Bulk and Surface Acoustic Waves in Piezoelectric Media

Introductory Course on Multiphysics Modelling

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Outline

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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**.

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)

Outline

Piezoelectricity

(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**

Piezoelectricity

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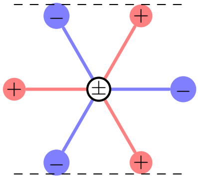
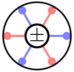
- **A simple molecular model** (of the direct piezoelectric effect)



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,
- as a result, an electrically neutral molecule appears.



neutral molecule

Piezoelectricity

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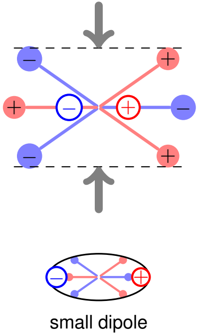

After exerting some pressure on the material:

- 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.

Piezoelectricity

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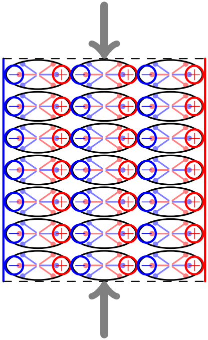


Eventually:

- 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.

Piezoelectricity

(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.

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

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.)

Piezoelectricity

(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.

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

- **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.

Piezoelectric equations

Elastodynamics

Equation of motion:

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

ρ – 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:

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

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

Constitutive relations for elasticity:

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

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

Boundary conditions:

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

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

Electrostatics

Gauss' law:

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

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

Maxwell's law:

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

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

Constitutive relations for dielectrics:

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

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

Boundary conditions:

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

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

Piezoelectric equations

- **Elastodynamics and electrostatics combined**

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

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

Kinematic relations and *Maxwell's law*:

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

Boundary conditions:

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

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

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

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

Piezoelectric equations

▶ Elastodynamics and electrostatics combined

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

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

Kinematic relations and *Maxwell's law*:

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

Boundary conditions: mechanical and electrical

▶ Piezoelectric coupling

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

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

$$\boldsymbol{D} = \underset{\text{direct effect}}{\boldsymbol{e} : \boldsymbol{S}} + \underset{\text{dielectricity}}{\boldsymbol{\epsilon} \cdot \boldsymbol{E}}$$

- $\boldsymbol{e}$ – 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 ($\boldsymbol{S} = \boldsymbol{0}$)

Piezoelectric equations in matrix notation

Voigt-Kelvin convention for index substitution:

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

This notation allows to represent:

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

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

$$\mathbb{T} = \begin{bmatrix} T_{11} & T_{22} & T_{33} & T_{23} & T_{31} & T_{12} \end{bmatrix}^{\mathsf{T}}$$

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

Piezoelectric equations in matrix notation

Voigt-Kelvin convention for index substitution:

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

$$\boldsymbol{c} \to \mathbb{c}_{(6\times 6)} \qquad \boldsymbol{e} \to \mathbb{e}_{(3\times 6)} \qquad \boldsymbol{\epsilon} \to \mathbb{\epsilon}_{(3\times 3)}$$

$$\boldsymbol{S} \to \mathbb{S}_{(6\times 1)} \qquad \boldsymbol{T} \to \mathbb{T}_{(6\times 1)} \qquad \boldsymbol{u}, \boldsymbol{D}, \boldsymbol{E} \to \mathbb{u}_{(3\times 1)}, \mathbb{D}_{(3\times 1)}, \mathbb{E}_{(3\times 1)}$$

- Constitutive relations:

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

- Kinematic relations and Maxwell's law:

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

- Sourceless field equations:

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

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

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

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

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

Outline

Crystalline materials

- 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).

Crystalline materials

The law of constant angles

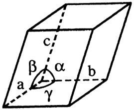
The normals to the crystal faces, drawn from a fixed point, form a geometrically invariant figure (the relative orientation of the faces is constant, although the crystal can be developed in very different forms).

