Polariton resonances in multilayered piezoelectric superlattices

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Abstract. Coupled electro-elastic SH waves propagating in a periodic piezoelectric finite-length superlattice with identical piezoelectric materials in a unit cell are considered in the framework of the full system of Maxwell's electrodynamic equations. In the long wavelength region, coupling between electro-magnetic and elastic waves creates frequency band gaps. It is shown that for piezoelectric superlattice at acoustic frequencies, acousto-optic coupling gives rise to polariton behavior at wavelengths much larger than the length of the unit cell. The results of the paper may be useful in design of narrow band filters or multi-channel piezoelectric filters.

1. Introduction
The interaction of waves with periodic structures, especially artificial superlattices, has recently attracted much attention. A periodic modulation of the dielectric or elastic material properties leads to absolute stop bands and ultimate control of propagation of waves in the structure. A piezoelectric or piezomagnetic superlattice made of a periodically domain-inverted dielectric crystal with periodically modulated piezoelectric or piezomagnetic coefficients, but a homogeneous refractive index, can be considered as a one-dimensional diatom ionic crystal with positive and negative ions arranged periodically [1]. The coupling between transverse lattice vibrations and electro-magnetic waves in an ionic crystal can lead to phonon polariton coupling with possible stop bands in the infrared region [2]. Analogously, piezoelectric and piezomagnetic periodic structures with periodicity of the lattice expanded from an atomic scale to microns can exhibit similar coupling and resonant band gap structure in the microwave region [3–7]. This coupling between the electromagnetic wave and the superlattice vibration takes place in the long wavelength region, where the superlattice can be considered as a deep subwavelength artificial material. Using the long wavelength approximation, it has been shown that the piezoelectric superlattice exhibits a new type of polariton, in which the resonance frequency is determined by the period of the superlattice and negative effective permittivity occurs near the high frequency side of resonance [8, 9]. Theoretical and experimental work has suggested that a different type of polariton is also possible in a piezoelectric superlattice that is coupling of electro-magnetic waves with longitudinal superlattice vibrations [10].

While the long-wave approximation only reveals the phonon-photon polariton at high acoustic frequencies in the middle of the Brillouin zone, the analytical solution shows that the coupling of photons and phonons is also possible at optical frequencies in the whole Brillouin zone [11, 12]. It also reveals a phonon-polariton gap in a piezoelectric phononic crystal with a unit cell made of
different constituent materials. The similarities and differences between artificial superlattices and real lattices suggest rich physics in artificial microstructures and gives a possibility to control and manipulate both photons and phonons simultaneously [10, 13].

The problem is more interesting in a periodic superlattice with full contact interfaces. The system in this case is described by two coupled electro-acoustic waves and exhibits a very interesting acousto-optic resonance (phonon-polariton) at high acoustic frequencies which cannot be observed in the previous problem. The dynamic setting for Maxwell’s equation, where both the optical effect and the effect from the rotational part of the electric field are taken into account, permits investigating this problem as well.

2. Statement of the problem
We investigate the reflection/transmission properties of a finite stack of transversely isotropic hexagonal piezoelectric crystals (6 mm), a periodically stratified piezoelectric crystal with the crystallographic axes directed along the $Oz$ direction (figure 1).

The anti-plane problem of interconnected elastic and electro-magnetic excitations can be written in terms of the variables $E_y(x, y)$, $u_z(x, y)$, $H_z(x, y)$, and $\sigma_{xz}(x, y)$ for which the interface boundary conditions are applied:

$$\frac{\partial u_z}{\partial x} = \sigma_{xz}G + \frac{e_{15}}{i\omega G\varepsilon_{11}} \frac{\partial H_z}{\partial y}, \quad (1)$$

$$\frac{\partial E_y}{\partial x} = -\frac{e_{15}}{G\varepsilon_{11}} \frac{\partial \sigma_{xz}}{\partial y} + \left(\frac{c_{44}}{i\omega G\varepsilon_{11}} \frac{\partial^2 H_z}{\partial y^2} - \frac{i\omega \mu_{33} H_z}{G}\right), \quad (2)$$

$$\frac{\partial \sigma_{xz}}{\partial x} = e_{15} \frac{\partial E_y}{\partial y} - \left(c_{44} \frac{\partial^2 u_z}{\partial y^2} + \rho \omega^2 u_z\right), \quad (3)$$

$$\frac{\partial H_z}{\partial x} = -i\omega \varepsilon_{11} E_y - i\omega e_{15} \frac{\partial u_z}{\partial y}, \quad G = c_{44} + \frac{e^2}{\varepsilon}. \quad (4)$$

