# Bulk and Surface Acoustic Waves in Piezoelectric Media

**Introductory Course on Multiphysics Modelling**

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# 1 Introduction

- **Surface Acoustic Waves (SAW)** are acoustic waves which travel along the surface of an elastic material; typically, their amplitude decays exponentially with depth into the substrate.

- **Wave propagation in anisotropic media is much more complex** than in isotropic materials.
- **Piezoelectric materials** are inherently **anisotropic**.

**Research milestones** – on anisotropic wave propagation and Surface Acoustic Waves:

- plane waves in anisotropic media (CHRISTOFFEL, 1877)
- surface wave in an isotropic elastic half-space (RAYLEIGH, 1885)
- double-surface, planar, isotropic, elastic waveguide (LAMB, 1917)
- Rayleigh wave on an anisotropic half-space with cubic crystal symmetry (STONELEY, 1955)
- "forbidden" directions for surface wave propagation do not exist! (LIM and FARNELL, 1968)
- pseudosurface waves (LIM, FARNELL and ROLLINS, 1968, 1969, 1970)
- Bleustein-Gulyaev surface piezoelectric wave (BLEUSTEIN, 1968; GULYAEV, 1969)
- Lamb waves in elastic, anisotropic (cubic) plates (SOLIE and AULD, 1973)
- (decoupling of) Rayleigh waves in orthorhombic, tetragonal, hexagonal, and cubic crystals (ROYER and DIEULESAINT, 1984)

# 2 Piezoelectricity

## 2.1 The piezoelectric phenomena

**(Direct) piezoelectric effect**

**Piezoelectricity** is the ability of some materials (notably crystals and certain ceramics) to generate an **electric charge** in response to applied **mechanical stress**. If the material is not short-circuited, the applied charge induces a **voltage** across the material.

**Elastic behaviour** $\xleftrightarrow[\textbf{coupling}]{\textbf{Piezoelectric}}$ **Dielectric behaviour**

► **A simple molecular model**

A simple molecular model of the direct piezoelectric effect is shown in Figure 1. The explanations are given below.

*Before* subjecting the material to some external stress:

- the centres of the negative and positive charges of each molecule coincide,
- the external effects of the charges are reciprocally cancelled,

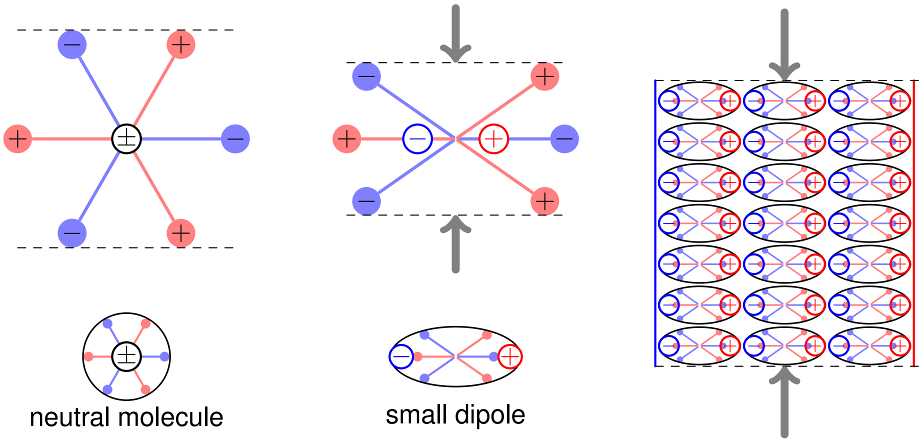



**FIGURE 1:** A molecular model of piezoelectricity

- as a result, an electrically neutral molecule appears.

*After* exerting some pressure on the material:

- the internal structure is deformed,
- that causes the separation of the positive and negative centres of the molecules,
- as a result, little dipoles are generated.

*Eventually*:

- the facing poles inside the material are mutually cancelled,
- a distribution of a linked charge appears in the material's surfaces and the material is polarized,
- the polarization generates an electric field and can be used to transform the mechanical energy of the material's deformation into electrical energy.

## ▶ Reversibility

The piezoelectric effect is **reversible**, that is, piezoelectric materials always exhibit both:

- **the direct piezoelectric effect** – the production of electricity when stress is applied,
- **the converse piezoelectric effect** – the production of stress and/or strain when an electric field is applied. (For example, lead zirconate titanate crystals will exhibit a maximum shape change of about 0.1% of the original dimension.)

## ▶ Some historical facts and etymology

- The (direct) piezoelectric phenomenon was discovered in 1880 by the brothers Pierre and Jacques Curie during experiments on quartz.

- The existence of the reverse process was predicted by Lippmann in 1881 and then immediately confirmed by the Curies.
- The word *piezoelectricity* means "*electricity by pressure*" and is derived from the Greek *piezein*, which means to squeeze or press.

## 2.2 Piezoelectric equations

### ▶ Elastodynamics

*Equation of motion* :

$$\rho \ddot{\boldsymbol{u}} = \nabla \cdot \boldsymbol{T} + \boldsymbol{f} \tag{1}$$

$\rho$ – the mass density of the material
$\boldsymbol{u}$ – the mechanical displacement vector
$\boldsymbol{T}$ – the 2nd-rank Cauchy stress tensor
$\boldsymbol{f}$ – the body force vector

*Kinematic relations* :

$$\boldsymbol{S} = \frac{1}{2}\Big(\nabla \boldsymbol{u} + (\nabla \boldsymbol{u})^{\mathsf{T}}\Big) \tag{2}$$

$\boldsymbol{S}$ – the 2nd-rank strain tensor

*Constitutive relations* for elasticity :

$$\boldsymbol{T} = \boldsymbol{c} : \boldsymbol{S} \tag{3}$$

$\boldsymbol{c}$ – the 4th-rank elasticity tensor

*Boundary conditions* :

$$\boldsymbol{T} \cdot \boldsymbol{n} = \hat{\boldsymbol{t}} \quad \text{or} \quad \boldsymbol{u} = \hat{\boldsymbol{u}} \tag{4}$$

$\hat{\boldsymbol{t}}$ – the surface load
$\hat{\boldsymbol{u}}$ – the prescribed displacements

### ▶ Electrostatics

*Gauss' law* :

$$\nabla \cdot \boldsymbol{D} = q \tag{5}$$

$\boldsymbol{D}$ – the electric displacement vector
$q$ – the body electric charge

*Maxwell's law* :

$$\boldsymbol{E} = -\nabla \phi \tag{6}$$

$\boldsymbol{E}$ – the electric filed vector
$\phi$ – the electric potential

*Constitutive relations* for dielectrics :

$$\boldsymbol{D} = \boldsymbol{\epsilon} \cdot \boldsymbol{E} \tag{7}$$

$\boldsymbol{\epsilon}$ – the 2nd-rank dielectric tensor

*Boundary conditions* :

$$\boldsymbol{D}\cdot\boldsymbol{n}=\hat{Q} \quad \text{or} \quad \phi=\hat{\phi} \tag{8}$$

$\hat{Q}$ – the surface charge
$\hat{\phi}$ – the prescribed electric potential

## ▶ Elastodynamics and electrostatics combined

**Sourceless** *equation of motion* and *Gauss' law* :

$$\rho\ddot{\boldsymbol{u}}=\nabla\cdot\boldsymbol{T}, \qquad \nabla\cdot\boldsymbol{D}=0 \tag{9}$$

*Kinematic relations* and *Maxwell's law* :

$$\boldsymbol{S}=\frac{1}{2}\Big(\nabla\boldsymbol{u}+(\nabla\boldsymbol{u})^{\mathsf{T}}\Big), \qquad \boldsymbol{E}=-\nabla\phi \tag{10}$$

*Boundary conditions* :

$$\text{– mechanical:} \quad \boldsymbol{T}\cdot\boldsymbol{n}=\hat{\boldsymbol{t}} \quad \text{or} \quad \boldsymbol{u}=\hat{\boldsymbol{u}} \tag{11}$$

$$\text{– electrical:} \quad \boldsymbol{D}\cdot\boldsymbol{n}=\hat{Q} \quad \text{or} \quad \phi=\hat{\phi} \tag{12}$$

**Piezoelectric materials are anisotropic!**
(There is *no* isotropic piezoelectric medium.)

The **piezoelectric** effects are realised by **coupling** terms
in the **anisotropic constitutive relations**.

## ▶ Piezoelectric coupling

*Constitutive relations* for piezoelectric materials (*stress-charge form*) :

$$\boldsymbol{T}=\underbrace{\boldsymbol{c}:\boldsymbol{S}}_{\text{elasticity}}-\underbrace{\boldsymbol{e}^{\mathsf{T}}\cdot\boldsymbol{E}}_{\text{inverse effect}} \tag{13}$$

$$\boldsymbol{D}=\underbrace{\boldsymbol{e}:\boldsymbol{S}}_{\text{direct effect}}+\underbrace{\boldsymbol{\epsilon}\cdot\boldsymbol{E}}_{\text{dielectricity}} \tag{14}$$

$\boldsymbol{e}$ – the 3rd-rank piezoelectric coupling tensor
$\boldsymbol{c}$ – the 4th-rank elasticity tensor in the absence of electric field ($\boldsymbol{E}=\boldsymbol{0}$)
$\boldsymbol{\epsilon}$ – the 2nd-rank dielectric tensor in the absence of strains ($\boldsymbol{S}=\boldsymbol{0}$)

## 2.3 Voigt-Kelvin notation

**Voigt-Kelvin convention** for index substitution:

$$11 \to 1, \quad 22 \to 2, \quad 33 \to 3, \quad 23 \to 4, \quad 31 \to 5, \quad 12 \to 6 \tag{15}$$

This notation allows to represent:

the 4th-rank tensor of elasticity $\boldsymbol{c}$ $\to$ $(6\times 6)$ matrix $\mathbb{c}$
the 3rd-rank tensor of piezoelectric coupling $\boldsymbol{e}$ $\to$ $(3\times 6)$ matrix $\mathbb{e}$
the 2nd-rank tensor of dielectric constants $\boldsymbol{\epsilon}$ $\to$ $(3\times 3)$ matrix $\mathbb{\epsilon}$
the 2nd-rank tensors of strain $\boldsymbol{S}$ and stress $\boldsymbol{T}$ $\to$ $(6\times 1)$ vectors:

$$\begin{aligned} \mathbb{S} &= \begin{bmatrix} S_{11} & S_{22} & S_{33} & 2S_{23} & 2S_{31} & 2S_{12} \end{bmatrix}^{\mathsf{T}} \\ \mathbb{T} &= \begin{bmatrix} T_{11} & T_{22} & T_{33} & T_{23} & T_{31} & T_{12} \end{bmatrix}^{\mathsf{T}} \end{aligned} \tag{16}$$

Consistently, denote also: $\mathbb{u} \equiv \boldsymbol{u}$, $\mathbb{D} \equiv \boldsymbol{D}$, $\mathbb{E} \equiv \boldsymbol{E}$, $\mathbb{n} \equiv \boldsymbol{n}$.

