Orientation of Piezoelectric Crystals and Acoustic Wave Propagation

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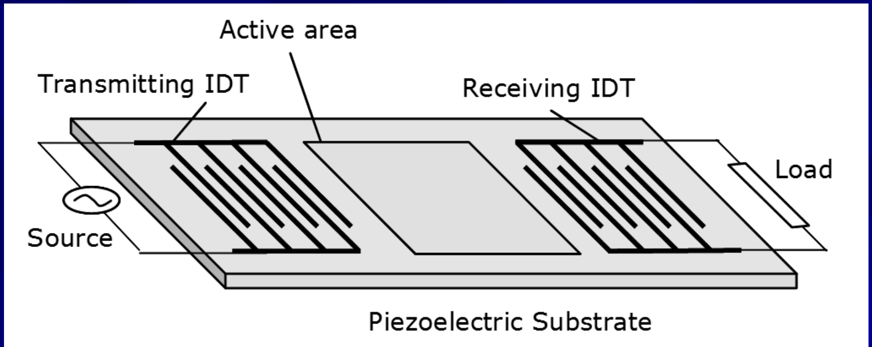
COMSOL CONFERENCE BOSTON 2012

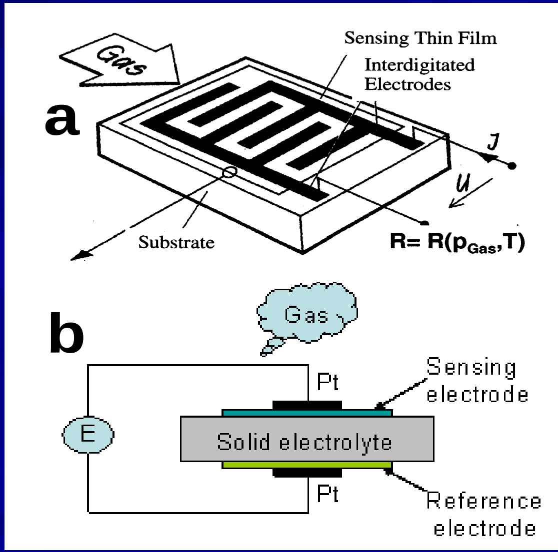
Overview

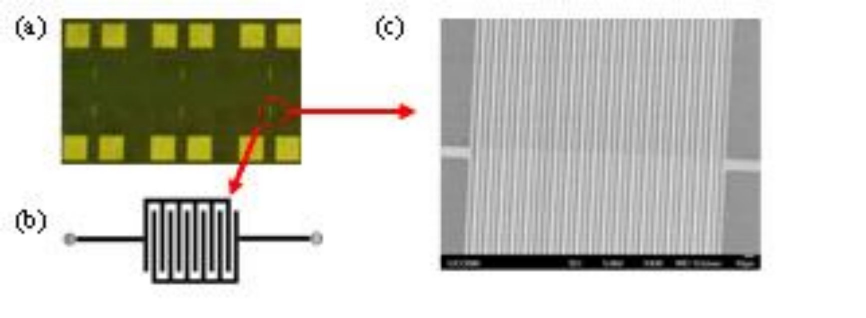
- Surface Acoustic Wave (SAW) devices
  - Wireless filters, resonators, sensors, etc.
- Confinement of acoustic energy near the surface of a piezoelectric substrate
- SAW sensors
  - Wireless remote operations
  - High temperature operations
  - Hazardous environment operations
  - High frequency, high precision and sensitivity

Overview

- SAW generation and signal measurement
  - One-port or two-port SAW devices
  - Interdigitated transducer (IDT): transmitting IDT and receiving IDT







Constitutive and Wave Equations

$$T = c \cdot S - e \cdot E \qquad D = e \cdot S + \varepsilon \cdot E$$

T , *S, E* and *D* are vectors of stress, strain, electric field and displacement;

c, *e* and *ε* are matrices of the elastic modulus (stiffness), piezoelectric stress constant and dielectric permittivity of the substrate material.

$$\nabla \cdot [e \nabla \Phi] + \nabla \cdot [c \nabla_s u] - \rho \ddot{u} = 0$$

$$\nabla \cdot [e \nabla_s u] = \nabla \cdot [\varepsilon \left(\nabla \Phi \right)]$$

ρ is density, u and ü are particle displacement and acceleration, and Φ is electric potential.

Wave field near the surface: $u = \beta \exp(-\alpha \omega z / V_s) \exp[i\omega(t - x / V_s)]$

Surface stresses: $T = c \cdot S - e \cdot E = c \cdot \nabla_s u + e \cdot \nabla \Phi$

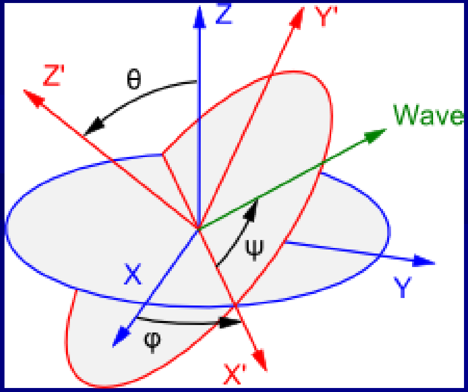
Surface electric displacements: $D = e \cdot \nabla_s u - \varepsilon \cdot \nabla \Phi$

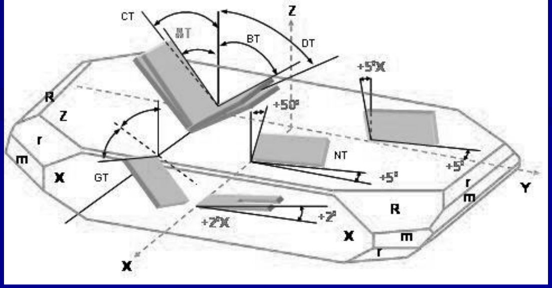
Anisotropy and Crystal Rotation

- Piezoelectric materials are anisotropic
  - Different orientation (or cut) of a piezoelectric substrate leads to different material properties, hence different wave characteristics

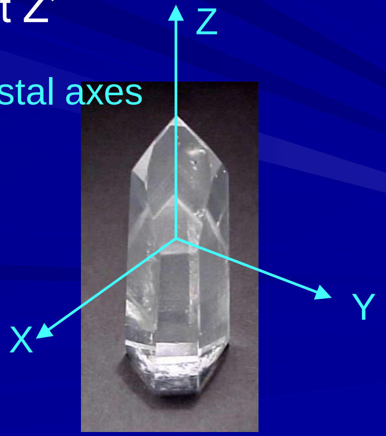
$$[c]=\begin{bmatrix} c_{11} & c_{12} & c_{13} & c_{14} & c_{15} & c_{16} \\ - & c_{22} & c_{23} & c_{24} & c_{25} & c_{26} \\ - & - & c_{33} & c_{34} & c_{35} & c_{36} \\ - & - & - & c_{44} & c_{45} & c_{46} \\ - & - & - & - & c_{55} & c_{56} \\ symm & - & - & - & - & c_{66} \end{bmatrix} \quad [e]=\begin{bmatrix} e_{11} & e_{12} & e_{13} & e_{14} & e_{15} & e_{16} \\ e_{21} & e_{22} & e_{23} & e_{24} & e_{25} & e_{26} \\ e_{31} & e_{32} & e_{33} & e_{34} & e_{35} & e_{36} \end{bmatrix} \quad [\varepsilon]=\begin{bmatrix} \varepsilon_{11} & \varepsilon_{12} & \varepsilon_{13} \\ - & \varepsilon_{22} & \varepsilon_{23} \\ symm & - & \varepsilon_{33} \end{bmatrix}$$