For the shear wave propagating in the $XY$ plane and polarized along the $Z$ axis, harmonic time dependence in the form $\exp(i\omega t)$ and plane-wave dependence in the form $\exp(ipy)$ for all time and space dependent variables is assumed with $\omega$ as the wave angular frequency and $p$ as a wave number. After introducing $e_{15} = e$, $\varepsilon_{11} = \varepsilon$, $H_z = H$, $u_z = u$, the vector functions

$$\mathbf{v}(x, y) = \mathbf{v}(x)e^{ipy} \quad \text{and} \quad \mathbf{v}(x) = (-\omega u, -iE, i\sigma, iH)^T, \quad (5)$$

Figure 1. Periodic piezoelectric superlattice.
and the matrix
\[
\hat{M} = \begin{pmatrix}
0 & 0 & \frac{\omega}{G} & \frac{ep}{G\varepsilon} \\
0 & 0 & \frac{-ep}{G\varepsilon} & \mu\omega - \frac{c_{44}p^2}{G\varepsilon} \\
\rho\omega - \frac{c_{44}p^2}{\omega} & -ep & 0 & 0 \\
-ep & \omega\varepsilon & 0 & 0
\end{pmatrix},
\]
the problem reduces to solving the following eigenvalue problem
\[
\frac{1}{i} \frac{d}{dx} \mathbf{v}(x) = \hat{M} \mathbf{v}(x).
\]
The eigenvalues of (8) are
\[
q = \pm \sqrt{\frac{\omega}{c_0^2} - p^2}, \quad s = \pm \sqrt{\frac{\varepsilon}{c_0^2} - p^2}, \quad c_0 = \sqrt{\frac{G}{\rho}}, \quad c = \sqrt{\varepsilon\mu},
\]
and the eigenvectors are
\[
\mathbf{v}_1 = \sqrt{\frac{Gq}{2\omega}} \left( \frac{\omega}{Gq}, \frac{ep}{Gq\varepsilon}, 1, 0 \right)^T, \quad \mathbf{v}_2 = i\sqrt{\frac{Gq}{2\omega}} \left( -\omega, -ep, 1, 0 \right)^T,
\]
\[
\mathbf{v}_3 = \sqrt{\frac{\varepsilon\omega}{2s}} \left( 0, \frac{s}{\varepsilon\omega}, -ep, 1 \right)^T, \quad \mathbf{v}_4 = i\sqrt{\frac{\varepsilon\omega}{2s}} \left( 0, -s, -ep, 1 \right)^T.
\]
For a periodic structure described in figure 1, the solution for (7) in the nth unit cell can be written in the form
\[
\mathbf{v}_n^{(j)}(x) = A_n^{(j)} \mathbf{v}_1^{(j)} e^{iq(x-n\beta)+B_n^{(j)} \mathbf{v}_2^{(j)} e^{-iq(x-n\beta)+C_n^{(j)} \mathbf{v}_3^{(j)} e^{is(x-n\beta)+D_n^{(j)} \mathbf{v}_4^{(j)} e^{-is(x-n\beta)}, \quad j = 1, 2, (11)}
\]
where $A_n^{(j)}$, $B_n^{(j)}$, $C_n^{(j)}$, and $D_n^{(j)}$ are the amplitudes of forward and backward travelling waves.

