

Acoustic Gain in Solids due to Piezoelectricity, Flexoelectricity, and Electrostriction

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A quantitative discussion of the combined influence of three electro-mechanical effects: piezoelectricity, flexoelectricity, and electrostriction in solids is provided for acoustic absorption and gain. While piezoelectricity occurs in non-centrosymmetric materials only, flexoelectricity and electrostriction exist in all materials. Two important new results are demonstrated: 1) the possibility to realize acoustic gain in all materials (centrosymmetric and non-centrosymmetric) when the acoustic Cherenkov condition is fulfilled, and 2) realization of acoustic gain in the presence of a strong dc electric field, even when the Cherenkov condition is not fulfilled, in the case of strong cross-coupling between piezoelectricity, flexoelectricity, and electrostriction. A simple analytical expression for the acoustic dispersion relation is derived for the combined effect of piezoelectricity, flexoelectricity, and electrostriction. At lower frequencies, the piezoelectric effect dominates for inversion-asymmetric materials. At high frequencies ($\approx >1$ MHz) flexoelectricity becomes increasingly important and eventually provides a major mechanism for gain and absorption in barium titanate (BaTiO_3). In the presence of strong electric fields ($\approx >1$ MV m^{-1}), electrostriction provides a dominant isolated contribution to absorption/gain in BaTiO_3 . Strong coupling between the three electromechanical contributions determines the total absorption/gain coefficient.

1. Introduction

Since the advent of graphene^[1] many new 2D materials with exotic physical properties and application potential have been fabricated. Several of these new solid materials may find use in device applications^[2–5] where electromechanical effects play an important yet different role compared to usual bulk or quantum-confined structures. Piezoelectricity is one characteristic intrinsic electromechanical property of many 2D materials^[6–8] that displays different qualitative and quantitative behavior than their bulk counterparts. For example, it has been shown experimentally and theoretically that the piezoelectric coefficient of MoS_2 changes drastically with the number of stacking layers.^[9] 2D MoS_2 structures with an even number of stacking layers are inversion symmetric and have a piezoelectric coefficient equal to zero while odd-layered structures show a non-zero but varying (usually decreasing) piezoelectric coefficient as the stacking number increases. Since 2D structures consist of one or a small number of single atomic

layers they are more flexible than bulk materials. Hence, flexoelectric effects are expected to play an important role in these materials. In addition, due to the small dimensions of nanodevices, electric fields may be as high as 1 GV m^{-1} such that electrostriction, manifesting itself as a mechanical stress proportional to the square of the electric field, can play a dominant role.

In the early sixties, Hutson, White, and McFee^[10–12] demonstrated experimentally and proved theoretically that piezoelectricity in bulk semiconductors provide a mechanism for acoustic gain due to the Cherenkov effect when the electron drift velocity, in the presence of a dc electric field, surpasses the speed of sound. Acoustic gain occurs as accelerated free electrons lose their kinetic energy, driven by the dc electric field, by emitting phonons. Recently, we demonstrated^[14] in the presence of epsilon-near-zero (ENZ) conditions acoustic gain due to piezoelectricity may become orders of magnitude higher than found in refs. [10–12]. We also showed in the context of parity–time symmetry acoustic metamaterials how amplified sound is an indispensable ingredient in many striking wave-based phenomena.^[15,16]

In this work, we make a systematic investigation of the combined effects of piezoelectricity, flexoelectricity, and electrostriction in solid materials for acoustic absorption (see **Figure 1**). We derive a closed form expression for the acoustic dispersion relation and show that typically, at low frequencies and electric fields,