- 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**.
- The atomic structure of crystal is determined by the **lattice** and the **atomic group** (a group of atoms) assigned to each node:

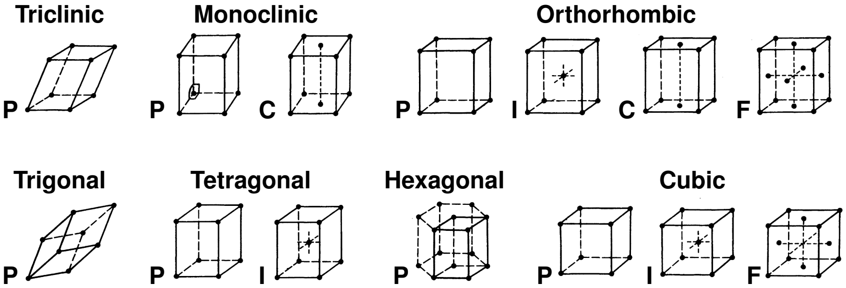
$$\textbf{Crystal} = \textbf{Lattice} + \textbf{Atomic group}$$

Crystalline materials

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	$\alpha = \beta = \gamma = 90^\circ$	$a = b = c$



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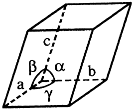

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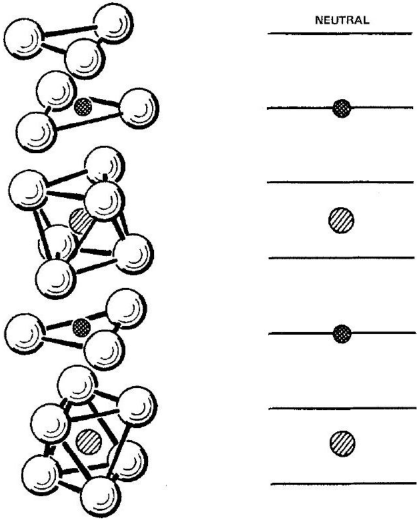
- The crystal symmetry is at most equal to that of the lattice $\rightarrow$ a crystal does not necessarily possesses a centre of symmetry.
- There are **32 point symmetry classes of crystals**.

Example: Lithium niobate ($LiNbO_3$)

Features:

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

To the right: Positions of the lithium and niobium atoms (double and singe cross-hatched circles, respectively) with respect to the oxygen octahedra



paraelectric

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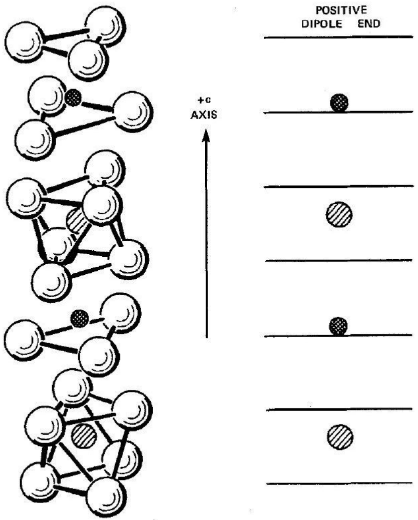
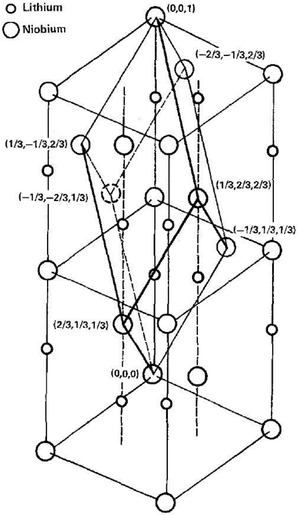
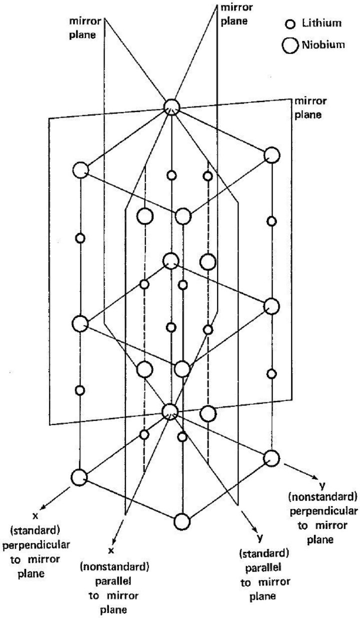