- Constitutive relations:

$$\mathbb{T} = \mathbb{c}\mathbb{S} - \mathbb{e}^{\mathsf{T}}\mathbb{E}, \qquad \mathbb{D} = \mathbb{e}\mathbb{S} + \mathbb{\epsilon}\mathbb{E}. \tag{17}$$

- Kinematic relations and Maxwell's law:

$$\mathbb{S} = \boldsymbol{\nabla}^{\mathsf{T}}\mathbb{u}, \qquad \mathbb{E} = -\nabla\phi. \tag{18}$$

- Sourceless field equations:

$$\boldsymbol{\nabla}\mathbb{T} - \rho\ddot{\mathbb{u}} = \mathbb{0}, \qquad \nabla^{\mathsf{T}}\mathbb{D} = 0. \tag{19}$$

Here:

$$\boldsymbol{\nabla} = \begin{bmatrix} \partial_{x_1} & 0 & 0 & 0 & \partial_{x_3} & \partial_{x_2} \\ 0 & \partial_{x_2} & 0 & \partial_{x_3} & 0 & \partial_{x_1} \\ 0 & 0 & \partial_{x_3} & \partial_{x_2} & \partial_{x_1} & 0 \end{bmatrix}, \qquad \nabla = \begin{bmatrix} \partial_{x_1} \\ \partial_{x_2} \\ \partial_{x_3} \end{bmatrix}, \qquad \mathbb{0} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}. \tag{20}$$

- Neumann boundary conditions – e.g., homogeneous:

$$\mathbb{N}\mathbb{T} = \mathbb{0}, \qquad \mathbb{n}^{\mathsf{T}}\mathbb{D} = 0, \tag{21}$$

where

$$\mathbb{N} = \begin{bmatrix} n_1 & 0 & 0 & 0 & n_3 & n_2 \\ 0 & n_2 & 0 & n_3 & 0 & n_1 \\ 0 & 0 & n_3 & n_2 & n_1 & 0 \end{bmatrix}, \qquad \mathbb{n} = \begin{bmatrix} n_1 \\ n_2 \\ n_3 \end{bmatrix}. \tag{22}$$

# 3 Anisotropic media

## 3.1 Crystalline materials

Crystalline materials are *homogeneous* – different macroscopic samples, with the same dimensions and crystalline orientation, behave identically.

At the atomic scale, where the medium is discontinuous, homogeneity remains in the sense described by Bravais – there are in the crystal three distinct directions each having an infinity of discrete points which are equivalent to any one point, that is, they possess the same environment.

- The crystal can be developed in very different forms, yet the relative orientation of the faces is constant.
- The angles between the various faces of a crystal remain unchanged throughout its growth a law. This is **the law of constant angles** in crystallography.

> **The law of constant angles**
>
> The normals to the crystal faces, drawn from a fixed point, form a geometrically invariant figure (the relative orientation of the faces is constant, although the crystal can be developed in very different forms).

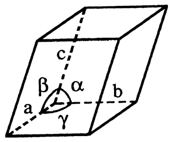
- The macroscopic properties of crystals suggest their classification according to the symmetry shown by the normals to the natural faces, known as the **point group**.
- The crystalline medium is characterized by an infinity of geometrical points (the **nodes**), which are **equivalent**, that is they have the same environment of other points. The set of these nodes forms a **three-dimensional lattice**, which expresses the periodicity of the crystal in all directions.
- There are **14 lattices** organized in **7 crystal systems** – see Table 1 and Figure 2.
- The atomic structure of crystal is determined by the **lattice** and the **atomic group** (a group of atoms) assigned to each node:

$$\textbf{Crystal} = \textbf{Lattice} + \textbf{Atomic group}$$

- The crystal symmetry is at most equal to that of the lattice $\rightarrow$ a crystal does not necessarily possesses a centre of symmetry.
- There are **32 point symmetry classes of crystals**.

**TABLE 1:** The **7 crystal systems** and **14 Bravais lattices**

| *System* | *Lattices* | | |
|---|---|---|---|
| 1. Triclinic | P | $\alpha \neq \beta \neq \gamma \neq 90^\circ$ | $a \neq b \neq c$ |
| 2. Monoclinic | P, C | $\alpha = \gamma = 90^\circ$, $\beta \neq 90^\circ$ | $a \neq b \neq c$ |
| 3. Orthorhombic | P, I, C, F | $\alpha = \beta = \gamma = 90^\circ$ | $a \neq b \neq c$ |
| 4. Trigonal (rhombohedral) | P (or R) | $\alpha = \beta = \gamma \neq 90^\circ$ | $a = b = c$ |
| 5. Tetragonal (quadratic) | P, I | $\alpha = \beta = \gamma = 90^\circ$ | $a = b \neq c$ |
| 6. Hexagonal | P | $\alpha = \beta = 90^\circ$, $\gamma = 120^\circ$ | $a = b \neq c$ |
| 7. Cubic | P, I, F | $\alpha = \beta = \gamma = 90^\circ$ | $a = b = c$ |



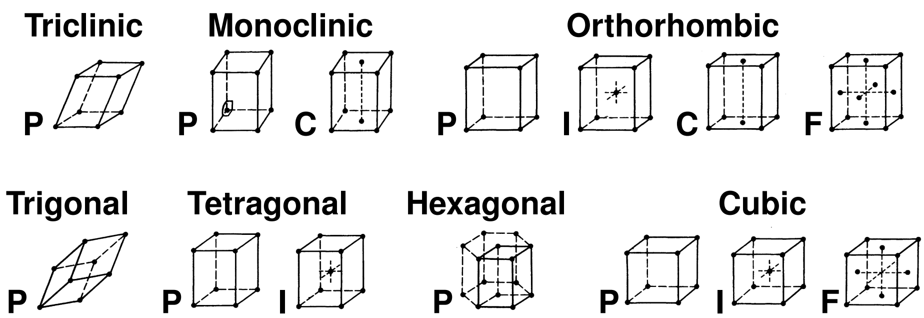




**FIGURE 2:** The **7 crystal systems** and **14 Bravais lattices**

### ▶ Example: Lithium niobate ($LiNbO_3$)

Figures 3 and 4 show the atomic and crystallographic structure of the lithium niobate crystal. A few characteristic features of this piezoelectric material are listed here:

- trigonal system, class 3m,
- strongly piezoelectric,
- large crystals available (cylinders of diameter 10 cm and length more than 10 cm).

## 3.2 Constitutive matrices for some classes of anisotropy

Figures 5-8 present non-zero components of the constitutive matrices for some symmetry classes. The number of independent material constants is given in every case, and in fact, for each of the constitutive matrices (see the numbers in parentheses at $c$, $e$, and $\epsilon$). The inter-dependencies between the relevant components are also shown, assuming that the system of reference is consistent with the material axes. This is demonstrated for four systems:

- cubic – see Figure 5,
- hexagonal – see Figure 6,
- orthorhombic – see Figure 7,
- trigonal – see Figure 8.

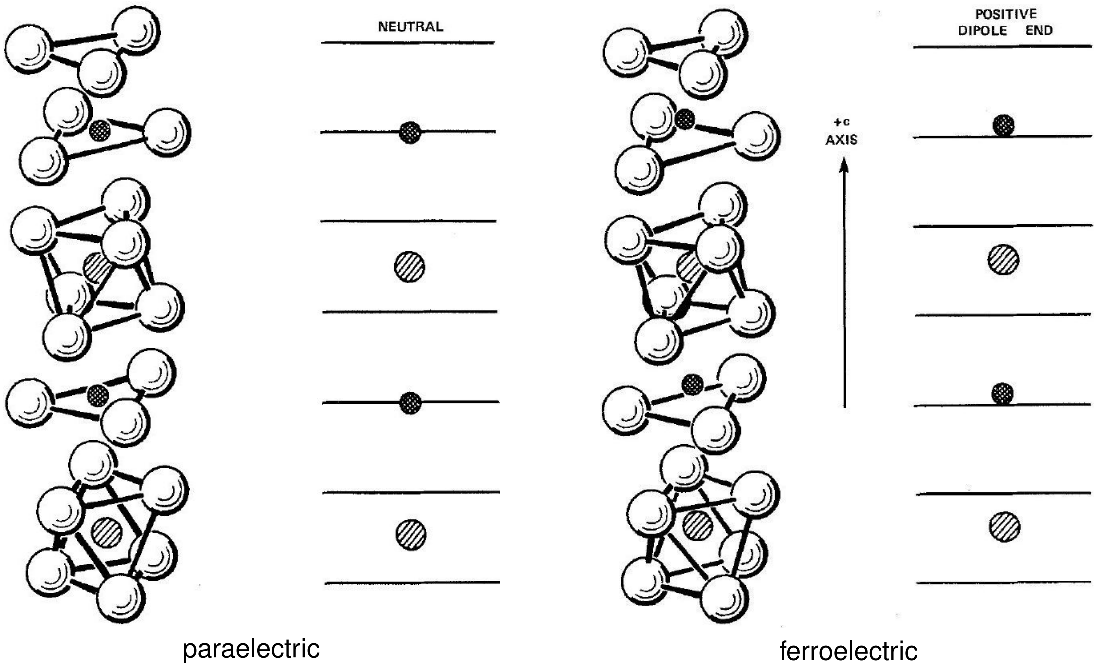



**FIGURE 3:** Lithium niobate crystal: positions of the lithium and niobium atoms (double and singe cross-hatched circles, respectively) with respect to the oxygen octahedra in the paraelectric and ferroelectric phase