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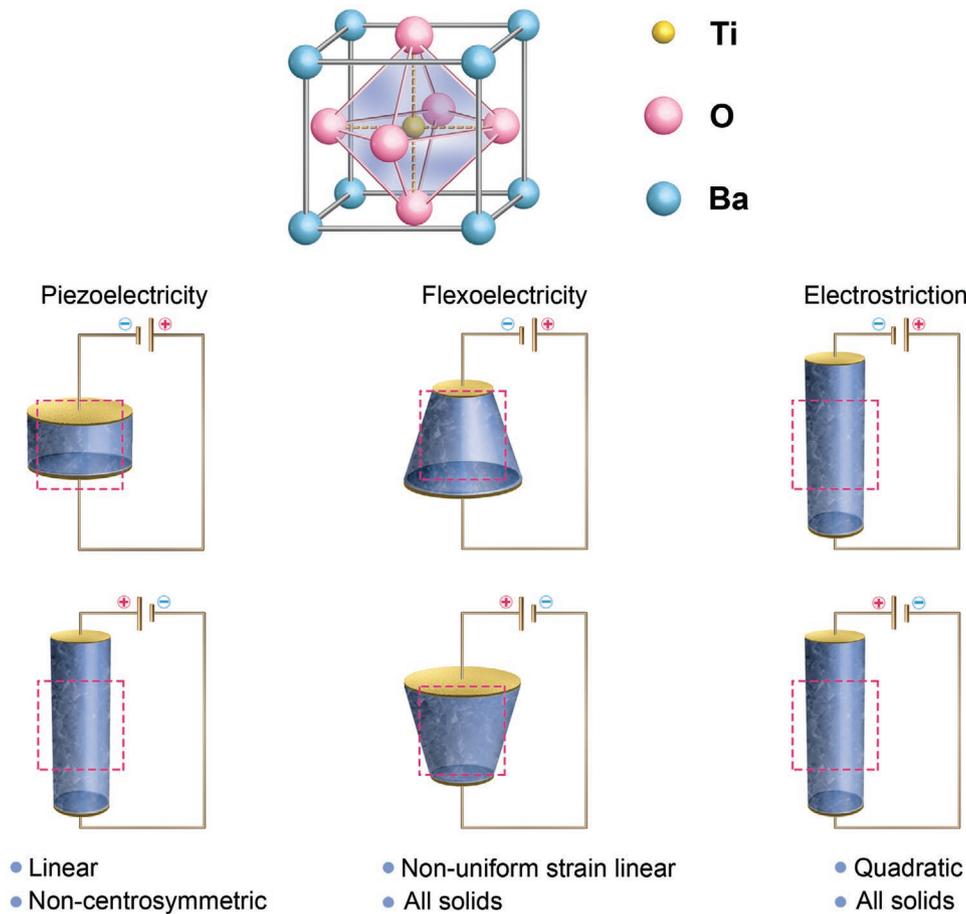


Figure 1. Schematic drawing of the BaTiO₃ crystal structure. The lower panel shows the isolated effects of piezoelectricity (left), flexoelectricity (middle), and electrostriction (right) for a cylinder-shaped BaTiO₃ structure with electrodes mounted at the top and bottom ends. The red dashed rectangle shows in profile the structure shape in the absence of an applied voltage.

piezoelectricity is the prevailing effect. In some materials, such as barium titanate (BaTiO₃), and at frequencies above ≈1 MHz or electric fields above ≈1 MV m⁻¹, flexoelectricity and electrostriction, respectively, contribute significantly to the acoustic absorption/gain. Interestingly, we demonstrate that couplings between the different electromechanical effects from piezoelectricity, flexoelectricity, and electrostriction are dominant and lead to absorption/gain coefficients that differ substantially from the sum of their individual contributions. We anticipate that for graphene and other 2D materials, due to these materials' small flexoelectric and electrostrictive coefficients, acoustic absorption/gain contributions from flexoelectricity and electrostriction first set in at high, yet realistic, frequencies and electric fields, respectively. In a recent work, the importance of flexoelectricity in pyramidal composite (Ba_xSr_{1-x}TiO₃) microstructures was investigated.^[17]

2. Theoretical Framework

For simplicity consider the constitutive relations of a 1D semiconductor including piezoelectricity, flexoelectricity, and electrostriction.