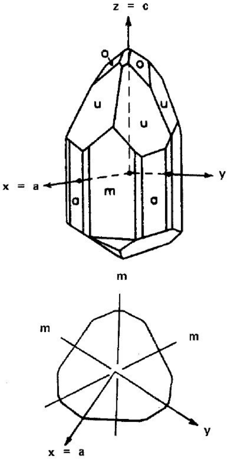
ferroelectric

Example: Lithium niobate ($LiNbO_3$)

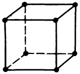
Orientations of the principal axes and the planes of mirror symmetry



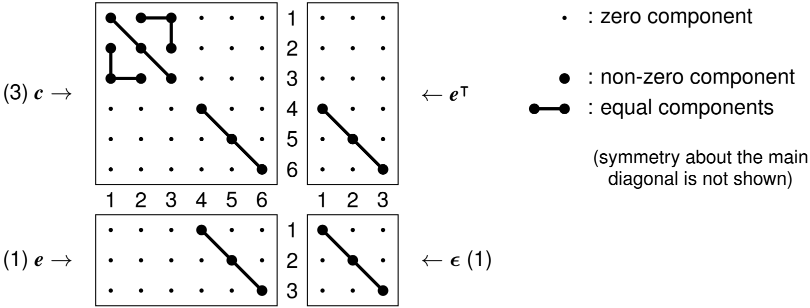




Constitutive matrices (for some classes of anisotropy)



Cubic system – class $\bar{4}3m$

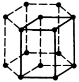


Materials:

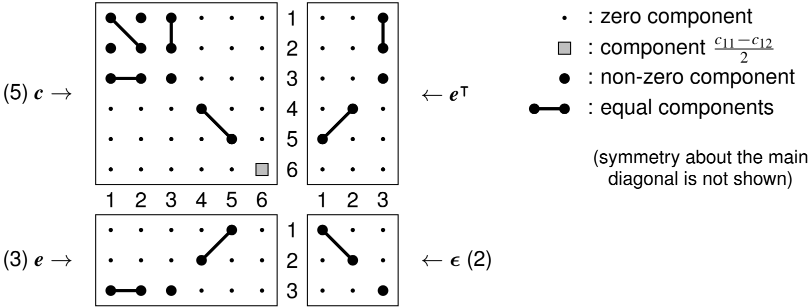
Gallium arsenide (GaAs) – class $\bar{4}3m$,

Bismuth and germanium oxide ($Bi_{12}GeO_{20}$) – class 23

Constitutive matrices (for some classes of anisotropy)

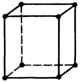


Hexagonal system – class 6mm



Materials:
Zinc oxide (ZnO), Cadmium sulphide (CdS), Ceramic PZT-4

Constitutive matrices (for some classes of anisotropy)



Orthorhombic system – class 2mm

(9) $c \rightarrow$ (left block, rows 1–6) and $\leftarrow e^{\mathsf{T}}$ (right block)

	1	2	3	4	5	6		1	2	3
1	●	●	●	·	·	·		·	·	●
2	●	●	●	·	·	·		·	·	●
3	●	●	●	·	·	·		·	·	●
4	·	·	·	●	·	·		·	●	·
5	·	·	·	·	●	·		●	·	·
6	·	·	·	·	·	●		·	·	·

(5) $e \rightarrow$ (left block, rows 1–3) and $\leftarrow \epsilon$ (3) (right block)

	1	2	3	4	5	6		1	2	3
1	·	·	·	·	●	·		●	·	·
2	·	·	·	●	·	·		·	●	·
3	●	●	●	·	·	·		·	·	●

· : zero component

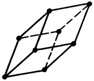
● : non-zero component

(symmetry about the main diagonal is not shown)

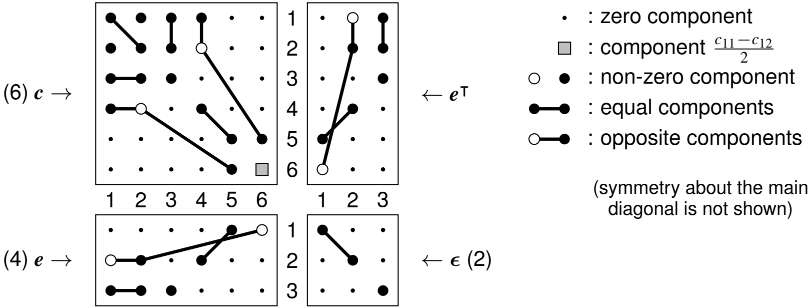
Materials:

Barium sodium niobate ($Ba_2NaNb_5O_{15}$)

Constitutive matrices (for some classes of anisotropy)



Trigonal system – class 3m



Materials:

Lithium niobate ($LiNbO_3$), Lithium tantalate ($LiTaO_3$)

Outline

Bulk acoustic waves in piezoelectric media

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 $\boldsymbol{x}$ and time t:

$$u_1 \equiv u(\boldsymbol{x},t) = A_u\,\mathcal{E}(\boldsymbol{x},t), \quad u_2 \equiv v(\boldsymbol{x},t) = A_v\,\mathcal{E}(\boldsymbol{x},t), \quad u_3 \equiv w(\boldsymbol{x},t) = A_w\,\mathcal{E}(\boldsymbol{x},t),$$

and for the electric potential:

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

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

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

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

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

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

Bulk acoustic waves in piezoelectric media

Using the Kelvin-Voigt notation, the mechanical strain and electric field vectors are expressed as

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

Notice that the polarization of electric field is longitudinal. The constitutive relations for the stress and electric displacement vectors are

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

When all these formulas are used for the field equations: $\boldsymbol{\nabla}\mathbb{T} - \rho\ddot{\mathbb{u}} = \mathbb{0}$ and $\nabla^\mathsf{T}\mathbb{D} = 0$, the following set of equations describing the plane wave propagation in piezoelectric media is obtained.

Equations for plane wave propagation in piezoelectric media

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

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

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

Bulk acoustic waves in piezoelectric media

Equations for plane wave propagation in piezoelectric media

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

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

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

The last equation in the set gives the following formula:

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

Christoffel matrix equation

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

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

Bulk acoustic waves in piezoelectric media

Christoffel matrix equation

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

***Observations*:**

- The **polarization is eigenvector of the Christoffel tensor** (matrix) $\mathbb{G}$ with eigenvalue ρV^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**.

Bulk acoustic waves in piezoelectric media

Christoffel matrix equation

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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.

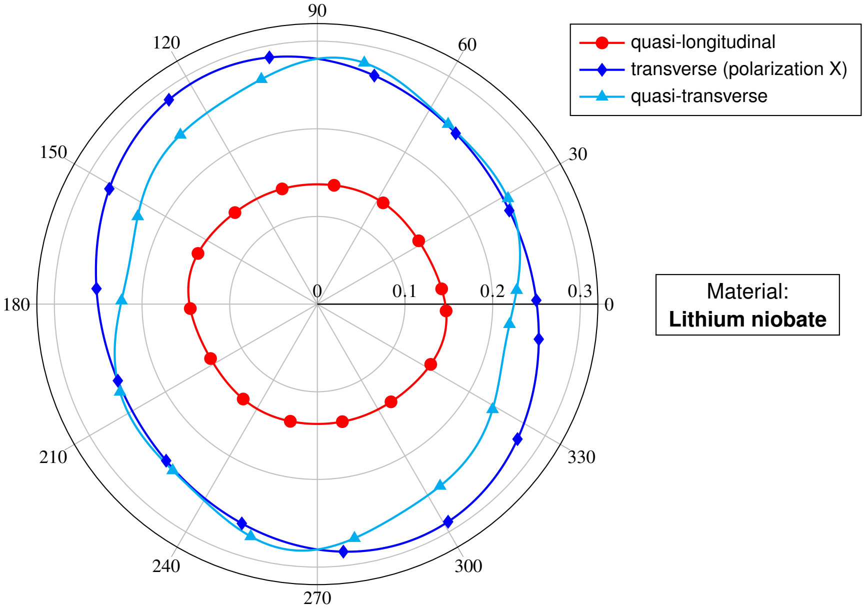
Characteristic surfaces

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**.