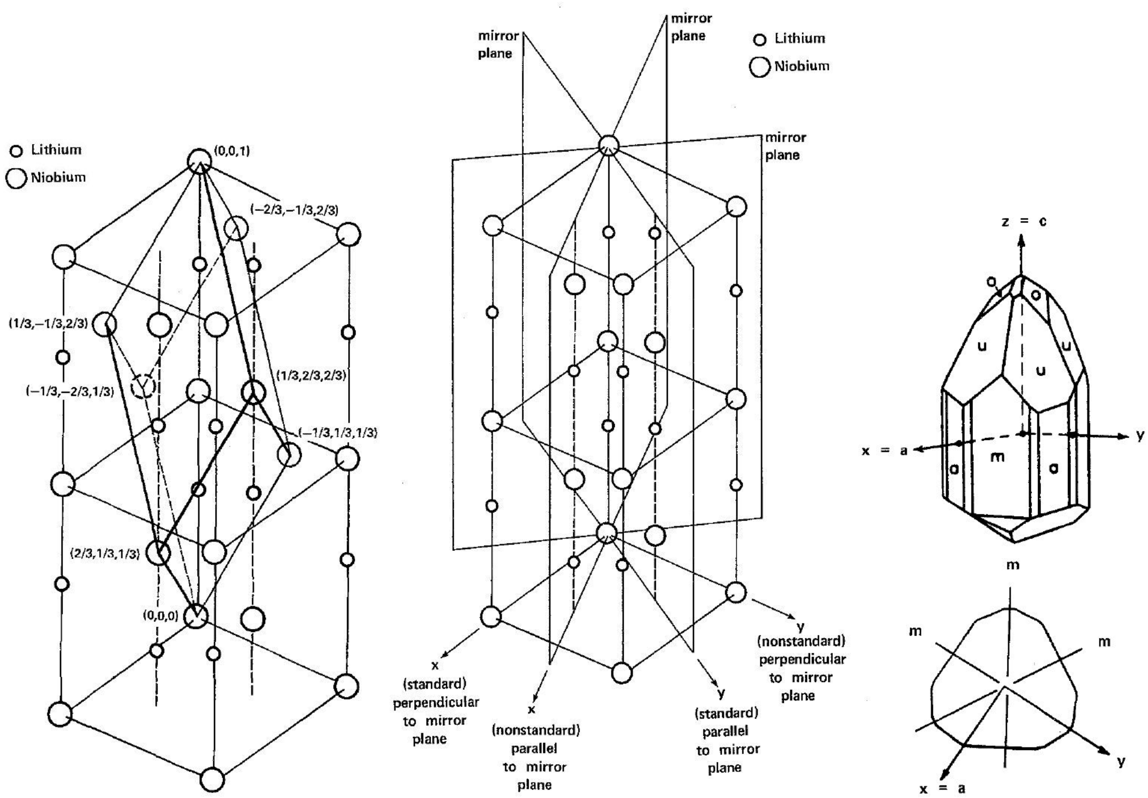



**FIGURE 4:** Lithium niobate crystal: (*left*) the conventional rhombohedral unit cell (shown with respect to the hexagonal unit cell), and (*middle & right*) the standard and nonstandard orientations of the principal axes and the planes of mirror symmetry