- Euler angles
  - A crystal cut is defined by a set of Euler angles (φ,θ,ψ)
    - φ defines the rotation about Z, θ about X' and ψ about Z'



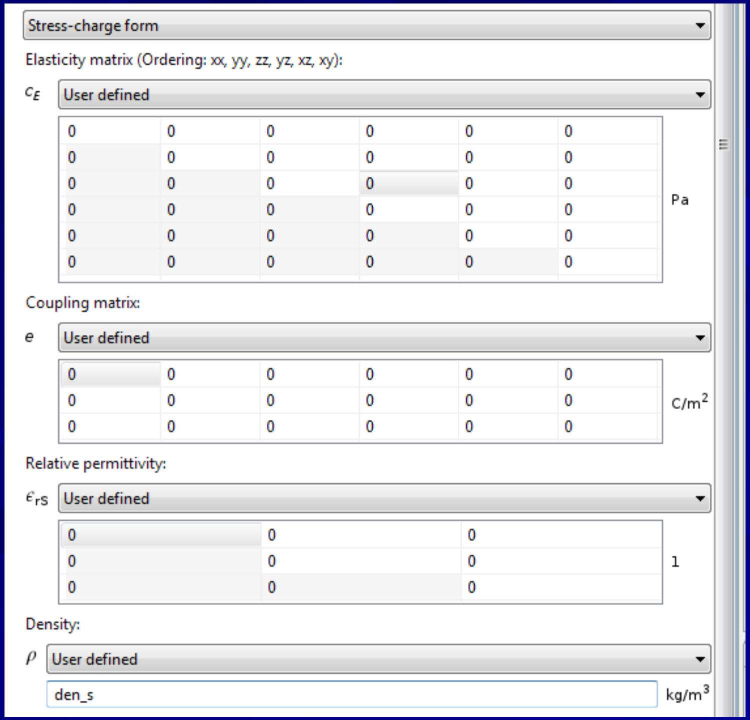


XYZ – crystal axes



Rotation and Transformation

- Transformation of material property matrices
  - The material matrices: [c] is 6×6, [e] is 3×6 and [ε] is 3×3
  - How to perform matrix transformation for 6×6, 3×6 and 3×3 matrices with only a 3×3 rotation matrix?



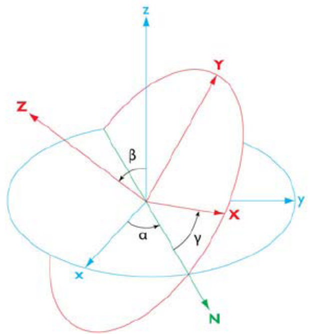
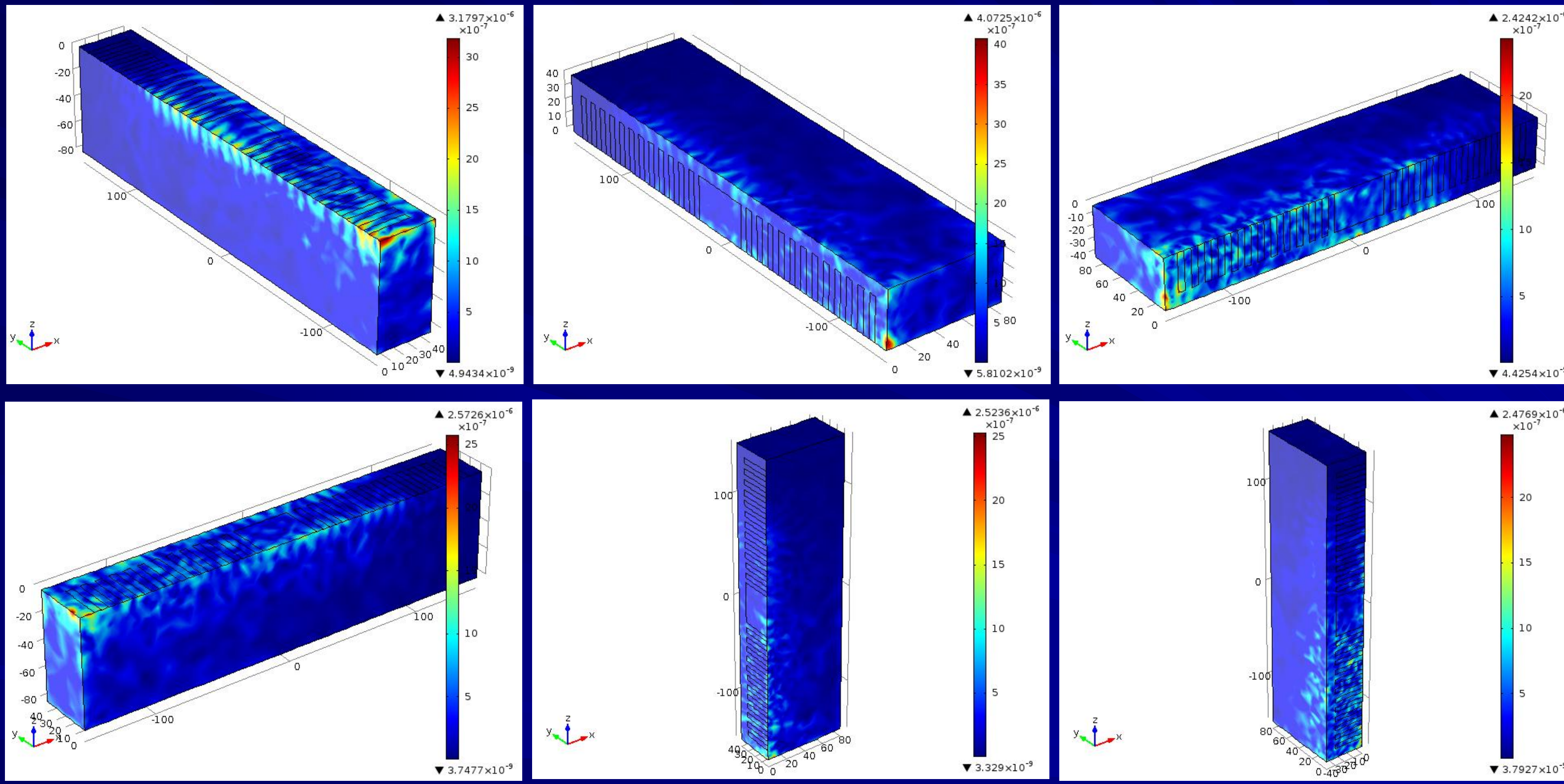


Figure 3-8: 3D Euler angles in a rotated coordinate system.