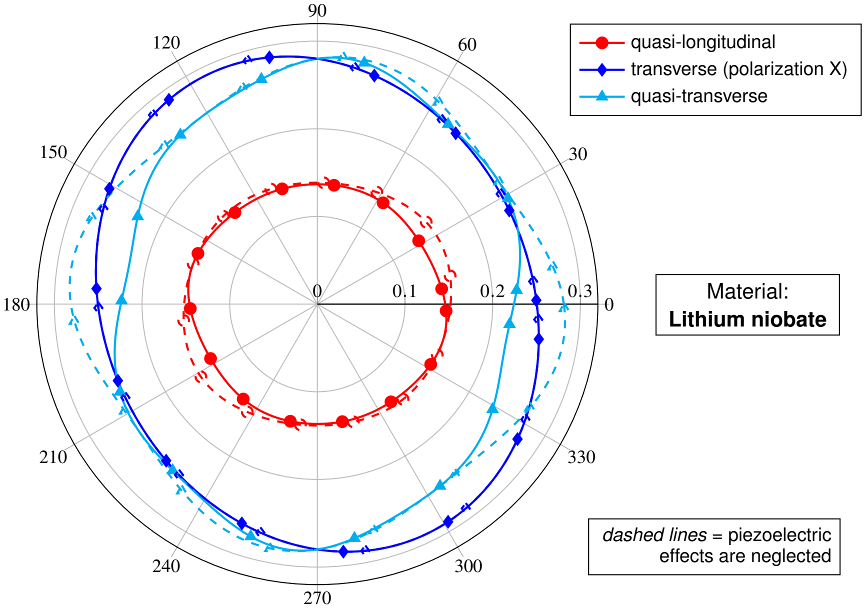
The wave surface is defined by the end of the **energy velocity vector** $V^{\mathrm{e}}(\boldsymbol{n})$, drawn from the origin, as the propagation direction $\boldsymbol{n}$ varies. It is an **equi-phase surface** and describes the points reached, at unit time, by the vibrations (energy) emitted at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

Characteristic surfaces (slowness surfaces [s/km] in the YZ-plane)



Material:
Lithium niobate

Characteristic surfaces (slowness surfaces [s/km] in the YZ-plane)



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dashed lines = piezoelectric effects are neglected

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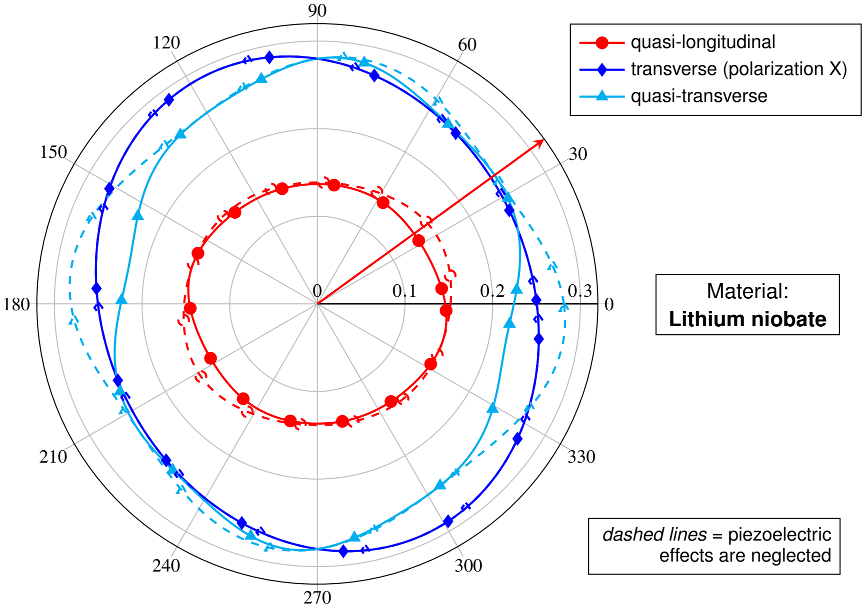