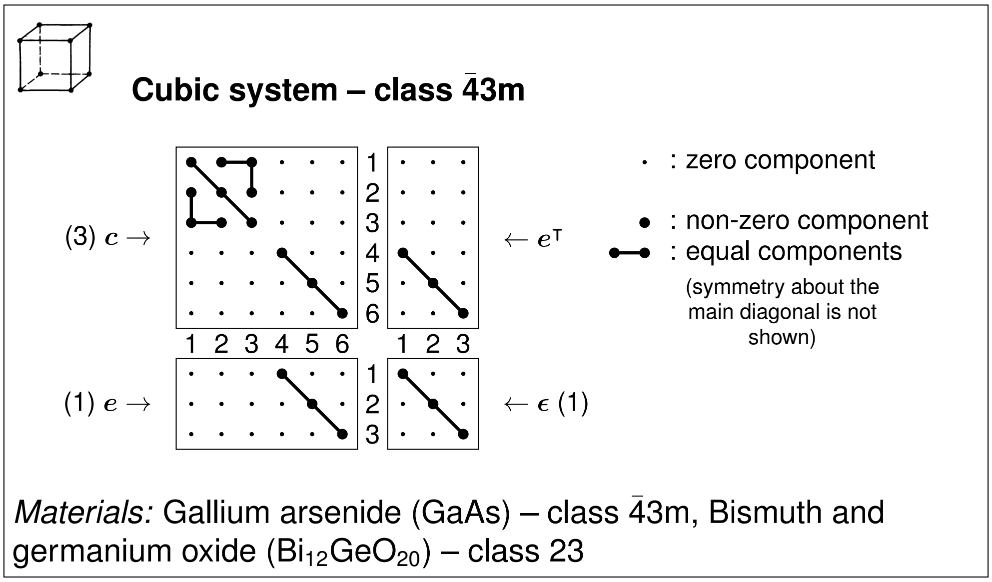



**FIGURE 5:** The components of constitutive matrices for the cubic system and symmetry class $\bar{4}3m$

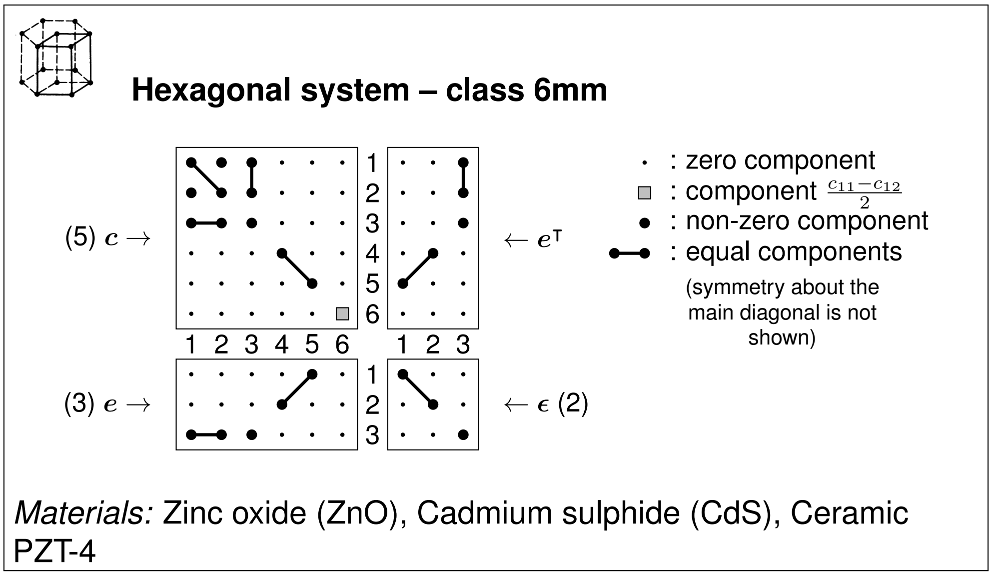



**FIGURE 6:** The components of constitutive matrices for the hexagonal system and symmetry class 6mm

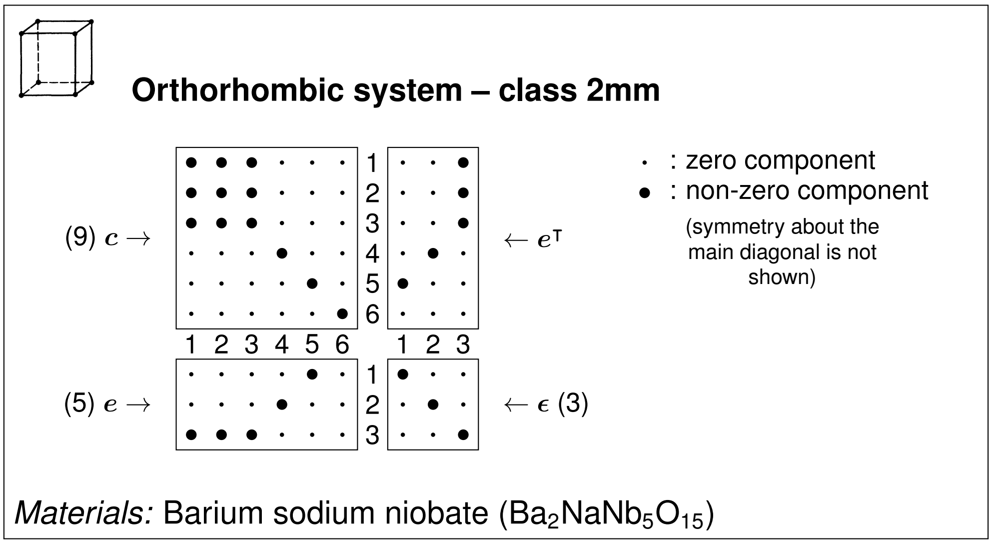



**FIGURE 7:** The components of constitutive matrices for the hexagonal system and symmetry class 6mm

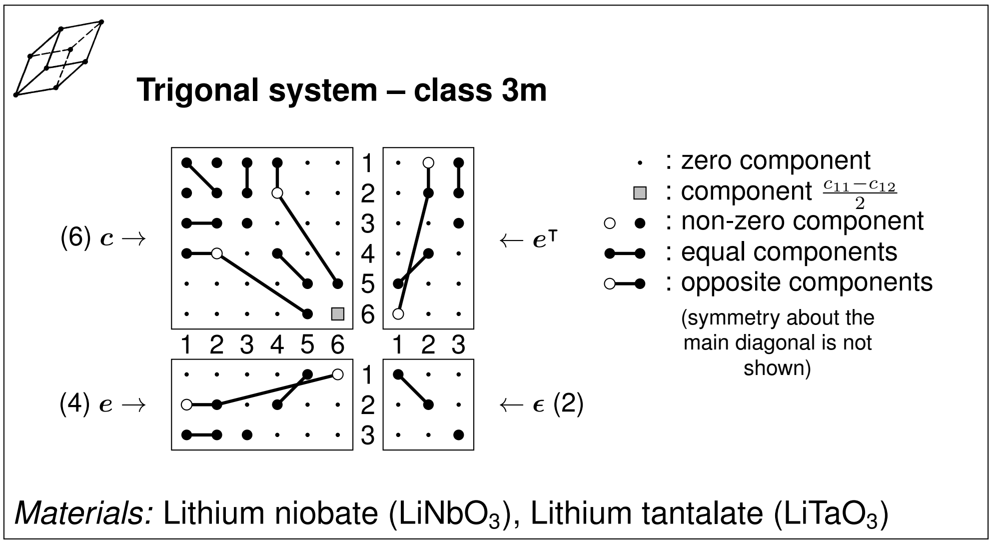



**FIGURE 8:** The components of constitutive matrices for the orthorhombic system and symmetry class 2mm

# 4 Bulk acoustic waves in anisotropic media

## 4.1 Mathematical description

The **plane wave propagation** along the **direction** $\boldsymbol{n}$ in a **piezoelectric medium** is described by the fields of mechanical displacement and electric potential which change with respect to the location $x$ and time $t$, accordingly to the forms presented below, namely, for the mechanical displacement components:

$$u_1 \equiv u(\boldsymbol{x}, t) = A_u\, \mathcal{E}(\boldsymbol{x}, t), \tag{23}$$

$$u_2 \equiv v(\boldsymbol{x}, t) = A_v\, \mathcal{E}(\boldsymbol{x}, t), \tag{24}$$

$$u_3 \equiv w(\boldsymbol{x}, t) = A_w\, \mathcal{E}(\boldsymbol{x}, t), \tag{25}$$

and for the electric potential:

$$\phi(\boldsymbol{x}, t) = A_\phi\, \mathcal{E}(\boldsymbol{x}, t), \tag{26}$$

where $A_u$, $A_v$, $A_w$, $A_\phi$ are constants independent of $x$ and $t$, and for the given waveform $\mathcal{F}$:

$$\mathcal{E}(\boldsymbol{x}, t) = \mathcal{F}(\boldsymbol{n} \cdot \boldsymbol{x} - Vt), \tag{27}$$

where $V$ is the **phase velocity**. These formulas can be rewritten in the matrix form as follows:

$$\mathbb{u} = \mathbb{A}_{\boldsymbol{u}}\, \mathcal{F}, \quad \phi = A_\phi\, \mathcal{F}, \quad \text{where} \quad \mathbb{A}_{\boldsymbol{u}} = \begin{bmatrix} A_u \\ A_v \\ A_w \end{bmatrix} \tag{28}$$

is the **wave polarization** vector (direction of the particle displacement).

Using the Kelvin-Voigt notation,i.e., the formulas and definitions introduced in Section 2.3, the mechanical strain and electric field vectors are expressed as

$$\mathbb{S} = \mathbb{N}^\mathsf{T} \mathbb{A}_{\boldsymbol{u}}\, \mathcal{F}', \qquad \mathbb{E} = -\mathbb{n} A_\phi\, \mathcal{F}'. \tag{29}$$

Notice that the polarization of electric field is longitudinal; the matrix $\mathbb{N}$ and vector $\mathbb{n}$ are defined as in (22), although here they are related to the direction of propagation $\boldsymbol{n}$ (and *not* to a vector normal to a boundary). The constitutive relations for the stress and electric displacement vectors are

$$\mathbb{T} = (\mathbb{c}\mathbb{N}^\mathsf{T} \mathbb{A}_{\boldsymbol{u}} + \mathbb{e}^\mathsf{T} \mathbb{n} A_\phi)\mathcal{F}', \qquad \mathbb{D} = (\mathbb{e}\mathbb{N}^\mathsf{T} \mathbb{A}_{\boldsymbol{u}} - \mathbb{\epsilon}\mathbb{n} A_\phi)\mathcal{F}'. \tag{30}$$

When all these formulas are used for the field equations (19),the following set of equations describing the plane wave propagation in piezoelectric media is obtained.

***Equations for plane wave propagation in piezoelectric media***

$$\begin{aligned} \left(\mathbb{N}\mathbb{c}\mathbb{N}^\mathsf{T} - \rho V^2 \mathbb{1}\right) \mathbb{A}_{\boldsymbol{u}} + \mathbb{N}\mathbb{e}^\mathsf{T} \mathbb{n} A_\phi = \mathbb{0}, \\ \mathbb{n}^\mathsf{T} \mathbb{e}\mathbb{N}^\mathsf{T} \mathbb{A}_{\boldsymbol{u}} - \mathbb{n}^\mathsf{T} \mathbb{\epsilon}\mathbb{n} A_\phi = 0, \end{aligned} \tag{31}$$

where $\mathbb{1}$ is the $(3\times3)$-identity matrix. Or, in the matrix form:

$$\begin{bmatrix} \mathbb{N}\mathbb{c}\mathbb{N}^\mathsf{T} - \rho V^2 \mathbb{1} & \mathbb{N}\mathbb{e}^\mathsf{T}\mathbb{n} \\ \mathbb{n}^\mathsf{T}\mathbb{e}\mathbb{N}^\mathsf{T} & -\mathbb{n}^\mathsf{T}\mathbb{\epsilon}\mathbb{n} \end{bmatrix} \begin{bmatrix} \mathbb{A}_{\boldsymbol{u}} \\ A_\phi \end{bmatrix} = \begin{bmatrix} \mathbb{0} \\ 0 \end{bmatrix}. \tag{32}$$

The last equation in the set gives the following formula:

$$A_\phi = \frac{\mathbb{n}^\mathsf{T}\mathbb{e}\mathbb{N}^\mathsf{T}}{\mathbb{n}^\mathsf{T}\mathbb{\epsilon}\mathbb{n}} \mathbb{A}_{\boldsymbol{u}} \tag{33}$$

which is used to derive the generalized **Christoffel matrix equation**.

**Christoffel matrix equation**

$$\left[\mathbb{G} - \rho V^2 \mathbb{1}\right] \mathbb{A}_{\boldsymbol{u}} = \mathbb{0}, \quad \text{where} \quad \mathbb{G} = \mathbb{N}\mathbb{c}\mathbb{N}^\mathsf{T} + \frac{\mathbb{N}\mathbb{e}^\mathsf{T}\mathbb{n}\mathbb{n}^\mathsf{T}\mathbb{e}\mathbb{N}^\mathsf{T}}{\mathbb{n}^\mathsf{T}\mathbb{\epsilon}\mathbb{n}} \tag{34}$$

is the matrix representation of the second-order **Christoffel tensor** (generalized for the case of piezoelectric medium).

***Observations***:

- The **polarization is eigenvector of the Christoffel tensor** (matrix) $\mathbb{G}$ with eigenvalue $\rho V^2$.
- The **phase velocities** and **polarizations** of plane waves propagating in the direction $\boldsymbol{n}$ in a crystal are given by the **eigenvalues** and **eigenvectors** of the corresponding **Christoffel tensor**.

The acoustic wave propagation in (anisotropic) solids is more complicated that in fluids, because of the following facts.

- **Three plane waves** with **mutually orthogonal polarizations** can propagate in **the same direction**, with **different velocities**.
- The elastic displacement vector is **not generally parallel or perpendicular to the propagation direction**. The waves are purely longitudinal or transverse only in particular directions.
- The wave with polarization closest to the propagation direction is called **quasi-longitudinal**, its velocity is usually higher than that of the two other waves, called **quasi-transverse**. Only in particular directions are the waves purely longitudinal or transverse.

A propagation direction is called an **acoustic axis**, when the transverse wave polarization has an arbitrary direction in the plane normal to the axis. The transverse waves are then degenerate and have the same velocity.

The **acoustic ray** is the direction of energy transport, that is the direction of the energy velocity vector. The projection of this vector onto the propagation direction is equal to the phase velocity of the plane wave. When the acoustic ray is perpendicular to the wave-fronts, and therefore parallel to the propagation direction, the mode (the wave) is described as *pure*, and the velocity of energy flow is equal to the phase velocity. A longitudinal wave is always pure; however, there may be transverse (degenerate) waves which are not pure. When the mode is pure, the directions of propagation and polarization are interchangeable (that is, switching them results in another pure mode).

## 4.2 Characteristic surfaces

**The velocity surface** is defined by the end of the vector $\boldsymbol{n}V(\boldsymbol{n})$, drawn from the origin in varied directions $\boldsymbol{n}$ (the length of this vector equals the phase velocity $V$ for waves with wavefronts perpendicular to it).

**The slowness surface** is defined by the end of vector $\boldsymbol{n}/V(\boldsymbol{n})$, drawn from the origin in varied directions $\boldsymbol{n}$. The **energy velocity** is, at all points, **normal to the slowness surface**.

**The wave surface** is defined by the end of the **energy velocity vector** $\boldsymbol{V}^{\mathrm{e}}(\boldsymbol{n})$, drawn from the origin, as the propagation direction $\boldsymbol{n}$ varies. It is an **equi-phase surface** and describes the points reached, at unit time, by the vibrations (energy) emitted at time zero by a point source at the origin.