The transformation matrix for the 3D case is then

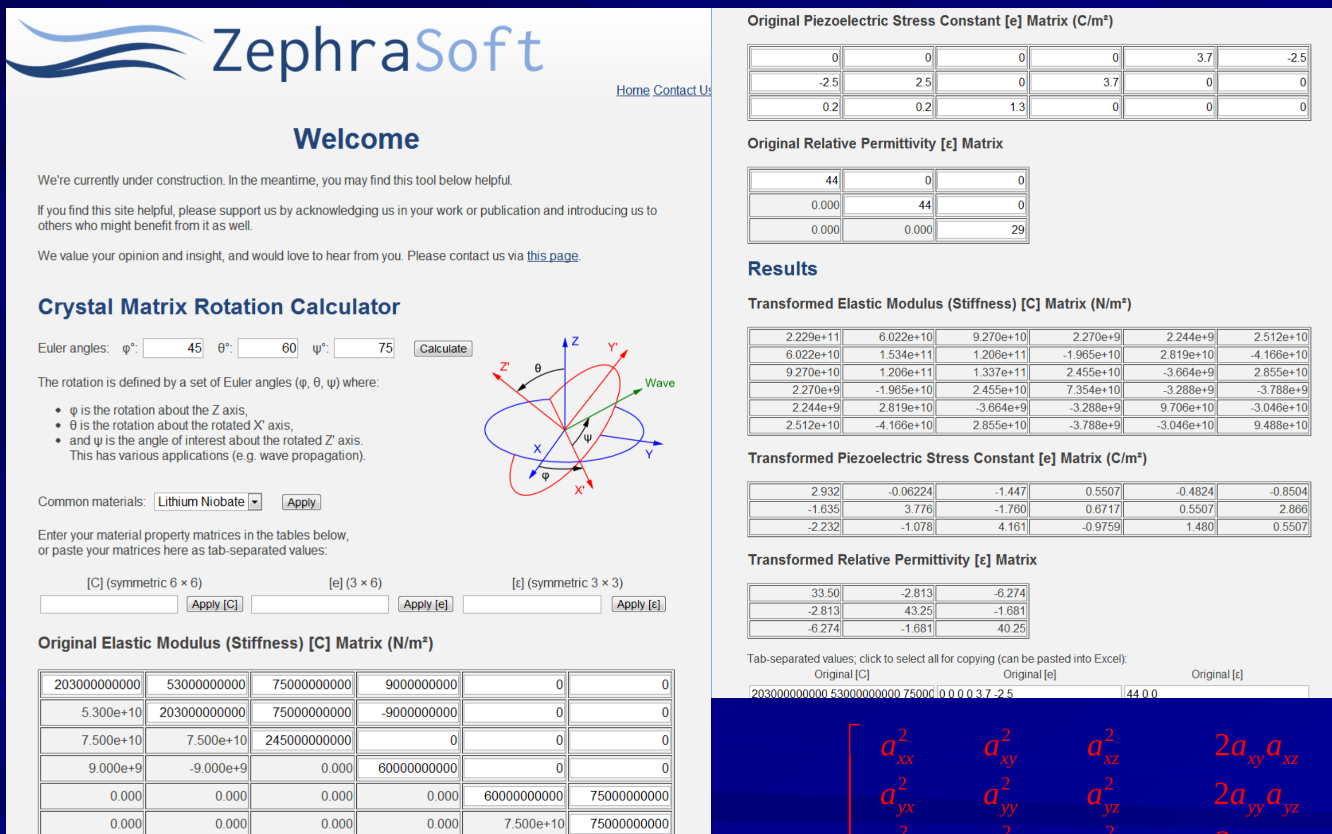
$$\begin{bmatrix} x_1 \\ y_1 \\ z_1 \end{bmatrix} = \begin{bmatrix} \cos\alpha\cos\gamma - \sin\alpha\cos\beta\sin\gamma & -\cos\alpha\sin\gamma - \sin\alpha\cos\beta\cos\gamma & \sin\beta\sin\alpha \\ \sin\alpha\cos\gamma + \cos\alpha\cos\beta\sin\gamma & -\sin\alpha\sin\gamma + \cos\alpha\cos\beta\cos\gamma & -\sin\beta\cos\alpha \\ \sin\beta\sin\gamma & \sin\beta\cos\gamma & \cos\beta \end{bmatrix}^T \cdot \begin{bmatrix} x \\ y \\ z \end{bmatrix}$$

Crystal Rotation: The Hard Way



Crystal Matrix Rotation Calculator

- Available at: zephrasoft.com



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Crystal Matrix Rotation Calculator

Euler angles: φ°: 45 θ°: 60 ψ°: 75 Calculate

The rotation is defined by a set of Euler angles (φ, θ, ψ) where:

- φ is the rotation about the Z axis,
- θ is the rotation about the rotated X' axis,
- and ψ is the angle of interest about the rotated Z' axis. This has various applications (e.g. wave propagation).

Common materials: Lithium Niobate Apply

Enter your material property matrices in the tables below, or paste your matrices here as tab-separated values:

[C] (symmetric 6 × 6) Apply [C] [e] (3 × 6) Apply [e] [ε] (symmetric 3 × 3) Apply [ε]

Original Elastic Modulus (Stiffness) [C] Matrix (N/m²)

203000000000	53000000000	75000000000	9000000000	0	0
5.300e+10	203000000000	75000000000	-9000000000	0	0
7.500e+10	7.500e+10	245000000000	0	0	0
9.000e+9	-9.000e+9	0.000	60000000000	0	0
0.000	0.000	0.000	0.000	60000000000	75000000000
0.000	0.000	0.000	0.000	7.500e+10	75000000000

Original Piezoelectric Stress Constant [e] Matrix (C/m²)

0	0	0	0	3.7	-2.5
-2.5	2.5	0	3.7	0	0
0.2	0.2	1.3	0	0	0

Original Relative Permittivity [ε] Matrix

44	0	0
0.000	44	0
0.000	0.000	29

Results

Transformed Elastic Modulus (Stiffness) [C] Matrix (N/m²)

2.229e+11	6.022e+10	9.270e+10	2.270e+9	2.244e+9	2.512e+10
6.022e+10	1.534e+11	1.206e+11	-1.965e+10	2.819e+10	-4.166e+10
9.270e+10	1.206e+11	1.337e+11	2.455e+10	-3.664e+9	2.855e+10
2.270e+9	-1.965e+10	2.455e+10	7.354e+10	-3.288e+9	-3.788e+9
2.244e+9	2.819e+10	-3.664e+9	-3.288e+9	9.706e+10	-3.046e+10
2.512e+10	-4.166e+10	2.855e+10	-3.788e+9	-3.046e+10	9.488e+10

Transformed Piezoelectric Stress Constant [e] Matrix (C/m²)

2.932	-0.06224	-1.447	0.5507	-0.4824	-0.8504
-1.635	3.776	-1.760	0.6717	0.5507	2.866
-2.232	-1.078	4.161	-0.9759	1.480	0.5507

Transformed Relative Permittivity [ε] Matrix

33.50	-2.813	-6.274
-2.813	43.25	-1.681
-6.274	-1.681	40.25

Tab-separated values; click to select all for copying (can be pasted into Excel):

Original [C] Original [e] Original [ε]

203000000000 53000000000 75000 0 0 0 0 3.7 -2.5 44 0 0

$$[c'] = [M][C][M]^T$$

$$[e'] = [a][e][M]^T$$

$$[\varepsilon'] = [a][\varepsilon][a]^T$$

$$[a] = \begin{bmatrix} a_{xx} & a_{xy} & a_{xz} \\ a_{yx} & a_{yy} & a_{yz} \\ a_{zx} & a_{zy} & a_{zz} \end{bmatrix}$$

$$[M] = \begin{bmatrix} a_{xx}^2 & a_{xy}^2 & a_{xz}^2 & 2a_{xy}a_{xz} & 2a_{xz}a_{xx} & 2a_{xx}a_{xy} \\ a_{yx}^2 & a_{yy}^2 & a_{yz}^2 & 2a_{yy}a_{yz} & 2a_{yz}a_{yx} & 2a_{yx}a_{yy} \\ a_{zx}^2 & a_{zy}^2 & a_{zz}^2 & 2a_{zy}a_{zz} & 2a_{zz}a_{zx} & 2a_{zx}a_{zy} \\ a_{yx}a_{zx} & a_{yy}a_{zy} & a_{yz}a_{zz} & a_{yy}a_{zz}+a_{yz}a_{zy} & a_{yx}a_{zz}+a_{yz}a_{zx} & a_{yy}a_{zx}+a_{yx}a_{zy} \\ a_{zx}a_{xx} & a_{zy}a_{xy} & a_{zz}a_{xz} & a_{xy}a_{zz}+a_{xz}a_{zy} & a_{xz}a_{zx}+a_{xx}a_{zz} & a_{xx}a_{zy}+a_{xy}a_{zx} \\ a_{xx}a_{yx} & a_{xy}a_{yy} & a_{xz}a_{yz} & a_{xy}a_{yz}+a_{xz}a_{yy} & a_{xz}a_{yx}+a_{xx}a_{yz} & a_{xx}a_{yy}+a_{xy}a_{yx} \end{bmatrix}$$