For perfectly bounded interfaces $x = n\beta + a_1$ and $x = (n+1)\beta$ between the layers $(n, 1)/(n, 2)$ and $(n, 2)/(n+1, 1)$, the unimodular propagator matrix $\hat{W}$ coupling the forward and backward travelling wave amplitudes $A_n^{(1)}$, $C_n^{(1)}$, $B_n^{(1)}$, and $D_n^{(1)}$ in layers (1) in two neighboring cells (n) and (n + 1) can be constructed directly as
\[
\begin{pmatrix}
A_n^{(1)} \\
B_n^{(1)} \\
C_n^{(1)} \\
D_n^{(1)}
\end{pmatrix} = \hat{W} \begin{pmatrix}
A_{n+1}^{(1)} \\
B_{n+1}^{(1)} \\
C_{n+1}^{(1)} \\
D_{n+1}^{(1)}
\end{pmatrix},
\]
For a superlattice with cells composed of identical but oppositely polarized piezoelectric material ($\varepsilon_1 = \varepsilon$, $\varepsilon_2 = -\varepsilon$) and with equal widths $a_1 = a_2 = a$, the propagator matrix $\hat{W}$ has the form
\[
\hat{W} = \begin{pmatrix}
e^{-2iaq} - \xi_1 e^{-ia(q+s)} & i\xi_1 e^{ia(q-s)} & e^{2iaq} & \xi_4 e^{-2iaq} \\
-i\xi_2 e^{-2ias} & e^{-2ias} + \xi_4 e^{2ias} & -\xi_2 e^{-ia(q+s)} & i\xi_2 e^{2ias} \\
e^{-2ias} & i\xi_4 e^{2ias} & e^{-2ias} - \xi_2 e^{-ia(q+s)} & -i\xi_2 e^{-ia(q-s)} \\
i\xi_2 e^{2ias} & -i\xi_2 e^{2ias} & -i\xi_2 e^{-ia(q-s)} & \xi_4 e^{-2ias}
\end{pmatrix},
\]
}\]
where
\[ \xi_1 = \gamma e^{i\theta}(e^{2ia-s} - 1), \quad \xi_2 = \gamma e^{i\theta}(e^{2iaq} - 1), \quad \xi_3 = \gamma e^{i\theta}(-e^{-i(s-q)} - 1), \quad \xi_4 = \gamma e^{i\theta}(-e^{-i(s+q)} - 1), \]
\[ \gamma = \frac{q^2}{q^s}, \quad \theta = \frac{e^2}{G\varepsilon^2}, \]
\[ \theta \] is the electro-mechanical coupling coefficient, and * in the superscript denotes the complex conjugate.

It now follows that the relationship between the amplitudes of forward and backward travelling wave fields in the first and last layers of the superlattice can be written as
\[ \begin{pmatrix} A_0^{(1)} \\ B_0^{(1)} \\ C_0^{(1)} \\ D_0^{(1)} \end{pmatrix} = \hat{W}^n \begin{pmatrix} A_n^{(1)} \\ B_n^{(1)} \\ C_n^{(1)} \\ D_n^{(1)} \end{pmatrix}, \]
\[ (15) \]

Due to the symmetry of the problem, the propagator matrix \( \hat{W} \) is unimodular with eigenvalues \( \lambda_{1,2} = e^{\pm ik_1\beta} \) and \( \lambda_{3,4} = e^{\pm ik_2\beta} \), where \( k_{1,2} \) are the Bloch–Floquet numbers [11]. The characteristic equation of the matrix \( \hat{W} \) gives the following dispersion equation for an elasto-electromagnetic wave propagation in a piezoelectric superlattice with \( \beta = 2\alpha \) [14]:
\[ \cos(k_{1,2}\beta) = \frac{\cos(q\beta) + \cos(s\beta)}{2} - 2\gamma^2\theta^2 \sin(ab\beta) \sin(sa) \pm \sqrt{\cos^2(qa) - \cos^2(sa)} \sqrt{1 - 4\gamma^2\theta^2 \frac{\sin(ab\beta) \sin(sa)}{\cos(qa) + \cos(sa)}}, \]
\[ (16) \]

It is clear from formula (16) that if the unit cell in the superlattice has oppositely polarised identical piezoelectric elements, it will allow the propagation of the Bloch–Floquet waves at acoustic frequencies. At optical frequencies, the opposite polarization does not generate band gaps, since the effect of piezoelectricity diminishes at such frequencies and the structure behaves as a homogeneous stricture with identical optical refractive indexes [11]. This means that only an acoustic incident wave will be considered for the investigation of the reflection/transmission properties in the superlattice. For an incident acoustic wave with amplitude \( A_I \), the partial amplitudes of the wave fields in the first layer and at the exit are related as
\[ \begin{pmatrix} A_I \\ B_R \\ 0 \\ D_R \end{pmatrix} = \hat{W}^n \begin{pmatrix} A_T \\ 0 \\ C_T \end{pmatrix}, \]
\[ (17) \]