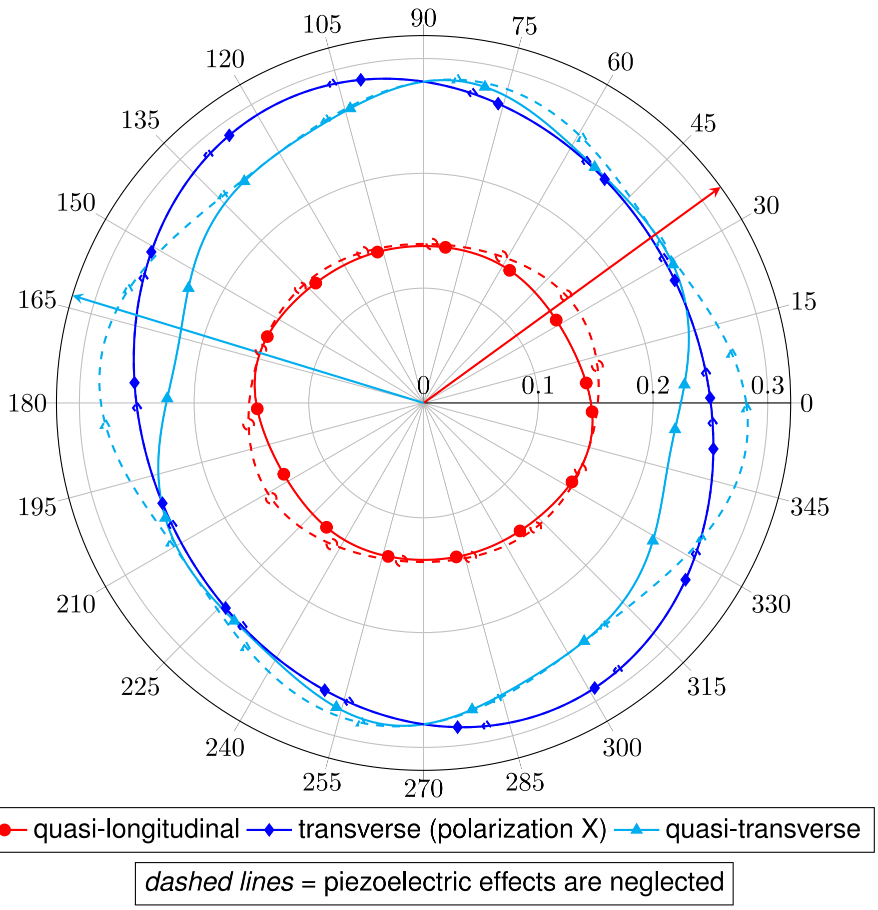



**FIGURE 9:** Slowness surfaces [s/km] in the **YZ**-plane for the lithium niobate crystal

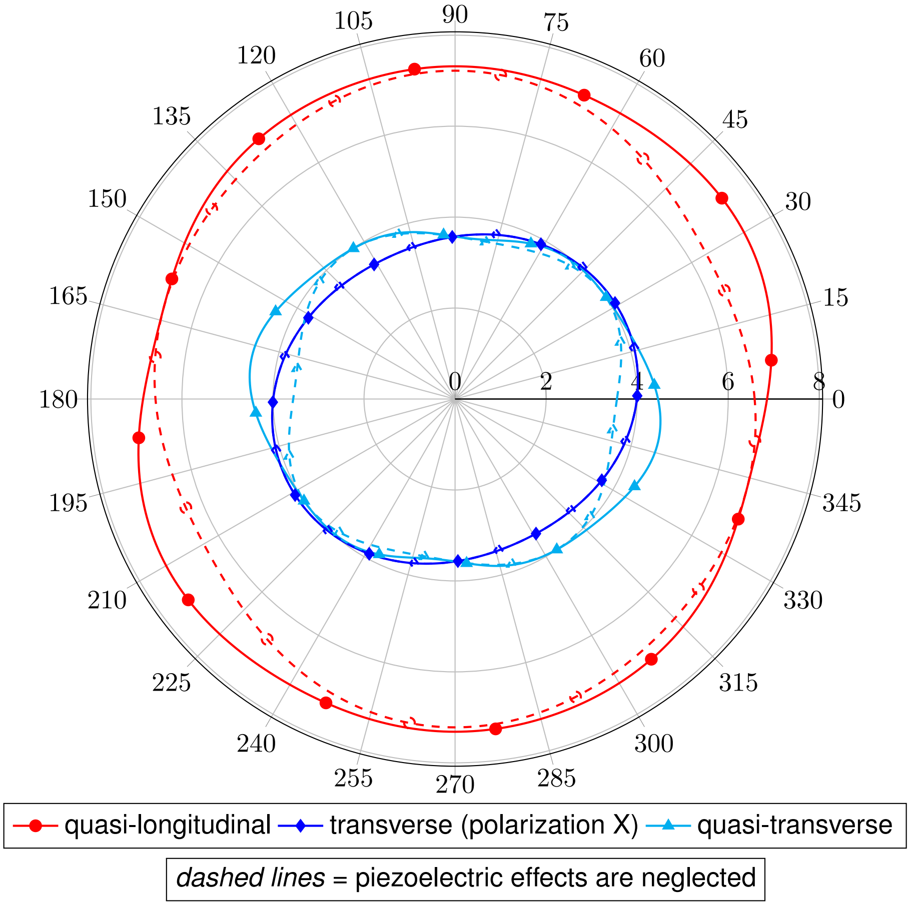



**FIGURE 10:** Velocity surfaces for lithium niobate [km/s] in the **YZ**-plane for the lithium niobate crystal

Examples of characteristic surfaces are given in Figures 9, 10, and 11 for the lithium niobate crystal which is characterised by a strong anisotropy of a trigonal class. Figure 9 shows the slowness surfaces in the YZ-plane and the corresponding velocity surfaces are presented in Figure 10. Figure 11 shows the slowness surfaces in the XY-plane; they are fairly different from their counterparts shown in Figure 9, although the pairs of corresponding curves presented in both Figures are the intersections of the same surface – this illustrates how far these '*anisotropic*' slowness surfaces are from the spherical shape typical for isotropy.

# 5 Surface Acoustic Waves (SAW)

## 5.1 Types of Surface Acoustic Waves

- **Rayleigh waves** – waves travelling near the surface of elastic solids
- **Lamb waves** – waves travelling in elastic plates (guided by the surfaces of these plates)
- **Love waves** – horizontally polarized shear waves guided by a thin elastic layer

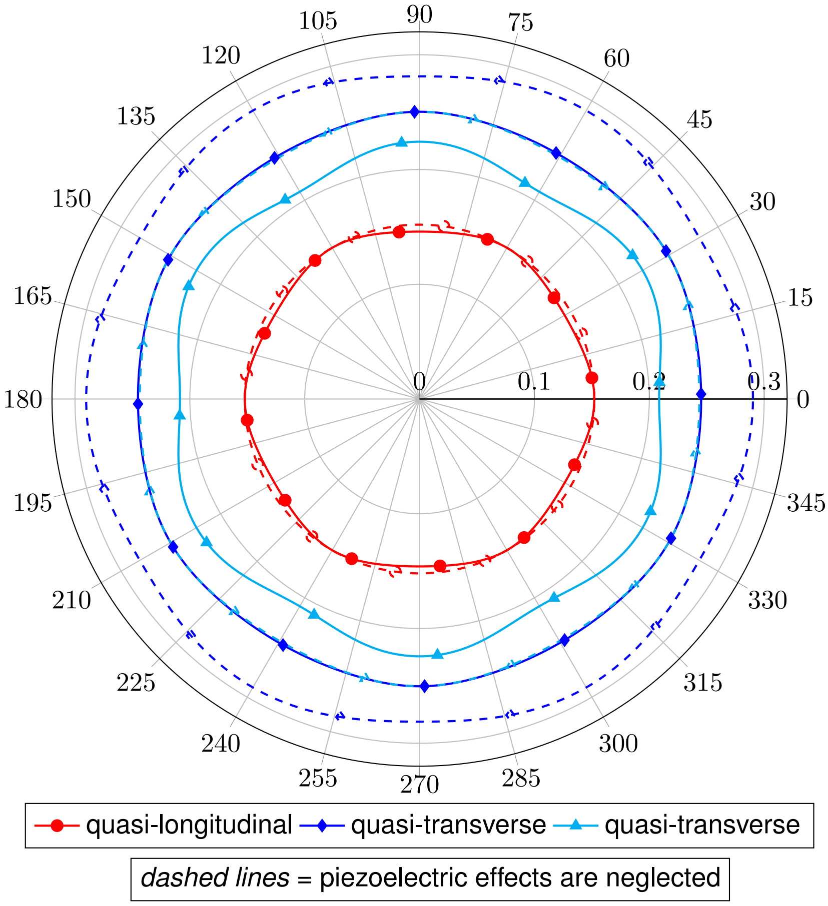



**FIGURE 11:** Slowness surfaces for lithium niobate [s/km] in the **XY**-plane for the lithium niobate crystal

set on another elastic solid (of higher acoustic wave velocity)

- **Stoneley waves** – waves travelling along solid-fluid or solid-solid interfaces

### ▶ Pseudo-surface waves

A pseudo-surface wave appears in certain crystals when, because of anisotropy, the Rayleigh wave velocity is greater than that of one of the bulk transverse waves.

## 5.2 Partial waves

For **harmonic wave propagation** in the **sagittal XZ-plane** the waveform is defined as follows:

$$\mathcal{E}(\boldsymbol{x}, t) = \exp\big[\mathrm{i}k(x + \beta z - Vt)\big], \quad \text{where} \quad V = \frac{\omega}{k}, \tag{35}$$

$\omega$ is the angular frequency, $k$ is the wavenumber, and $\beta$ is a constant value which defines the direction of propagation in the XZ-plane, namely, the angle between this direction and the X-axis is $\arctan(\beta)$. Therefore:

$$\mathcal{F}(.) = \exp\big[\mathrm{i}k(.)\big], \qquad \mathcal{F}'(.) = \mathrm{i}k\mathcal{F}(.). \tag{36}$$

Now, when the matrix $\mathbb{N}$ and vector $\mathbb{n}$ are related to the direction of propagation $\boldsymbol{n}$, they can be specified as follows

$$\mathbb{N} \to \mathbb{B} = \begin{bmatrix} 1 & 0 & 0 & 0 & \beta & 0 \\ 0 & 0 & 0 & \beta & 0 & 1 \\ 0 & 0 & \beta & 0 & 1 & 0 \end{bmatrix}, \qquad \mathbb{n} \to \mathbb{b} = \begin{bmatrix} 1 \\ 0 \\ \beta \end{bmatrix}. \tag{37}$$

Therefore, the strain, electric field, stress, and electric displacement vectors are

$$\mathbb{S} = \mathbb{B}^\mathsf{T} \mathbb{A}_{\boldsymbol{u}} \mathrm{i}k\mathcal{E}, \qquad \mathbb{E} = -\mathbb{b} A_\phi \mathrm{i}k\mathcal{E}, \tag{38}$$

$$\mathbb{T} = (\mathbb{c}\mathbb{B}^\mathsf{T}\mathbb{A}_{\boldsymbol{u}} + \mathbb{e}^\mathsf{T}\mathbb{b}A_\phi)\mathrm{i}k\mathcal{E}, \qquad \mathbb{D} = (\mathbb{e}\mathbb{B}^\mathsf{T}\mathbb{A}_{\boldsymbol{u}} - \mathbb{\epsilon}\mathbb{b}A_\phi)\mathrm{i}k\mathcal{E}, \tag{39}$$

and the final set of equations is as follows.