Material Properties in Crystal Axes

- Trigonal 32 and 3m crystals
  - 32 crystal: Langasite ($La_3Ga_3SiO_{14}$)

$$[c]=\begin{bmatrix} c_{11} & c_{12} & c_{13} & c_{14} & 0 & 0 \\ - & c_{22} & c_{23} & -c_{14} & 0 & 0 \\ - & - & c_{33} & 0 & 0 & 0 \\ - & - & - & c_{44} & 0 & 0 \\ - & - & - & - & c_{44} & c_{14} \\ - & - & - & - & - & (c_{11}-c_{12})/2 \end{bmatrix}$$

$$[e]=\begin{bmatrix} e_{11} & -e_{11} & 0 & e_{14} & 0 & 0 \\ 0 & 0 & 0 & 0 & -e_{14} & -e_{11} \\ 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

$$\varepsilon = \begin{pmatrix} \varepsilon_{11} & 0 & 0 \\ 0 & \varepsilon_{11} & 0 \\ 0 & 0 & \varepsilon_{33} \end{pmatrix}$$

Langasite: $(\phi,\theta,\psi) = (0°, 0°, 0°)$	
C_{11}	18.89×10^{10} Nm^{-2}
C_{12}	10.42×10^{10} Nm^{-2}
C_{13}	10.15×10^{10} Nm^{-2}
C_{14}	1.44×10^{10} Nm^{-2}
C_{33}	26.83×10^{10} Nm^{-2}
C_{44}	5.33×10^{10} Nm^{-2}
e_{11}	-0.437 Cm^{-2}
e_{14}	0.104 Cm^{-2}
e_{31}	0.2 Cm^{-2}
ε_{11}	19.05
ε_{33}	51.81
ρ	5739 Kg m^{-3}

  - 3m crystal: Lithium Niobate ($LiNbO_3$)

$$[c]=\begin{bmatrix} c_{11} & c_{12} & c_{13} & c_{14} & 0 & 0 \\ - & c_{22} & c_{23} & -c_{14} & 0 & 0 \\ - & - & c_{33} & 0 & 0 & 0 \\ - & - & - & c_{44} & 0 & 0 \\ - & - & - & - & c_{44} & c_{14} \\ - & - & - & - & - & (c_{11}-c_{12})/2 \end{bmatrix}$$

$$[e]=\begin{bmatrix} 0 & 0 & 0 & 0 & e_{15} & -e_{22} \\ -e_{22} & e_{22} & 0 & e_{15} & 0 & 0 \\ e_{31} & e_{31} & e_{33} & 0 & 0 & 0 \end{bmatrix}$$

$$\varepsilon = \begin{pmatrix} \varepsilon_{11} & 0 & 0 \\ 0 & \varepsilon_{11} & 0 \\ 0 & 0 & \varepsilon_{33} \end{pmatrix}$$

Lithium Niobate: $(\phi,\theta,\psi) = (0°, 0°, 0°)$	
C_{11}	20.3×10^{10} Nm^{-2}
C_{12}	5.3×10^{10} Nm^{-2}
C_{13}	7.5×10^{10} Nm^{-2}
C_{14}	0.9×10^{10} Nm^{-2}
C_{33}	24.5×10^{10} Nm^{-2}
C_{44}	6.0×10^{10} Nm^{-2}
e_{15}	3.7 Cm^{-2}
e_{22}	2.5 Cm^{-2}
e_{31}	0.2 Cm^{-2}
e_{33}	1.3 Cm^{-2}
ε_{11}	44
ε_{33}	29
ρ	4600 Kg m^{-3}

$IL = 20\times\log_{10}|V_{output}/V_{input}|$

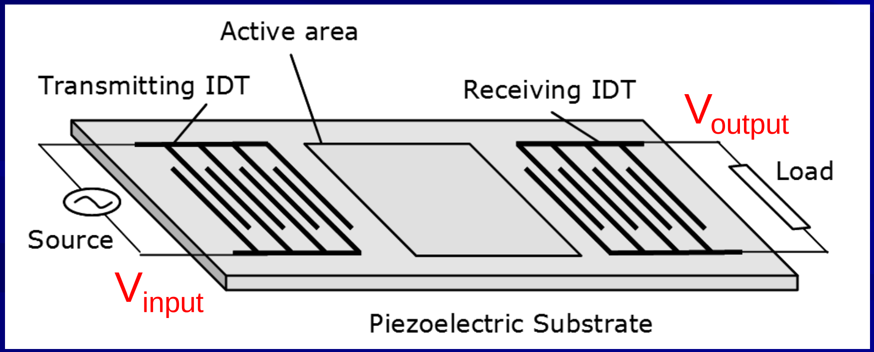
Modeling Consideration

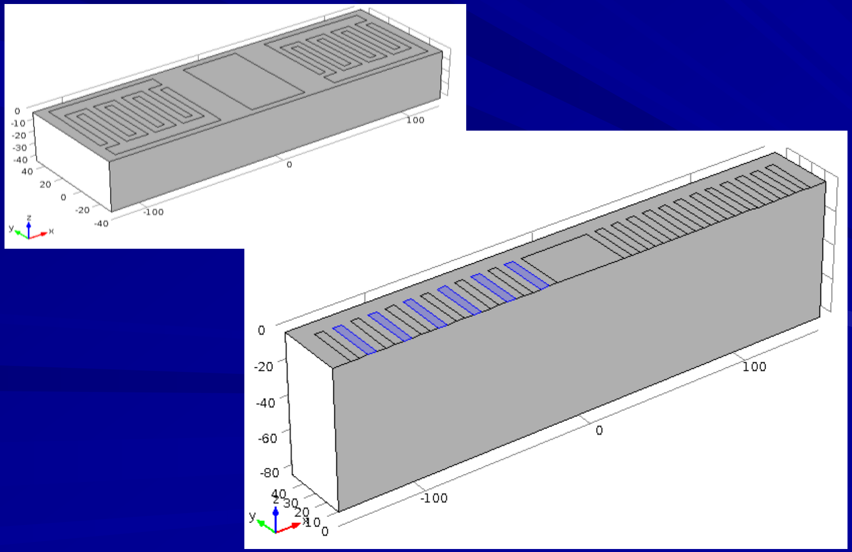
- Two-port delay-line SAW sensor
  - Reciprocal and symmetric design:
    - S11=S22, S12=S21
  - Insertion loss (IL): 20log|S12|
  - SAW travel velocity $V_s = \lambda f_0$, λ is wavelength (λ=20 μm) *and* f_0 is resonant frequency

$$IL = 20\times\log_{10}\left|\frac{\mathrm{F}\{V_{output}\}}{\mathrm{F}\{V_{input}\}}\right|$$

