Acoustic and Optical Phonon Field Couplings in Piezoelectric Semiconductors

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Outline

- Elastic Equations for a Cubic Crystal
- Coupled Acoustic and Optical Phonons in Piezoelectric Materials
- Boundary Conditions
- New Results
- Acoustic Dispersion and Anisotropy
- Results
- Summary

Constitutive Stress-Strain Relations

$$
\begin{aligned}
T_1 &= c_{11}S_1 + c_{12}S_2 + c_{12}S_3, \\
T_2 &= c_{12}S_1 + c_{11}S_2 + c_{12}S_3, \\
T_3 &= c_{12}S_1 + c_{12}S_2 + c_{11}S_3, \\
T_4 &= c_{44}S_4 - e_{14}E_1,\ T_5 = c_{44}S_5 - e_{14}E_2,\ T_6 = c_{44}S_6 - e_{14}E_3, \\
D_1 &= \epsilon_{11}E_1 + e_{14}S_4,\ D_2 = \epsilon_{11}E_2 + e_{14}S_5,\ D_3 = \epsilon_{11}E_3 + e_{14}S_6. \qquad (1)
\end{aligned}
$$

T_I : Stress tensor (in Voigt notation)
S_I : Strain tensor (in Voigt notation)
E_i : Electric field ($i = 1$ for x etc.)
c_{IJ} : Stiffness tensor
ϵ_{ij} : Permittivity tensor
e_{iJ} : Piezoelectric e tensor

Strain and Displacement

$$S_1 = \frac{\partial u_x}{\partial x},\ S_2 = \frac{\partial u_y}{\partial y},\ S_3 = \frac{\partial u_z}{\partial z},$$
$$S_4 = \frac{\partial u_y}{\partial z} + \frac{\partial u_z}{\partial y},\ S_5 = \frac{\partial u_x}{\partial z} + \frac{\partial u_z}{\partial x},$$
$$S_6 = \frac{\partial u_x}{\partial y} + \frac{\partial u_y}{\partial x}. \tag{2}$$

u_i : Displacement

We assume the in-plane phonon wavevector is directed along the x axis and low frequencies (quasi-static approximation)

$$\mathbf{u}(\mathbf{r}, t) = e^{iq_x x}\mathbf{u}_n(q_x, z),$$
$$\mathbf{E} = -\nabla\phi. \tag{3}$$

and get

$$\begin{aligned}
\left(-q_x^2 c_{11} + c_{44}\frac{\partial^2}{\partial z^2} + \rho\omega^2\right) u_x + iq_x\left(c_{12}+c_{44}\right)\frac{\partial u_z}{\partial z} &= 0,\\
\left(-q_x^2 c_{44} + c_{44}\frac{\partial^2}{\partial z^2} + \rho\omega^2\right) u_y + 2iq_x e_{14}\frac{\partial \phi}{\partial z} &= 0,\\
iq_x\left(c_{12}+c_{44}\right)\frac{\partial u_x}{\partial z} + \left(-q_x^2 c_{44} + c_{11}\frac{\partial^2}{\partial z^2} + \rho\omega^2\right) u_z &= 0,\\
2iq_x e_{14}\frac{\partial u_y}{\partial z} + \epsilon_{11}\left(q_x^2 - \frac{\partial^2}{\partial z^2}\right)\phi &= 0.
\end{aligned} \tag{4}$$

Phonons in a GaAs Slab

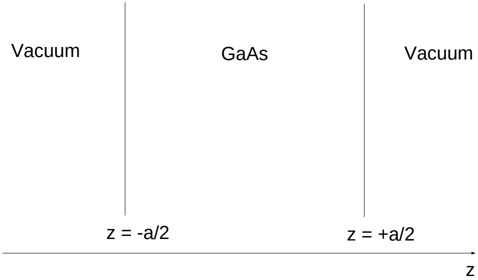

Figure: Schematic drawing of a GaAs slab embedded in semi-infinite layers of vacuum. The slab thickness is a.