**Plane harmonic wave propagation in piezoelectric media**

$$\begin{aligned} \left(\mathbb{B}\mathbb{c}\mathbb{B}^\mathsf{T} - \rho V^2 \mathbb{1}\right)\mathbb{A}_{\boldsymbol{u}} + \mathbb{B}\mathbb{e}^\mathsf{T}\mathbb{b}A_\phi &= \mathbb{0}, \\ \mathbb{b}^\mathsf{T}\mathbb{e}\mathbb{B}^\mathsf{T}\mathbb{A}_{\boldsymbol{u}} - \mathbb{b}^\mathsf{T}\mathbb{\epsilon}\mathbb{b}A_\phi &= 0. \end{aligned} \tag{40}$$

- This **plane-wave eigensystem** depends now also on $\beta$.
- Eigenproblem is solved for $\beta$ with $V$ treated as parameter. The secular equation is an 8th-order polynomial (or a 6th-order polynomial for purely elastic media).
- The 8 eigenvalues and eigenvectors form 8 **partial waves**. In case of the Rayleigh wave, 4 of them are discarded on the basis of boundary conditions at $-\infty$ (see Section 5.3).
- The solution is a linear combination of partial waves which are coupled by the **boundary conditions** on the surface(s), see Sections 5.3 and 5.4. That gives **another eigensystem**.
- Its secular equation must be zero for the velocity $V$ to be the correct surface wave velocity – this condition is checked and eventually satisfied by an adjusting procedure which changes $V$ in a loop.

## 5.3 Rayleigh waves

A Rayleigh wave propagates along the surface of a medium, see Figure 12. The relevant boundary conditions are specified below.

Mechanical boundary conditions:

$$\text{for } z \to -\infty: \quad \boldsymbol{u} = \mathbf{0} \tag{41}$$

$$\text{for } z = 0: \quad \boldsymbol{T} \cdot \boldsymbol{n} = \mathbf{0} \tag{42}$$

Electrical boundary conditions:

$$\text{for } z \to -\infty: \quad \phi = 0 \tag{43}$$

$$\text{for } z = 0: \quad \boldsymbol{D} \cdot \boldsymbol{n} = 0 \tag{44}$$

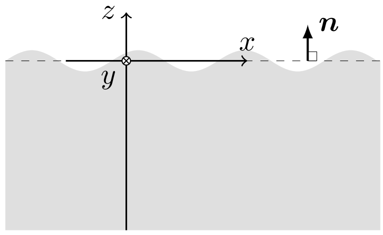



**FIGURE 12:** A Rayleigh wave

**Features:**

- the partial waves are coupled at the surface;
- for a particular material and orientation (the cut and direction of propagation) there is actually **only one velocity**, i.e., there is only **one Rayleigh wave**;
- longitudinal and transverse **motions decrease exponentially** in amplitude **as distance from the surface increases** (there is a phase difference between these component motions);
- the Rayleigh wave is **non-dispersive**.

## 5.4 Lamb waves

Lamb waves are driven by a plate of finite thickness – see, for example, Figure 13. There are many kinds (modes) and velocities of such propagation obtained by applying on both surfaces the boundary conditions given below.

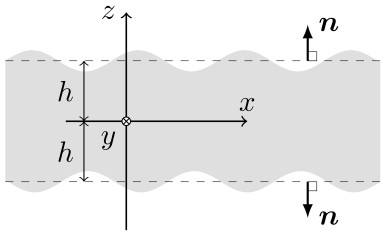



**FIGURE 13:** A Lamb wave

Mechanical boundary conditions:

$$\text{for } z = +h: \quad \boldsymbol{T} \cdot \boldsymbol{n} = \boldsymbol{0} \tag{45}$$

$$\text{for } z = -h: \quad \boldsymbol{T} \cdot \boldsymbol{n} = \boldsymbol{0} \tag{46}$$

Electrical boundary conditions:

$$\text{for } z = +h: \quad \boldsymbol{D} \cdot \boldsymbol{n} = 0 \tag{47}$$

$$\text{for } z = -h: \quad \boldsymbol{D} \cdot \boldsymbol{n} = 0 \tag{48}$$

*Comment*: Electrical boundary conditions here are for the case of the surface(s) covered with a hypothetical medium with *zero electrical permittivity*; however, for materials with relatively high permittivity (such as lithium niobate), if the adjacent medium is vacuum (or air) the results are very similar.

**Features:**

- partial waves are coupled and also reflected back and fourth by the boundaries of the plate;
- **coupled waves** results from the **travelling waves** along the plate and **standing waves** in the direction across the plate thickness;
- there are **many modes** (symmetric and antisymmetric) with **different velocities**;
- **dispersion** (the wave velocities depend on the frequency and the plate thickness).

## 5.5 Decoupling of Rayleigh waves in piezoelectric media

There are two such cases:

1. When the sagittal plane is normal to a direct binary axis of crystal, there exists the possibility for:
   - a non-piezoelectric Rayleigh wave $\mathrm{R}_2$ polarized in this plane $(u_2 = 0)$,
   - a piezoelectric transverse horizontal wave $\overline{\mathrm{TH}}$ (BLEUSTEIN & GULYAEV, 1968) which can propagate independently.
2. When the sagittal plane is parallel to a mirror plane of crystal, there exists the possibility for:
   - a piezoelectric Rayleigh wave $\overline{\mathrm{R}}_2$ polarized in the sagittal plane $(u_2 = 0)$,
   - a non-piezoelectric transverse horizontal wave TH which can propagate independently and is not a surface wave.

- The symmetries of these two cases can be satisfied only for **orthorhombic**, **tetragonal**, **hexagonal**, and **cubic** crystals. With respect to the crystallographic axes there are **16 possible combinations**, that is, orientations of the propagation direction $x_1$ and the sagittal plane normal $x_2$.
- Decoupling is also possible in **trigonal** crystals: for the so-called Y-cut (i.e., the free surface is parallel to the XZ-plane) when the propagation is along the Z-axis (the sagittal plane is YZ).
- Figure 14 shows non-zero components of the constitutive matrices for the trigonal system, class 3m, with respect to any system of reference rotated around the X-axis; although no inter-dependencies between these components are shown, one should remember that there are only 12 independent components.

# 6 SAW examples

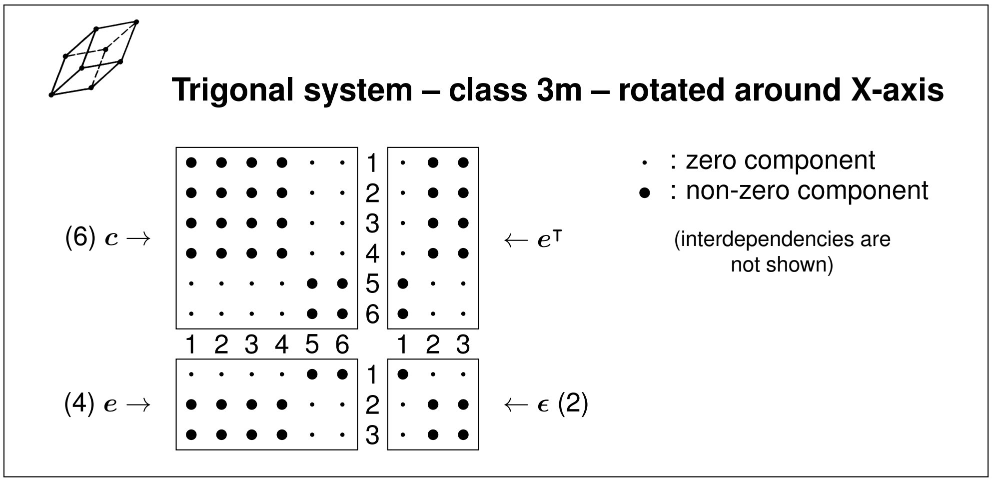



**FIGURE 14:** The components of constitutive matrices for the trigonal system and symmetry class 3mm – for any system of reference rotated around the X-axis

## 6.1 Piezoelectric Rayleigh wave in lithium niobate

- Figure 15 presents the Rayleigh wave $\overline{\mathrm{R}}_2$ in lithium niobate ($LiNbO_3$), Y-cut, propagation along the Z-axis; the wave velocity is $V =$ **3485** m/s.
- The electric potential of the associated electric field (phase angle: 0°) is shown in Figure 16.
- There is no dispersion – the wave velocity is the same whatever would be the wave frequency $f$; the wavelength is therefore: $\lambda = V/f$.

## 6.2 Lamb waves in a lithium niobate plate

Now, the wave propagation is considered in a lithium niobate plate of sufficiently small thickness (with respect to the wavelengths), which should allow to distinctly observe Lamb modes. The thickness of plate is 0.5 mm.