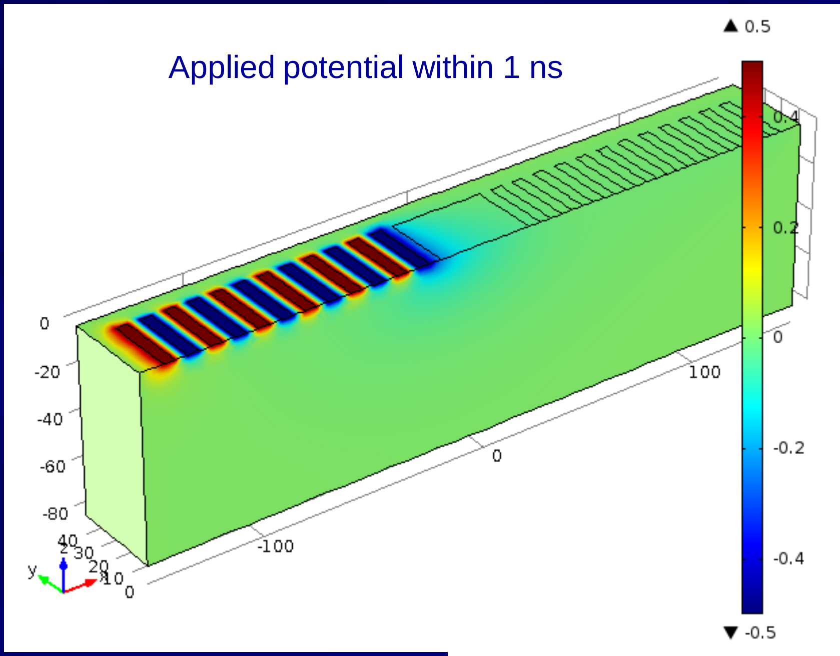
$\mathrm{F} - \mathit{FourierTransform}$