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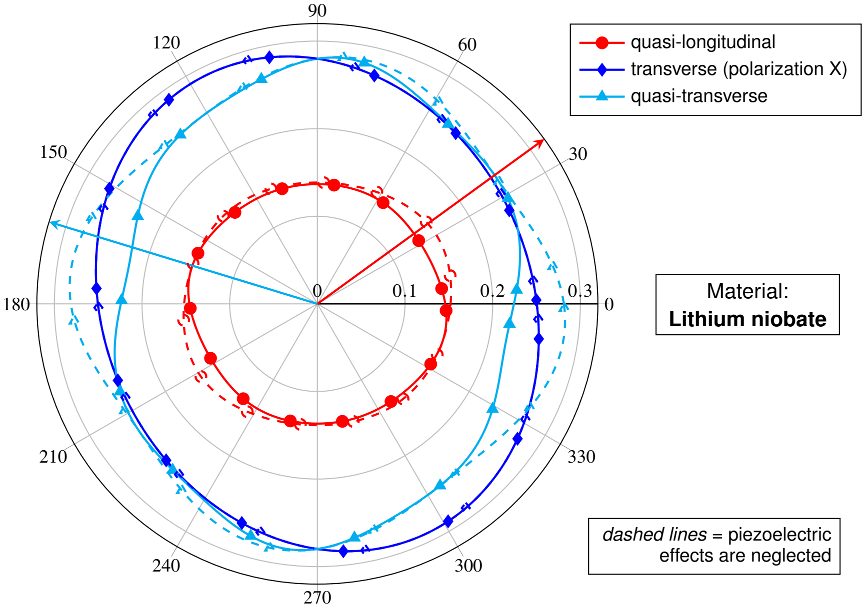
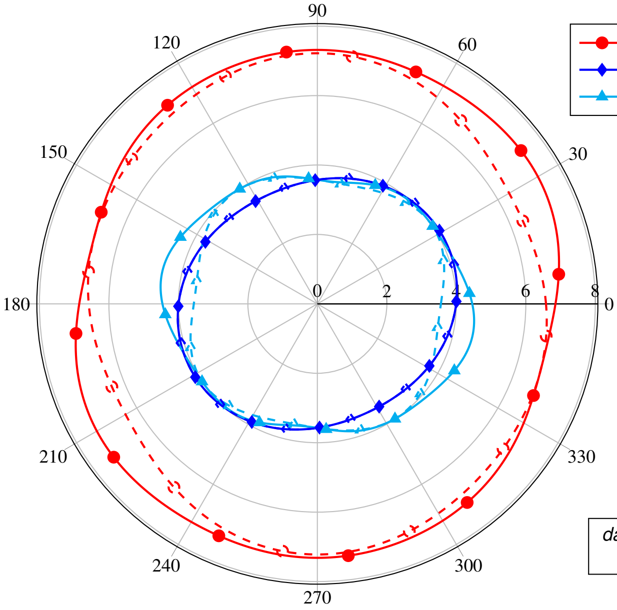


Material:
Lithium niobate

dashed lines = piezoelectric effects are neglected

Characteristic surfaces (velocity surfaces [km/s] in the YZ-plane)



Material:
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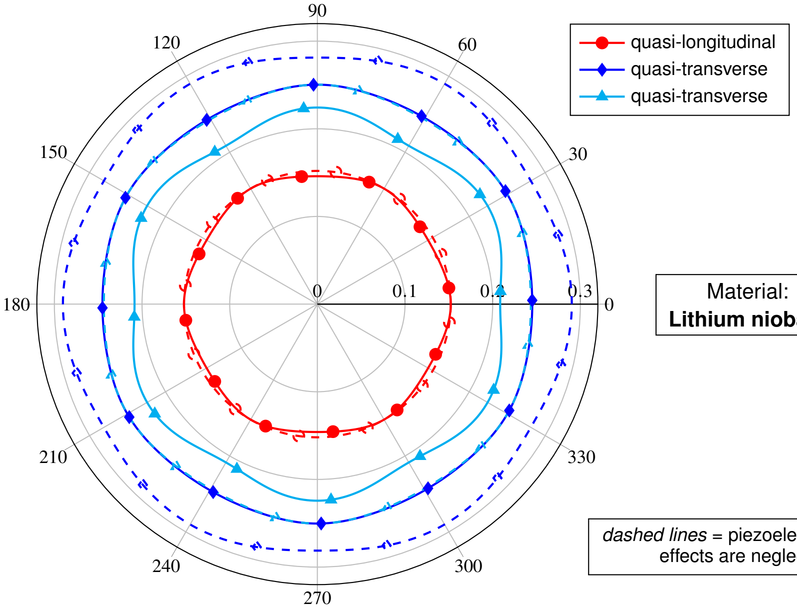
Characteristic surfaces (slowness surfaces [s/km] in the XY-plane)



Material:
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Outline

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 set on another elastic solid (of higher acoustic wave velocity)
- **Stoneley waves** – waves travelling along solid-fluid or solid-solid interfaces

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► **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.