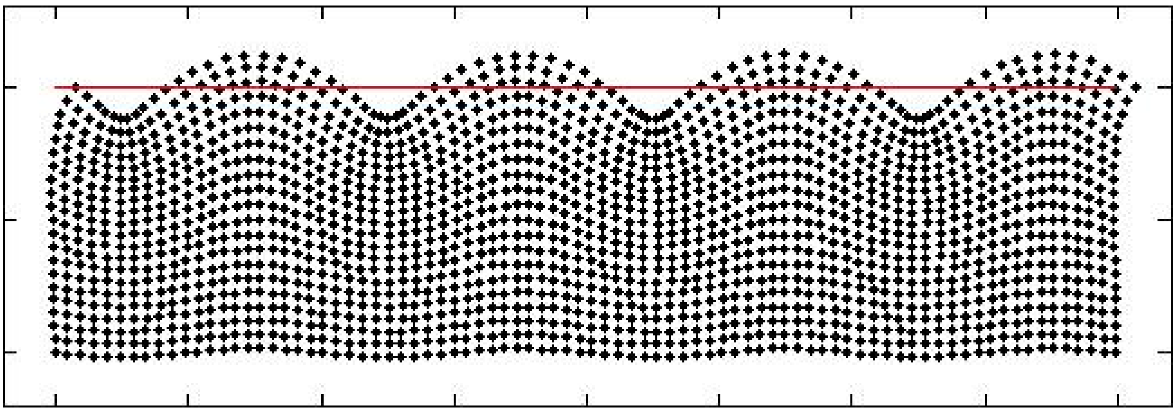


**FIGURE 15:** Rayleigh wave $\overline{\mathrm{R}}_2$ in lithium niobate (Y-cut, propagation along the Z-axis)

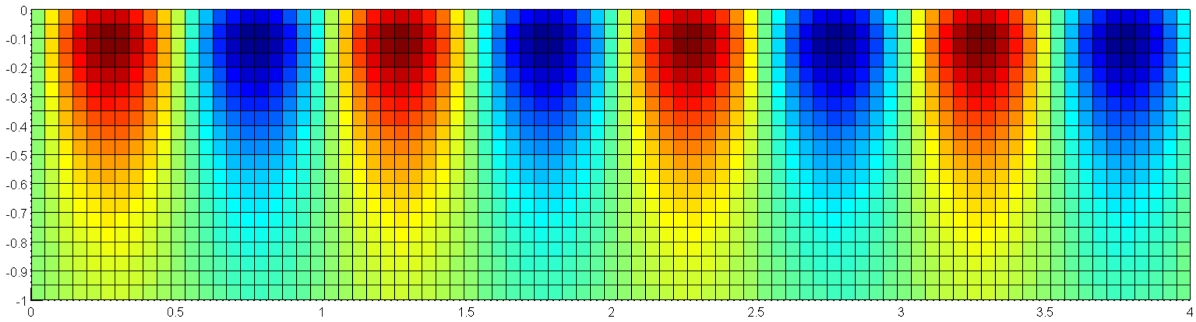


**FIGURE 16:** The electric potential of the associated electric field for the Rayleigh wave shown in Figure 15

Figure 17 shows findings of the velocities of Lamb waves propagating along the Z-axis in a Y-cut lithium niobate plate with thickness 0.5 mm. The found velocities are marked by the peaks. The results for two wave frequencies are shown, namely, for $f = 11.6$ MHz and $f = 15.0$ MHz. In the considered scope below $6$ km/s, four mode velocities were found for both cases (another modes may be found with higher velocities).

**Observations:**

- For both considered frequencies (see Figure 17), and in fact, for any frequency, the lowest wave velocity is slightly lower than the velocity of Rayleigh wave ($V = 3485$ m/s) propagating on the surface of the same Litium niobate material with the

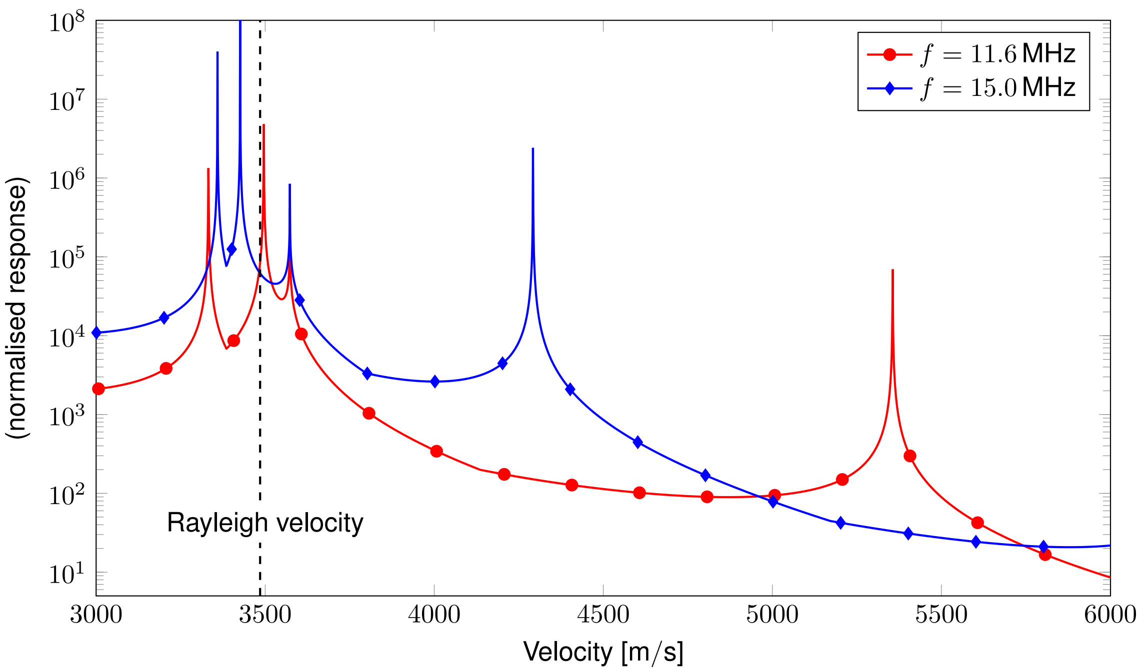



**FIGURE 17:** Findings of the velocities (marked by the peaks) of Lamb waves in a 0.5 mm-thick lithium niobate plate (Y-cut, propagation along the Z-axis): four modes are found (under $6$ km/s) for each of the considered frequencies

same cut and propagation direction.

- This lowest velocity is for the first Lamb mode which is antisymmetric, see Figure 18.
- The second velocity is found for a symmetric mode (see Figure 19) and it is – for any frequency – slightly higher than the velocity of the corresponding Rayleigh wave.
- The difference between the velocities of these first two modes is larger for lower frequencies (see Figure 17). When the frequency increases this difference decreases since the velocities for both modes are becoming closer to the Rayleigh velocity, i.e., the slower mode velocity increases and the faster mode velocity decreases.
- With the frequency increase, the corresponding wavelengths are getting shorter and may become much smaller that the plate thickness, so that in fact, eventually one may observe a practically independent, uncoupled propagation of two Rayleigh waves along both sides of the *comparatively* thick plate.

Figure 18 shows the first Lamb mode of propagation (i.e., with the slowest possible velocity) in the considered lithium niobate plate (Y-cut, propagation along the Z-axis); this mode is antisymmetric. Another antisymmetric mode for the same plate is shown in Figure 20; it is a higher-velocity mode.

The symmetric mode of Lamb wave propagation is presented in Figure 19; here, the plate motion in the sagittal plane (i.e., across the plate) as well as the motion of plate surface (i.e., ‘top view’) are shown to illustrate that for this cut and propagation direction (i.e., Y-cut, propagation along the Z-axis) the wave polarization is in the sagittal plane. This is true for any Lamb mode, in particular, for the modes presented in Figures 18

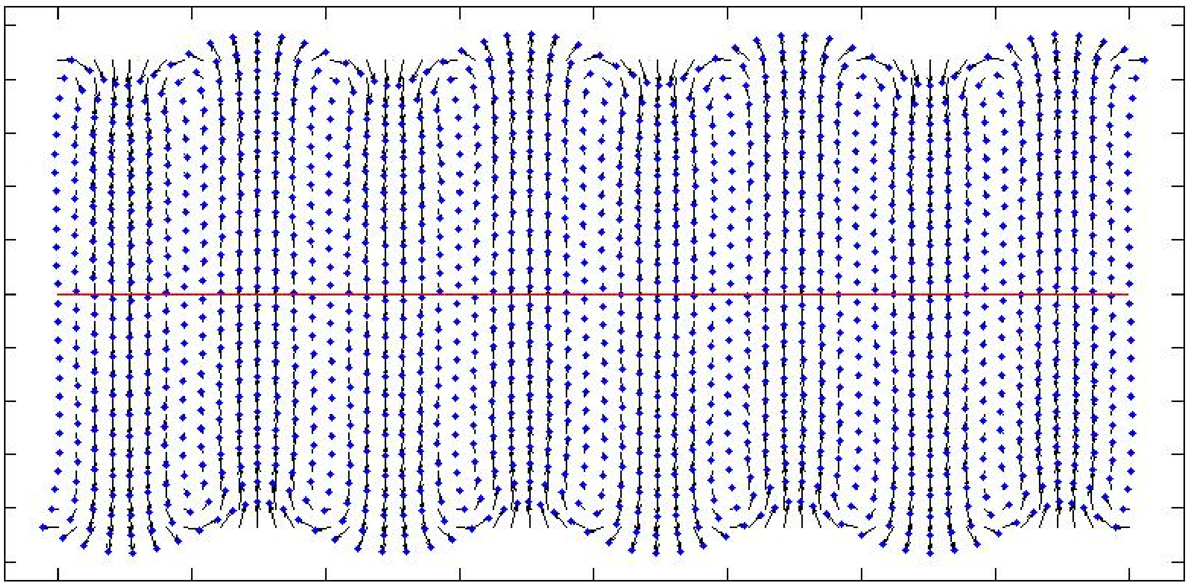



**FIGURE 18:** The first (antisymmetric) mode of Lamb wave in a 0.5 mm-thick lithium niobate plate (Y-cut, propagation along the Z-axis)

