CIRCUIT

Features in the electric circuits interface are connected by specifying connecting node numbers for each port of the device.

## Ground Node I

A ground node is automatically added to the circuit, with the default node number of 0.

Next add a voltage source between the ground node and a (newly created) node with number 2 .

## Voltage Source I

I In the Model Builder window, right-click Electrical Circuit and choose Voltage Source.
2 In the Voltage Source settings window, locate the Node Connections section.

3 In the table, enter the following settings:

| Label | Node names |
| :--- | :--- |
| P | 2 |

4 Locate the Device Parameters section. From the Source type list, choose AC-source.
5 In the $V_{\text {src }}$ edit field, type 10.
Add a capacitor between the voltage source output (node 2 ) and a new node, 1 .

## Capacitor I

I Right-click Electrical Circuit and choose Capacitor.
2 In the Capacitor settings window, locate the Node Connections section.
3 In the table, enter the following settings:

| Label | Node names |
| :--- | :--- |
| P | 2 |
| n | 1 |

4 Locate the Device Parameters section. In the $C$ edit field, type Cs.
Connect node 1 to the terminal feature in the model using the external I-terminal feature.

## External I-Terminal I

I Right-click Electrical Circuit and choose External I-Terminal.
The terminal node in the piezoelectric devices interface needs to be changed to a circuit type terminal.

## PIEZOELECTRIC DEVICES

## Terminal I

I In the Model Builder window, under Model I>Piezoelectric Devices click Terminal I.
2 In the Terminal settings window, locate the Terminal section.
3 From the Terminal type list, choose Circuit.
Next, couple the electric potential from the terminal node back into the model.

## ELECTRICAL CIRCUIT

## External I-Terminal I

I In the Model Builder window, under Model I>Electrical Circuit click External I-Terminal I.

2 In the External I-Terminal settings window, locate the External Terminal section.
3 From the $V$ list, choose Terminal voltage (pzd/termI).
Finally set up a study to compute the frequency response of the device with different capacitors added in series.

## STUDY 2

## Step I: Frequency Domain

I In the Model Builder window, under Study 2 click Step I: Frequency Domain.
2 In the Frequency Domain settings window, locate the Study Settings section.
3 Click the Range button.
4 Go to the Range dialog box.
5 In the Start edit field, type 5.09e6.
6 In the Step edit field, type 1 e 3.
7 In the Stop edit field, type 5.125e6.
8 Click the Replace button.

## Parametric Sweep

I In the Model Builder window, right-click Study 2 and choose Parametric Sweep.
2 In the Parametric Sweep settings window, locate the Study Settings section.
3 Click Add.
4 In the table, enter the following settings:

## Parameter value list

$0.1 \mathrm{e}-12 \quad 0.4 \mathrm{e}-12 \quad 1 \mathrm{e}-12$
5 In the Model Builder window, click Study 2.
6 In the Study settings window, locate the Study Settings section.
7 Clear the Generate default plots check box.
8 Click the Compute button.

## RESULTS

Re-plot the mechanical response with the additional series capacitance.

## Mechanical Response I

I In the Model Builder window, under Results right-click Mechanical Response and choose Duplicate.
2 In the ID Plot Group settings window, locate the Data section.
3 From the Data set list, choose Solution 3.
4 Click to expand the Legend section. From the Position list, choose Upper left.
5 In the Model Builder window, expand the Mechanical Response I node, then click Point Graph 1 .
6 In the Point Graph settings window, click to expand the Legends section.
7 Select the Show legends check box.
8 Click the Plot button.
Note how the mechanical resonant frequency is 'pulled' by the series capacitance.