Partial waves (for SAW)

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

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

ω is the angular frequency, k is the wavenumber, and β is a constant value which defines the direction of propagation in the XZ-plane. Therefore:

$$\mathcal{F}(.) = \exp\left[\mathrm{i}k(.)\right], \qquad \mathcal{F}'(.) = \mathrm{i}k\mathcal{F}(.).$$

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

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

Partial waves (for SAW)

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

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ω is the angular frequency, k is the wavenumber, and β is a constant value which defines the direction of propagation in the XZ-plane. Therefore, the strain, electric field, stress, and electric displacement vectors are

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

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

and the final set of equations is as follows.

Plane harmonic wave propagation in piezoelectric media

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

Partial waves (for SAW)

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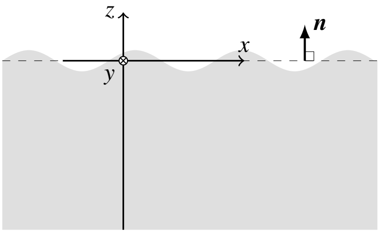
- This **plane-wave eigensystem** depends now also on β.
- Eigenproblem is solved for β with V treated as parameter. The secular equation is an 8th-order polynomial (or a 6th-order polynomial for purely elastic media).
- The 8 eigenvalues and eigenvectors form 8 **partial waves**. In case of the Rayleigh wave, 4 of them are discarded on the basis of boundary conditions at $-\infty$.
- The solution is a linear combination of partial waves which are coupled by the **boundary conditions** on the surface(s). 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.

Rayleigh waves

A Rayleigh wave propagates along the surface of a medium.



Mechanical boundary conditions:

$$\text{for } z \to -\infty : \quad \boldsymbol{u} = \boldsymbol{0}$$
$$\text{for } z = 0 : \quad \boldsymbol{T} \cdot \boldsymbol{n} = \boldsymbol{0}$$

Electrical boundary conditions:

$$\text{for } z \to -\infty : \quad \phi = 0$$
$$\text{for } z = 0 : \quad \boldsymbol{D} \cdot \boldsymbol{n} = 0$$

Rayleigh waves

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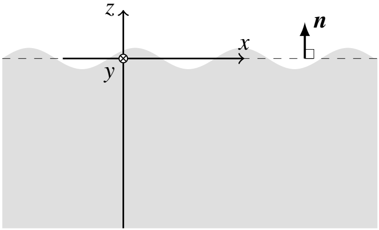
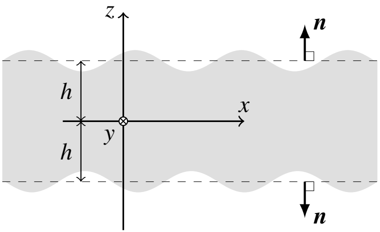


Features:

- 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**.

Lamb waves

Lamb waves are driven by a plate of finite thickness.



Mechanical boundary conditions:

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

Electrical boundary conditions:

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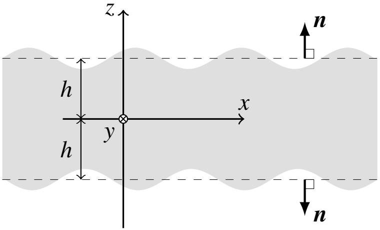

Features:

- 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).

Decoupling of Rayleigh-type piezoelectric waves

1. When the sagittal plane is normal to a direct binary axis of crystal, there exists the possibility for:
   - a non-piezoelectric Rayleigh wave R_2 polarized in this plane $(u_2 = 0)$,
   - a piezoelectric transverse horizontal wave $\overline{\text{TH}}$ (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 $\overline{R}_2$ 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.