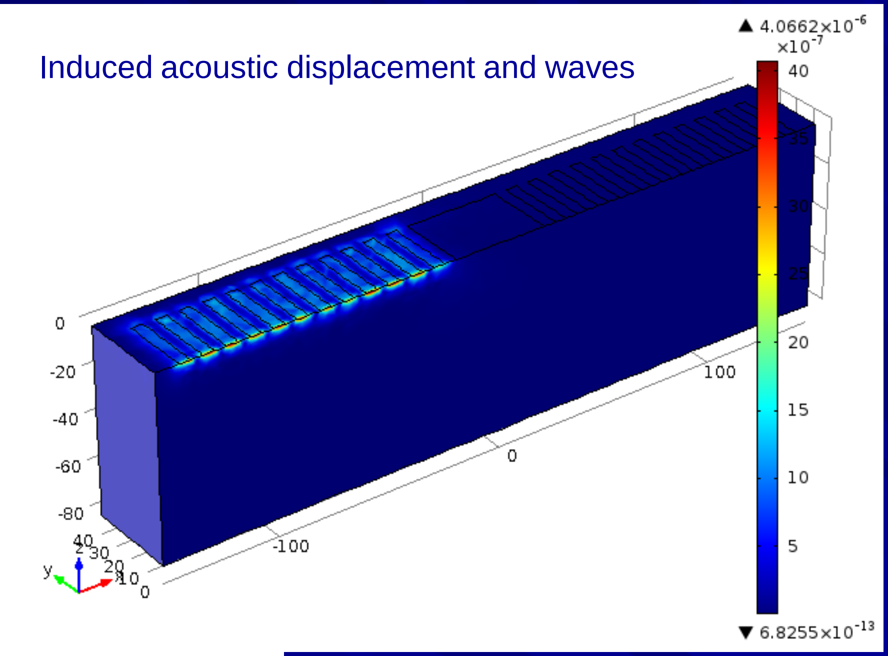
$$V_S = \lambda f_0$$

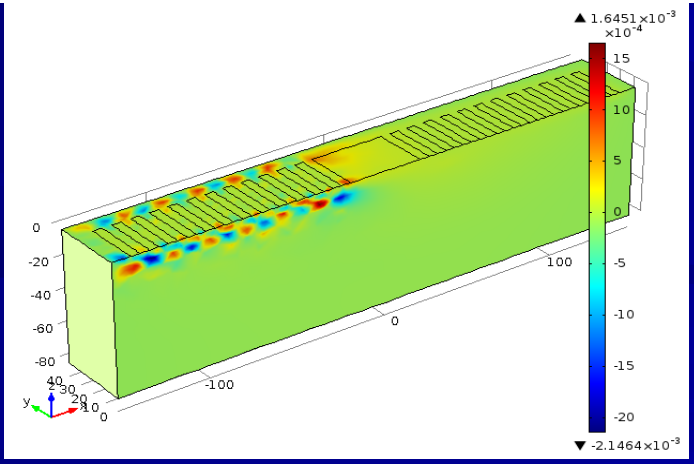




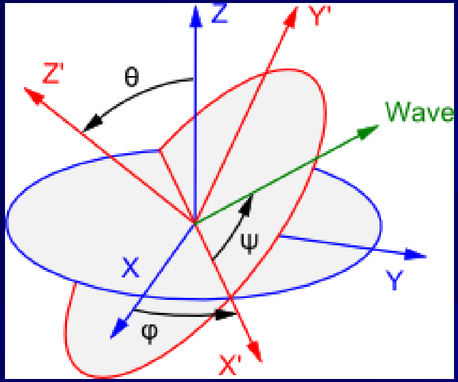
Electric-Excited Acoustic Waves

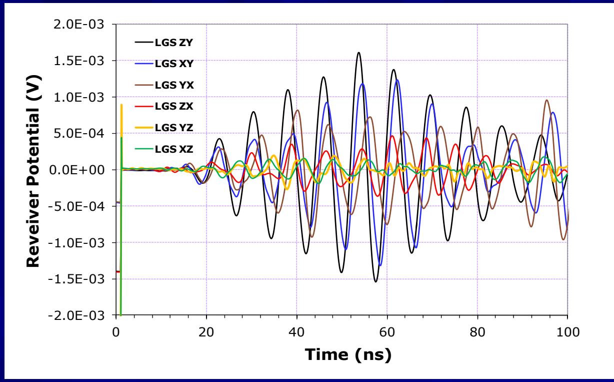


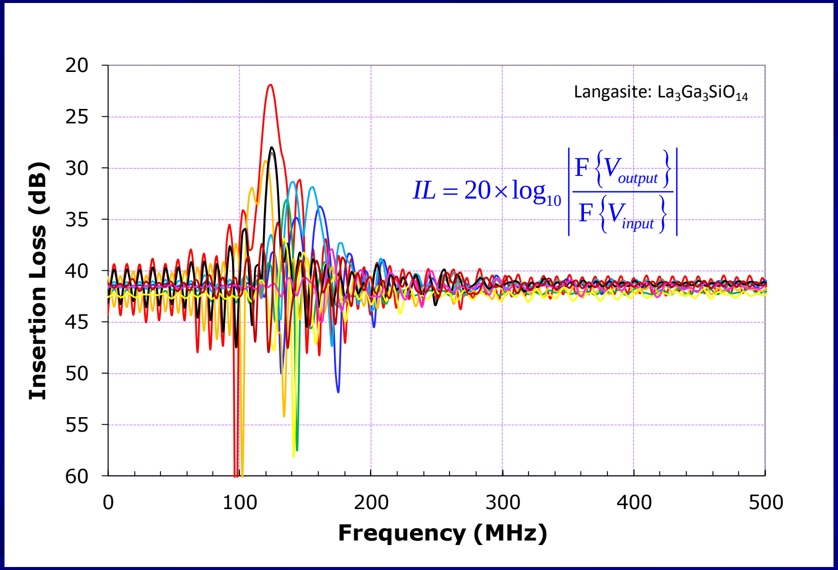


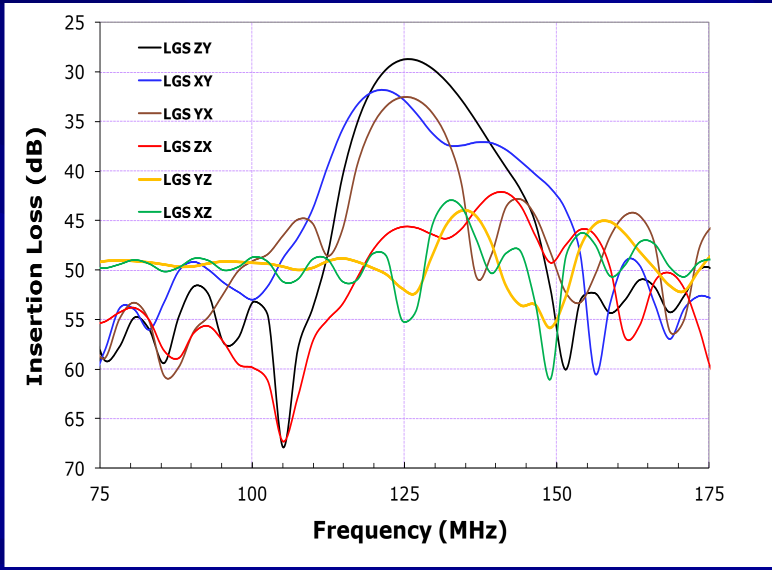


SAW Signal and Insertion Loss



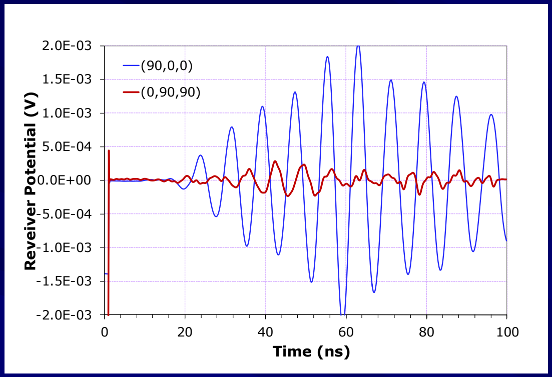


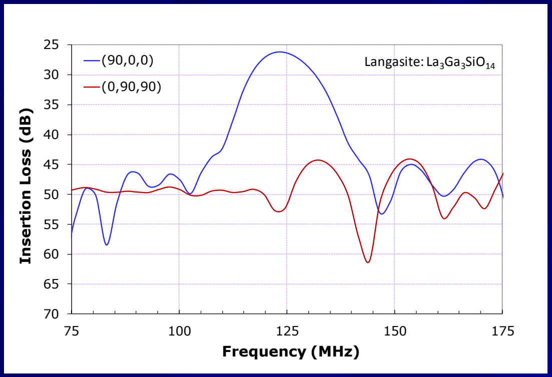


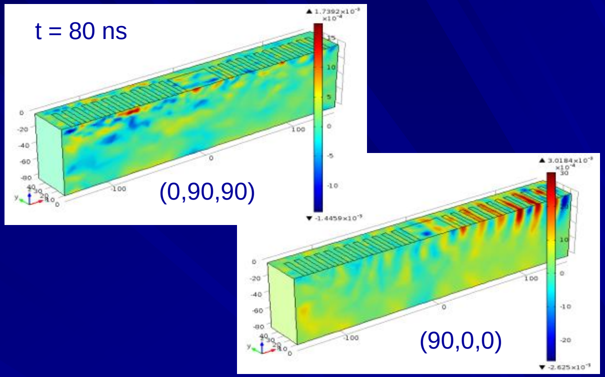


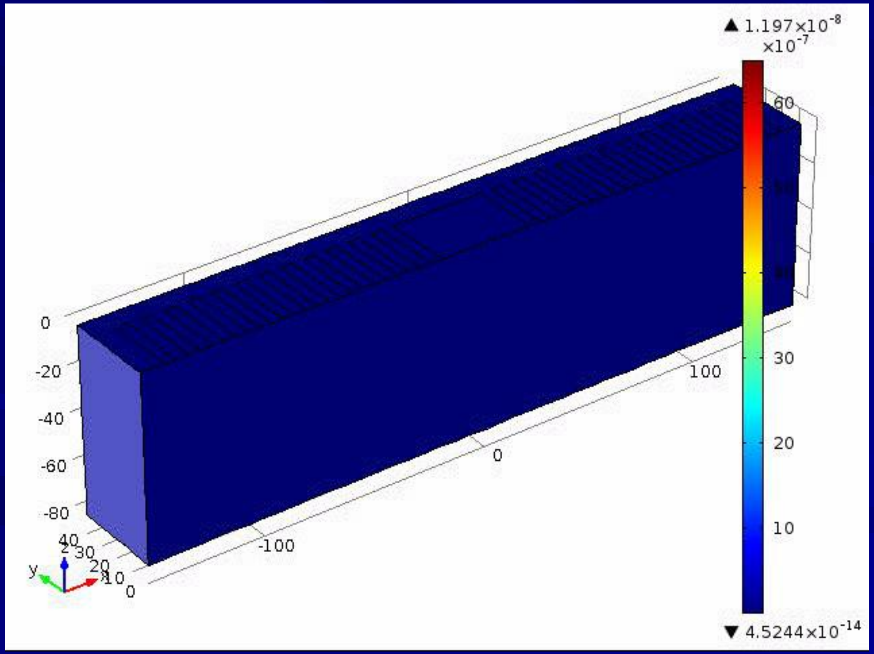
$$V_S = \lambda f_0 = 20(\mu m) \times [120 - 125](MHz) = 2400 - 2500(m/s)$$

Good and Bad Crystal Cuts

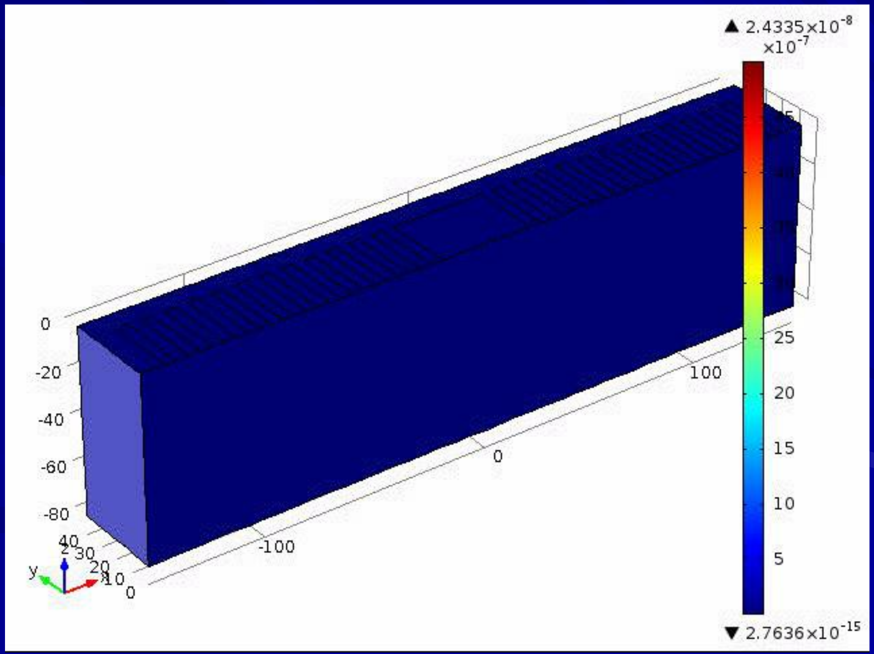








(90,0,0)