Phonons in a GaAs Slab

Two solution types (I and II) exist for $u_x - u_z$ coupled acoustic phonons.
For type I:

$$u_x = \sum_{j=1}^{2} A_{x,j} \cos \gamma_j z, \;\; u_z = \sum_{j=1}^{2} A_{z,j} \sin \gamma_j z, \tag{5}$$

Similarly two solution types (I and II) exist for $u_y - \phi$ coupled acousto-optical phonons.
For type I:

$$\begin{aligned} u_y &= A_{y,1} \cos\left(\delta_1 z\right) + A_{y,2} \cosh\left(\delta_2 z\right), \\ \phi &= A_{\phi,1} \sin\left(\delta_1 z\right) + A_{\phi,2} \sinh\left(\delta_2 z\right), \end{aligned} \tag{6}$$

Electric Field

For vacuum the Maxwell-Poisson equation becomes ($|z| > a/2$),

$$-\epsilon_0 \nabla^2 \phi = \epsilon_0 \left(q_x^2 - \frac{\partial^2}{\partial z^2} \right) \phi = 0, \tag{7}$$

and

$$\begin{aligned} \phi(z) &= \phi_+ e^{-|\mathbf{q}_\parallel| z} e^{i\mathbf{q}_\parallel \cdot \mathbf{r}} \text{ if } z > a/2, \\ \phi(z) &= \phi_- e^{|\mathbf{q}_\parallel| z} e^{i\mathbf{q}_\parallel \cdot \mathbf{r}} \text{ if } z < -a/2. \end{aligned} \tag{8}$$

Mechanical and Electric Interface Conditions

$$T_{xz}(z = \pm a/2) = 0; \; T_{zz}(z = \pm a/2) = 0. \tag{9}$$

$$T_{yz}(z = \pm a/2) = c_{44}\frac{\partial u_y}{\partial z} + e_{14}\frac{\partial \phi}{\partial x}|_{z=\pm a/2} = 0, \tag{10}$$

$$\mathbf{E}_{\parallel} \text{ continuous,} \tag{11}$$

$$\mathbf{D}_{\perp} \text{ continuous.} \tag{12}$$

Optical Phonons

Optical phonon modes are determined from the ionic displacement:

$$\mathbf{u}_{ion} = \mathbf{u}_{+} - \mathbf{u}_{-}, \tag{13}$$

and can be found from the Born-Huang equations

$$\mathbf{u}_{ion} = -\sqrt{\frac{\Omega}{m_r}} \frac{\sqrt{\epsilon(0) - \epsilon(\infty)}\omega_{TO}}{\omega^2 - \omega_{TO}^2} \mathbf{E}. \tag{14}$$

Ω: Unit cell volume
m_r: Unit cell reduced mass

Coupled Acousto-Optic Phonon Normalization

$$\int d\mathbf{r} \left[\sqrt{\frac{m_r}{\Omega}} \mathbf{u}^*_{ion}(\mathbf{r}, t) \right] \left[\sqrt{\frac{m_r}{\Omega}} \mathbf{u}_{ion}(\mathbf{r}, t) \right] + \int d\mathbf{r} \, [\sqrt{\rho} \mathbf{u}^*(\mathbf{r}, t)] \, [\sqrt{\rho} \mathbf{u}(\mathbf{r}, t)] = \frac{\hbar}{2\omega_n}. \tag{15}$$

ω_n : Phonon mode frequency

Proof I: Coupled $u_y - \phi$ modes cannot exist at the LO phonon frequency in piezoelectric materials

In this case $\epsilon = 0$ and:

$$u_y = A_y e^{iq_x x}, \tag{16}$$

and

$$\phi = (\phi_0 + \phi_1 z)\, e^{iq_x x}; \quad \phi_0 = \phi_1 = 0. \tag{17}$$

Continuity of the transverse electric field component:

$$\phi_+ = \phi_- = 0. \tag{18}$$

Continuity in the normal electric displacement:

$$A_y = 0. \tag{19}$$

The electric potential ϕ and the phonon u_y component are both zero.
New Result: It is not possible to excite coupled $u_y - \phi$ modes at the LO phonon frequency in piezoelectric materials!

Proof II: Confined coupled acousto-optical $u_y - \phi$ modes cannot exist in piezoelectric media except at certain discrete q_x wavenumber values

A confined phonon mode is characterized by an electric field that vanishes at the slab interfaces (for type I):

$$u_y = A_y \cos\left(\frac{m\pi}{a} z\right) e^{iq_x x}; \quad \phi = A_\phi \sin\left(\frac{m\pi}{a} z\right) e^{iq_x x}, \qquad (20)$$

where $m = 2, 4, 6, \ldots$.

From the elastic equations:

$$\left(-q_x^2 c_{44} - \left(\frac{m\pi}{a}\right)^2 c_{44} + \rho\omega^2\right) A_y + 2iq_x e_{14} \left(\frac{m\pi}{a}\right) A_\phi = 0, \qquad (21)$$

and from the Maxwell-Poisson equation:

$$-2iq_x e_{14} \left(\frac{m\pi}{a}\right) A_y + \epsilon_{11} \left(q_x^2 + \left(\frac{m\pi}{a}\right)^2\right) A_\phi = 0. \qquad (22)$$

Proof II...