$$T = cS - eE - v \frac{\partial E}{\partial x} - gE^2 \quad (1)$$

$$D = \epsilon E + P + eS + v \frac{\partial S}{\partial x} + 2gES \quad (2)$$

where T , S , D , E , P , c , ϵ , e , v , and g are the stress, strain, electric displacement, electric field, spontaneous polarization, stiffness, permittivity, piezoelectric e constant, flexoelectric coefficient, and electrostriction coefficient, respectively. In deriving the relations between electrostrictive terms in Equations (1) and (2), we used the 1D thermodynamic relations^[13]

$$\tilde{H} = U - ED \quad (3)$$

$$d\tilde{H} = \Theta d\Omega + TdS - DdE \quad (4)$$

where \tilde{H} is the electric enthalpy, Ω is the entropy, and

$$T = \frac{\partial \tilde{H}}{\partial S} \quad (5)$$

$$D = -\frac{\partial \tilde{H}}{\partial E} \quad (6)$$

Similarly, the relation between flexoelectric terms in Equations (1) and (2) is obtained by use of the following

expression for the differential electric enthalpy assuming constant entropy

$$d\frac{\partial\tilde{H}}{\partial x} = \frac{\partial d\tilde{H}}{\partial x} = \frac{\partial T}{\partial x} dS + Td\left(\frac{\partial S}{\partial x}\right) - \frac{\partial D}{\partial x} dE - Dd\left(\frac{\partial E}{\partial x}\right) \quad (7)$$

thus

$$v = \frac{\partial D}{\partial\left(\frac{\partial S}{\partial x}\right)} = -\frac{\partial\left(\frac{\partial\tilde{H}}{\partial x}\right)}{\partial\left(\frac{\partial S}{\partial x}\right)\partial\left(\frac{\partial E}{\partial x}\right)} = -\frac{\partial\left(\frac{\partial\tilde{H}}{\partial x}\right)}{\partial\left(\frac{\partial E}{\partial x}\right)\partial\left(\frac{\partial S}{\partial x}\right)} = -\frac{\partial T}{\partial\left(\frac{\partial E}{\partial x}\right)} \quad (8)$$

Consider next electromechanical wave motion along the x direction. The equation of motion for a solid is

$$\rho \frac{\partial^2 u}{\partial t^2} = \frac{\partial T}{\partial x} = c \frac{\partial^2 u}{\partial x^2} - e \frac{\partial E}{\partial x} - v \frac{\partial^2 E}{\partial x^2} - 2gE \frac{\partial E}{\partial x} \quad (9)$$

where ρ is the mass density, and $s = \frac{\partial u}{\partial x}$ with u the material displacement due to the wave motion.

The continuity equation becomes

$$\frac{\partial J}{\partial x} = -\frac{\partial \rho_e}{\partial t} \quad (10)$$

where J and ρ_e are the current density and the free charge density, respectively. Let n_s be the carrier density due to the presence of the acoustic wave. The total density n of electrons in the conduction band is

$$n = n_0 + fn_s \quad (11)$$

where f denotes the fraction of the acoustically generated electrons that are free to move, and n_0 is the conduction band electron density in equilibrium. Since the ion background exactly compensates for the electron density in equilibrium, the free charge satisfies

$$\rho_e = -qn_s \quad (12)$$

The current density J due to electrons has drift and diffusion contributions. Two drift terms arise due to the presence of flexoelectricity (strain gradients), that is,

$$J = q\mu_c n E - q\mu_c n \frac{B}{q} \frac{\partial S}{\partial x} + qfD_n \frac{\partial n_s}{\partial x} \quad (13)$$

where μ_c is the electron mobility and B is the conduction band deformation potential in eV. Note that the flexoelectric drift terms arises from the contribution, $\frac{B}{q} S$, to the electric potential ϕ in the presence of strain and use of $E = -\frac{\partial \phi}{\partial x}$. The diffusion constant D_n is assumed to obey the Einstein relation

$$D_n = \frac{\mu_c k_B \Theta}{q} \quad (14)$$

where k_B and Θ are Boltzmann's constant and the absolute temperature, respectively.

We must supplement the above set of equations by the Maxwell–Poisson equation

$$\frac{\partial D}{\partial x} = \rho_e = -qn_s \quad (15)$$

Before we proceed it is important to notice that the influence of holes is neglected. The argument is simply that for semiconductors holes are usually much heavier than electrons. Hence, in a first approximative model, we will neglect their contribution to charge transport and acoustic dynamics.