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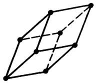
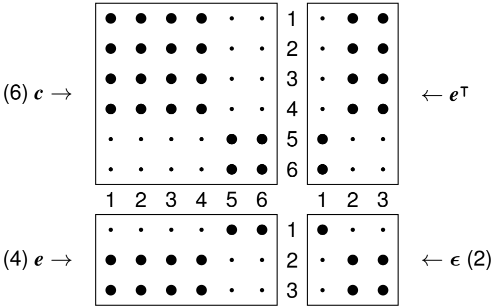
- The symmetries of these two cases can be satisfied only for **orthorhombic**, **tetragonal**, **hexagonal**, and **cubic** crystals. With respect to the crystallographic axes there are **16 possible combinations**, that is, orientations of the propagation direction x_1 and the sagittal plane normal 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).

Decoupling of Rayleigh-type piezoelectric waves



Trigonal system – class 3m – rotated around X-axis



· : zero component

● : non-zero component

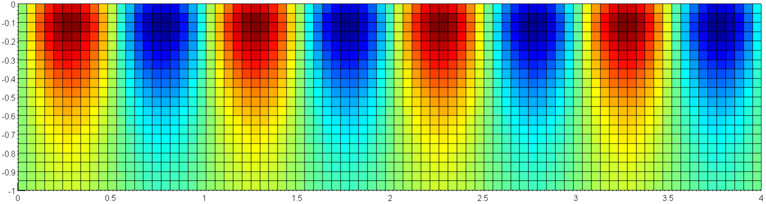
(interdependencies are not shown)

Outline

Example 1: Rayleigh wave

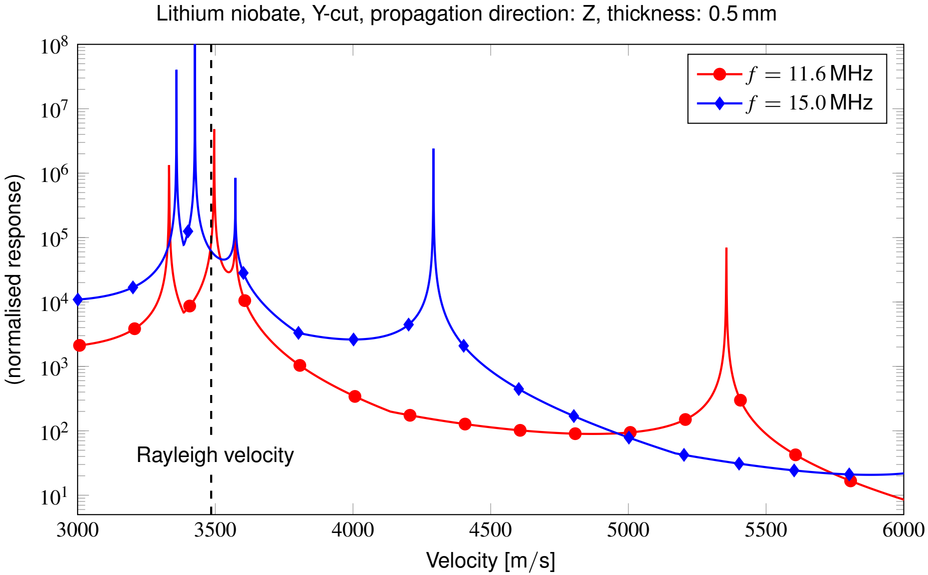
Rayleigh wave $\overline{\mathrm{R}}_2$ (Litium niobate, Y-cut, propagation-Z, velocity: **3485** m/s)

Electric potential of the associated electric field (phase angle: $0°$)



Example 2: Lamb waves

Wave velocities ($LiNbO_3$ Y-cut, propagation direction Z)



Example 2: Lamb waves

Antisymmetric modes ($LiNbO_3$ Y-cut, propagation direction Z)

1st antisymmetric mode (sagittal plane)

another antisymmetric mode (sagittal plane)

Example 2: Lamb waves

Symmetric mode ($LiNbO_3$ Y-cut, propagation direction Z)

sagittal plane

the wave polarization is in the sagittal plane

free surface

Example 2: Lamb waves

Symmetric mode ($LiNbO_3$ Y+128°-cut, propagation direction X)

sagittal plane

the wave polarization is OUT of the sagittal plane

free surface