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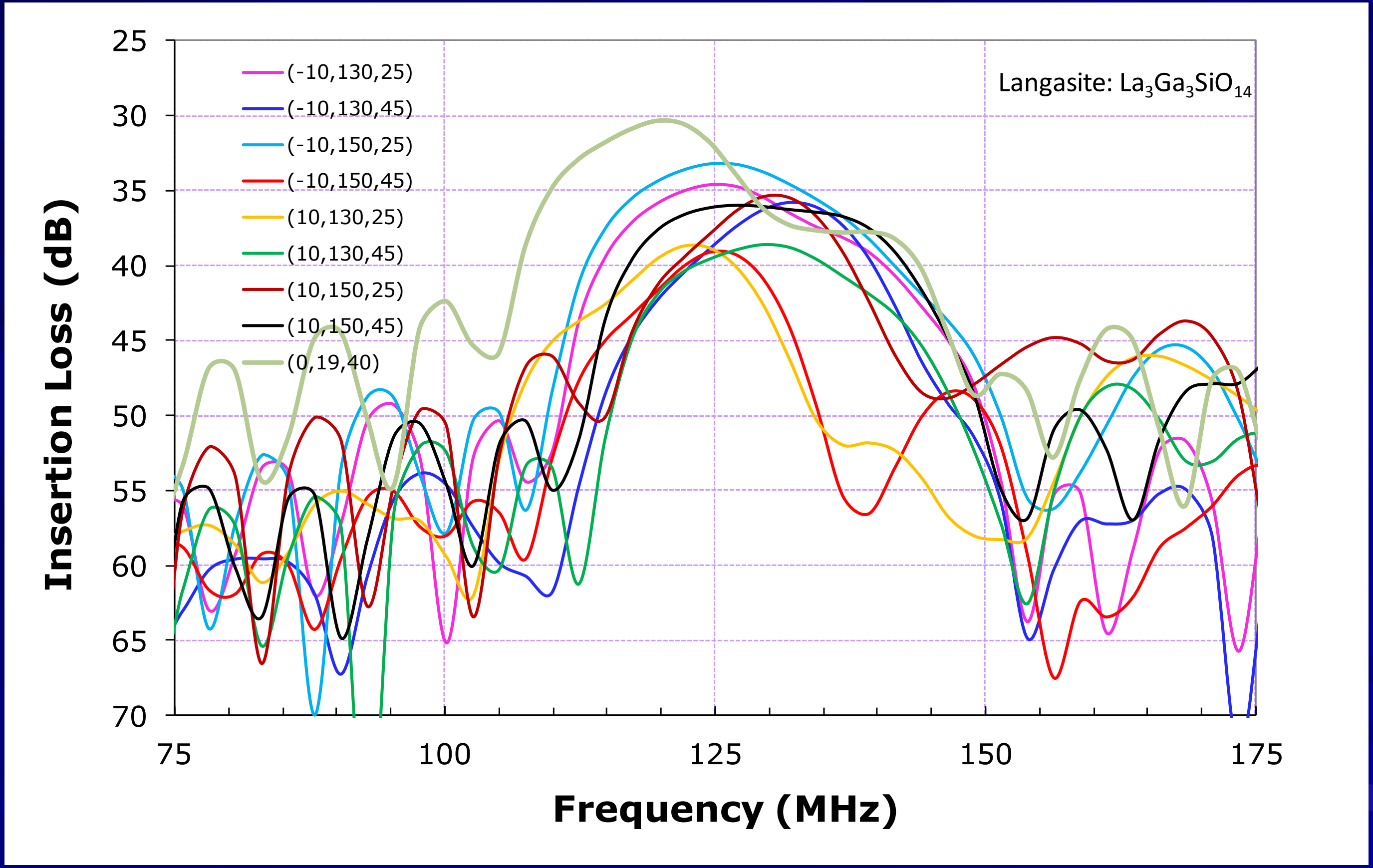
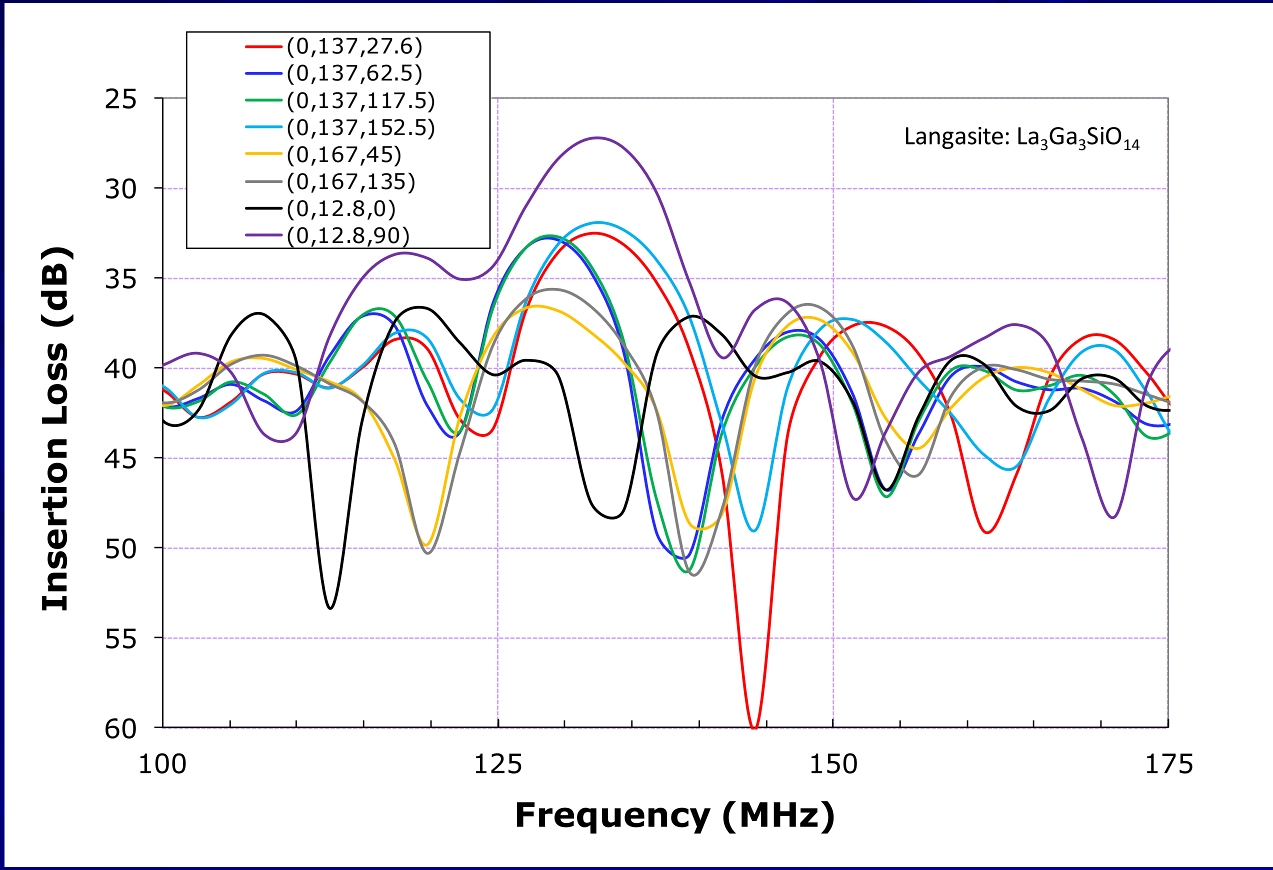
Crystal Cuts and SAW Behavior