Hence the possible mode frequencies are

$$\omega_m = \sqrt{\frac{c_{44}}{\rho}} \left[q_x^2 + \left(\frac{m\pi}{a}\right)^2 + \frac{4q_x^2 e_{14}^2 \left(\frac{m\pi}{a}\right)^2}{\epsilon_{11} c_{44} \left(q_x^2 + \left(\frac{m\pi}{a}\right)^2\right)} \right]^{1/2} . \qquad (23)$$

Continuity in the transverse electric field and normal displacement yield $\phi_+ = 0$ and

$$A_\phi = \frac{i q_x e_{14}}{\epsilon_{11} \left(-1\right)^{m/2} \left(\frac{m\pi}{a}\right)} A_y . \qquad (24)$$

Combining Eqs. (22) and (24):

$$2\left(-1\right)^{m/2} \left(\frac{m\pi}{a}\right)^2 = q_x^2 + \left(\frac{m\pi}{a}\right)^2 , \qquad (25)$$

New Result: Possible only at certain discrete q_x values $\{q_{x,m}\}$!

Degree of anisotropy for GaAs

$$\alpha = \left| \frac{\frac{c_{11}-c_{12}}{2} - c_{44}}{c_{44}} \right| = 45\% \ . \qquad (26)$$

Dispersion I

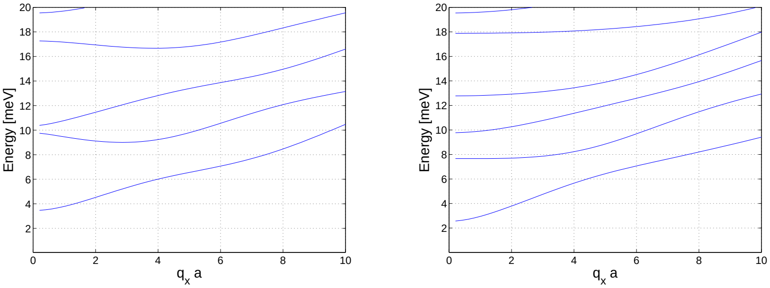

Figure: Dispersion relations for the coupled $u_x - u_z$ acoustic phonon modes of a 2 nm GaAs slab. (Left plot) GaAs and (right plot) GaAs but using the isotropic assumption: $c_{44} = \frac{c_{11} - c_{12}}{2} = 3.25 \cdot 10^{10}$ Pa. The first axis is $q_x a$ and the second axis the phonon band energy in meV.

Dispersion II

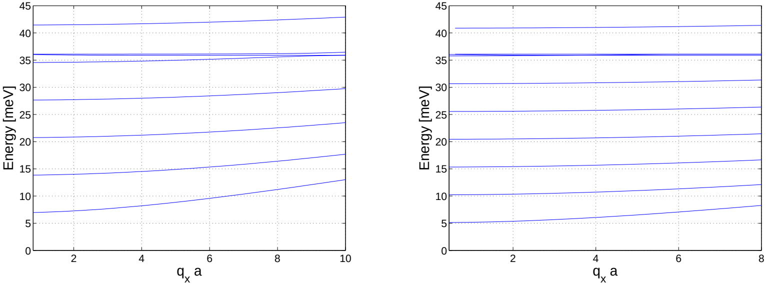

Figure: Dispersion relations for the coupled $u_y - u_{ion}$ acousto-optical phonon modes of a 2 nm GaAs slab. (Left plot) GaAs including piezoelectricity and anisotropy and (right plot) GaAs but using the isotropic non-piezoelectric assumption: $c_{44} = \frac{c_{11} - c_{12}}{2} = 3.25 \cdot 10^{10}$ Pa and $e_{14} = 0$.

Conclusion

- New model for coupled acousto-optic phonons in zincblende crystals
- Pure $u_x - u_z$ acoustic phonon modes exist
- Pure $u_y - u_{ion}$ acousto-optic phonon modes exist
- Proof 1: Coupled $u_y - u_{ion}$ modes cannot exist at the LO phonon frequency in piezoelectric materials
- Proof 2: Confined coupled acousto-optical $u_y - u_{ion}$ modes cannot exist in piezoelectric media except at certain discrete q_x wavenumber values