where \( B_R \) and \( D_R \) are the amplitudes of the reflected elastic and electromagnetic waves and \( A_T \) and \( C_T \) are the amplitudes of the transmitted acoustic and electromagnetic waves. It follows from (17) that the reflection/transmission coefficients \( R_{ac}, R_{el}, T_{ac}, T_{el} \) for acoustic and electromagnetic waves in terms of the propagator matrix are
\[ R_{ac} = \frac{B_R}{A_I}, \quad T_{ac} = \frac{A_T}{A_I}, \quad R_{el} = \frac{D_R}{A_I}, \quad T_{el} = \frac{C_T}{A_I}, \]
\[ (18) \]
\[ (19) \]
Figure 2. (a) Dispersion diagram of an infinite superlattice at acoustic frequencies near the center of the Brillouin zone. The horizontal lines correspond to the dimensionless phase velocity $k\beta/\pi$ of the acoustic wave enhanced by piezoelectricity, the vertical axis is the dimensionless frequency $\omega\beta/c_0$. The linear oblique dotted line corresponds to the phase velocity of a pure electromagnetic wave. (b) Transmitted acoustic (blue line), electromagnetic (red line), reflected acoustic (blue dashed line), and reflected electromagnetic (red dashed line) energy diagrams, $n = 200$.

3. Results and Discussion

Due to the electro-mechanical coupling in a piezoelectric superlattice, an incident acoustic wave generates a propagating electromagnetic wave. At specific frequencies in the long wavelength region, the elastic and generated electromagnetic waves resonate with each other creating a new form of a sub-wavelength band gap which is not associated with the Bragg reflection.

Since the dispersion curve of photons at acoustic frequencies is too close to the vertical axis, the coupling between the electromagnetic wave and the superlattice vibration can be seen in the long-wavelength region [12].

The solution of the dispersion equation (16) describes both coupled elastic and electromagnetic waves for the infinite piezoelectric superlattice. Here $k_1\beta$ describes the coupled acoustic wave field for frequencies lower than the pure electromagnetic wave frequency, and $k_2\beta$ describes the coupled acoustic and electromagnetic waves for frequencies higher than or equal to the frequencies of the pure electromagnetic wave. The resonant phonon polariton coupling appears when the square root in (16) becomes zero, i.e., $k_1\beta = k_2\beta$.

The first panel in figure 2 shows the subwavelength resonant bands described by dispersion curves (16) for an infinite superlattice at acoustic frequencies near the center of the Brillouin zone. The horizontal lines correspond to the phase velocity of the acoustic wave enhanced by the piezoelectric coupling. The linear oblique dotted line computed by the equation $k\beta/\omega = \sqrt{1/c^2 - \sin^2\phi/c_0^2}$ corresponds to the phase velocity of a pure electromagnetic wave uncoupled with the lattice vibrations. The region of crossover of these two lines is the resonance region, where neither an electromagnetic nor an acoustic wave can propagate for a very narrow range of the wave number.

As can be seen from the first panel in figure 2, the acousto-optic coupling for equal length layers in the cell takes place only for odd multiples of the fundamental resonance frequency $(\omega\beta/(c_0\pi)) = n$, $n = 1, 3, 5, \ldots$). For even $n$, the polariton is not excited. Here the red line corresponds to the $k_1\beta$ in (16), and the blue line corresponds to the $k_2\beta$. 

Conclusions
Due to the electromechanical coupling, the piezoelectric superlattice exhibits unique reflection/transmission properties even when the unit cell is made of identical piezoelectric materials. When the interfaces in the superlattice are perfectly bonded, the two identical elements in the unit cell can be oppositely polarized to make the structure behave as a phononic crystal. This however occurs only at acoustic frequencies, since the piezoelectric effect does not affect the band structure at optic frequencies where, in this case, the structure will act as a homogeneous material. The piezoelectric superlattice structure demonstrates an interesting coupling effect between the electro-magnetic wave and the superlattice vibration. The dispersion equation (16) contains information about this coupling which, in the long wavelength region, results in phonon-polariton gaps, where the resonance frequency is determined by the period of the superlattice.

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