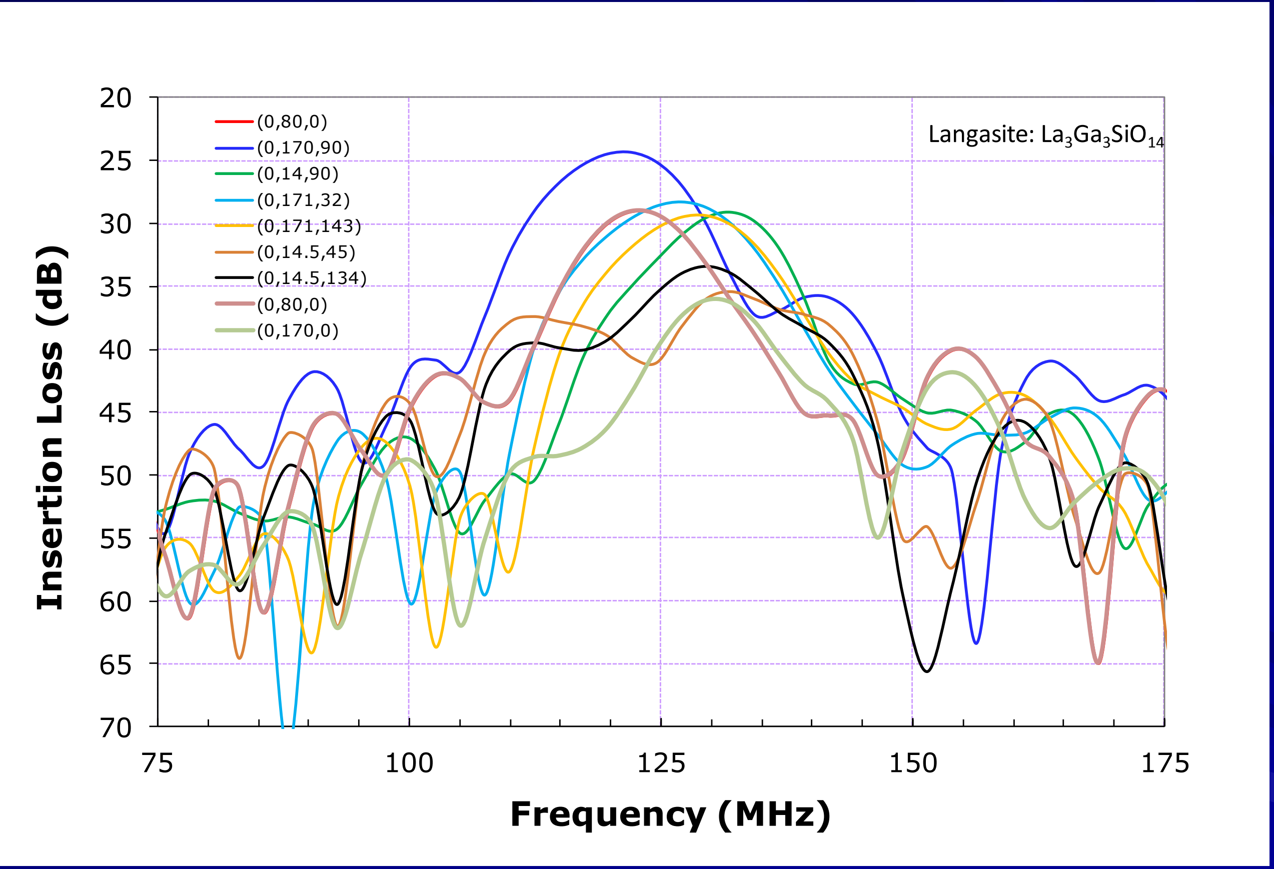
$$V_S = \lambda f_0 = 20(\mu m) \times [120 - 125](MHz) = 2400 - 2500(m/s)$$

Crystal Cuts and SAW Behavior



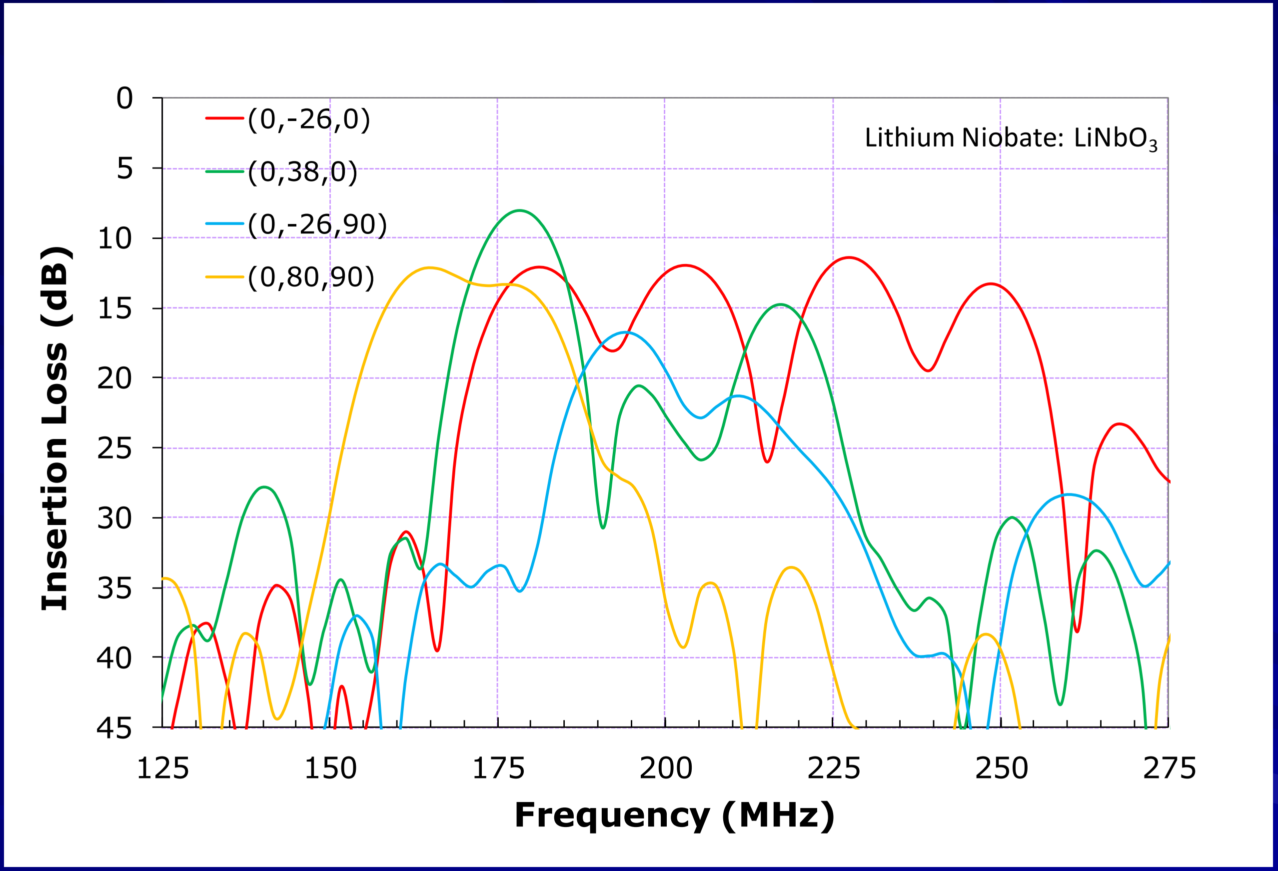
$$V_S = \lambda f_0 = 20(\mu m) \times [130 - 133](MHz) = 2600 - 2660(m/s)$$

Crystal Cuts and SAW Behavior



$$V_S = \lambda f_0 = 20(\mu m) \times [120 - 133](MHz) = 2400 - 2660(m/s)$$

Crystal Cuts and SAW Behavior



$$V_S = \lambda f_0 = 20(\mu m) \times \left[165 - 250\right](MHz) = 3300 - 5000(m/s)$$

Summary

- Crystal cut angles and wave propagation direction affect SAW velocity and insertion loss significantly
- Selection of an appropriate crystal cut is crucial to deriving desired performances for SAW devices
- Computer simulation provides a quick and cost-effective way to identify optimal crystal cuts for the development of high-performance SAW devices
- Acknowledgement

  - Institute for Biological Interface of Engineering
  - Clemson Palmetto Cluster Super Computing Facility
  - zephrasoft.com for the use of the Crystal Matrix Rotation Calculator

Thank You!