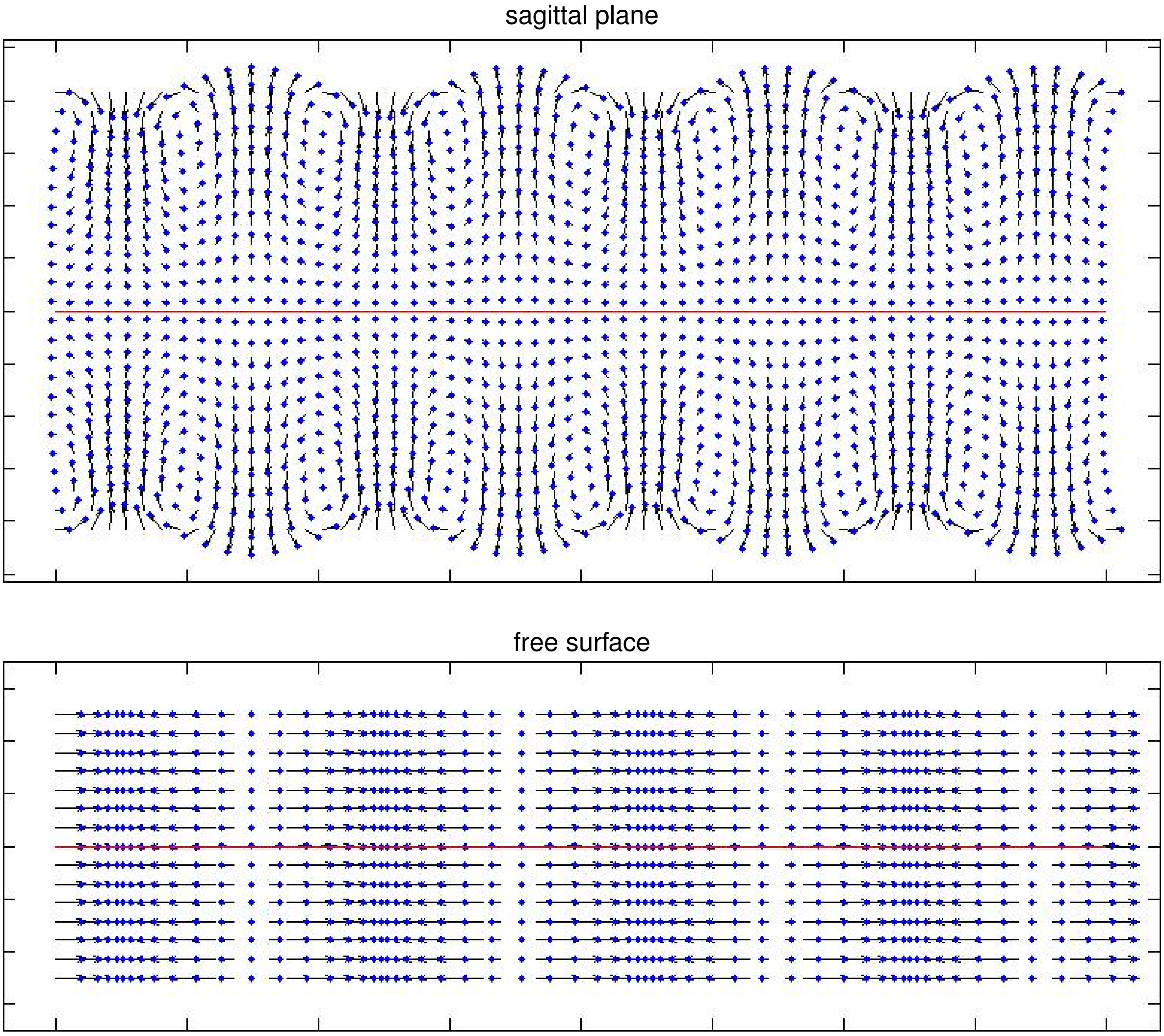



**FIGURE 19:** The second (the first symmetric) mode of Lamb wave in a 0.5 mm-thick lithium niobate plate (Y-cut, propagation along the Z-axis); the motion of free surface ('top view') shows that the wave is polarized in the sagittal plane

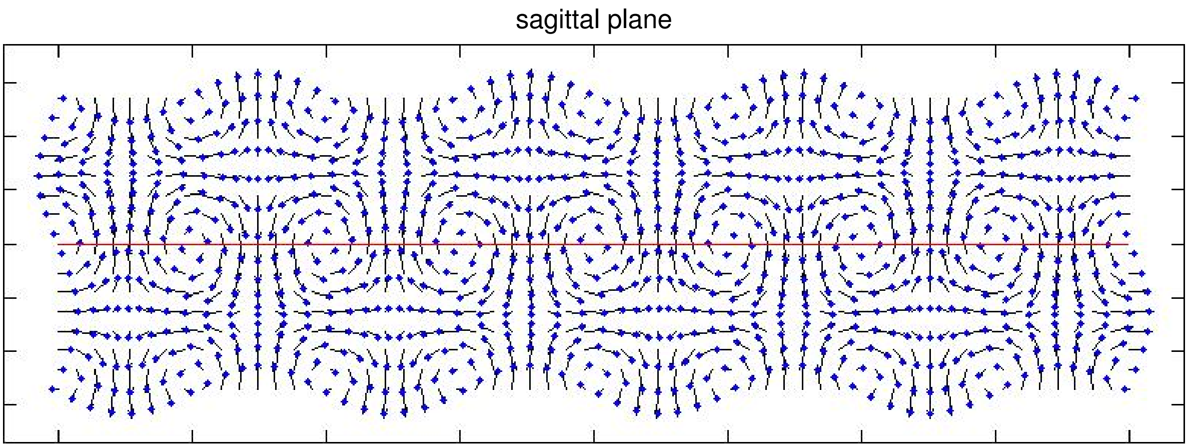



**FIGURE 20:** Another antisymmetric mode of Lamb wave in a 0.5 mm-thick lithium niobate plate (Y-cut, propagation along the Z-axis)

and 20.

The wave polarization is out of the sagittal plane for the lithium niobate cut at angle Y+128°. This is illustrated in Figure 21 where the first symmetric mode is presented (in fact, this is the second mode – the slowest mode is antisymmetric).

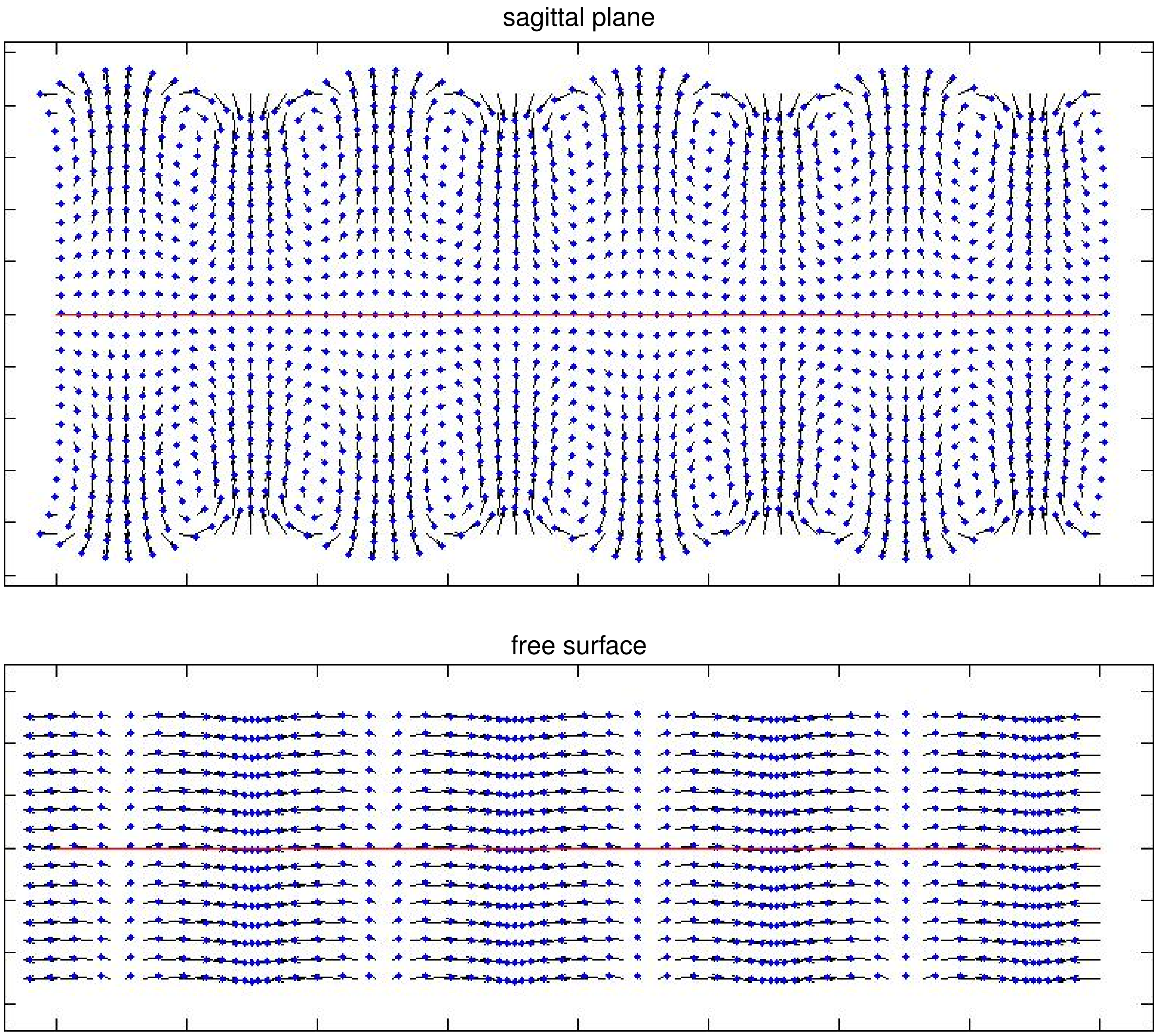



**FIGURE 21:** The second (the first symmetric) mode of Lamb wave in a 0.5 mm-thick lithium niobate plate cut at angle Y+128° (propagation along the Z-axis); the motion of free surface ('top view') clearly shows that the wave is the wave polarization is out of the sagittal plane