2.1. Continuity Equation

It follows from the continuity equation and the Maxwell–Poisson equation that

$$\begin{aligned} \frac{\partial J}{\partial x} &= q\mu_c \left(n_0 \frac{\partial E}{\partial x} + f \frac{\partial n_s}{\partial x} E + fn_s \frac{\partial E}{\partial x} \right) + qfD_n \frac{\partial^2 n_s}{\partial x^2} + \mu_c B \left(n \frac{\partial^3 u}{\partial x^3} + \frac{\partial n}{\partial x} \frac{\partial^2 u}{\partial x^2} \right) \\ &= -\frac{\partial \rho_e}{\partial t} = -\frac{\partial^2 D}{\partial x \partial t} \end{aligned} \quad (16)$$

Terms involving n_s can be augmented by using the Maxwell–Poisson equation, that is,

$$\begin{aligned} \frac{\partial^2 D}{\partial x \partial t} &= -q\mu_c n_0 \frac{\partial E}{\partial x} + \mu_c f \frac{\partial^2 D}{\partial x^2} E + f\mu_c \frac{\partial D}{\partial x} \frac{\partial E}{\partial x} + fD_n \frac{\partial^3 D}{\partial x^3} - \\ &\mu_c B \left(n_0 \frac{\partial^3 u}{\partial x^3} - \frac{f}{q} \frac{\partial D}{\partial x} \frac{\partial^3 u}{\partial x^3} - \frac{f}{q} \frac{\partial^2 D}{\partial x^2} \frac{\partial^2 u}{\partial x^2} \right) \end{aligned} \quad (17)$$

We now proceed to solve Equation (17) for the case where the electric field consists of a dc term E_0 and a small acoustic term E_1

$$E(x, t) = E_0 + E_1 \exp(i\omega t - ikx) \quad (18)$$

where k is the wavenumber associated with the acoustic wave of frequency $\frac{\omega}{2\pi}$. We also make the ansatz

$$D(x, t) = D_0 + D_1 \exp(i\omega t - ikx) \quad (19)$$

$$u(x, t) = u_0(x) + u_1 \exp(i\omega t - ikx) \quad (20)$$

where E_0 , D_0 are constants, and u_0 is a time-independent function of x . The coefficients D_1 and u_1 are constant (small) acoustic amplitudes for the electric displacement and the displacement, respectively.

Since acoustic amplitudes are small, we neglect all terms involving products of acoustic amplitudes. Collecting first-order plane wave terms in acoustic amplitudes we find from Equation (17)

$$\omega k D_1 = q\mu_c n_0 ik E_1 - k^2 \mu_c f E_0 D_1 + ik^3 f D_n D_1 - \mu_c n_0 B ik^3 u_1 \quad (21)$$

Similarly, collecting terms to first order in acoustic amplitudes yields from Equation (9)

$$-\rho \omega^2 u_1 = -ck^2 u_1 + ike E_1 + vk^2 E_1 + 2ikg E_0 E_1 \quad (22)$$

and from Equation (2) we obtain

$$D_1 = \epsilon E_1 - ike u_1 - vk^2 u_1 - 2ikg E_0 u_1 \quad (23)$$

From the latter three equations, a determinantal equation in the acoustic amplitudes (D_1, E_1, u_1) is obtained by specifying the $\omega - k$ dispersion relation. Attempting instead a direct solution, Equation (21) gives

$$D_1 = \frac{iq\mu_c n_0}{\omega + f\mu_c E_0 k - ifD_n k^2} E_1 - \frac{ik^2 \mu_c n_0 B}{\omega + f\mu_c E_0 k - ifD_n k^2} u_1 \quad (24)$$

then from Equation (23)

$$\left(\varepsilon - \frac{iq\mu_c n_0}{\omega + f\mu_c E_0 k - ifD_n k^2} \right) E_1 = \left(ik\varepsilon + vk^2 + 2ikgE_0 - \frac{ik^2 \mu_c n_0 B}{\omega + f\mu_c E_0 k - ifD_n k^2} \right) u_1 \quad (25)$$

Using the latter expression in Equation (22) yields the dispersion equation

$$\rho\omega^2 = ck^2 + \frac{(ik\varepsilon + vk^2 + 2ikgE_0) \left(ik\varepsilon + vk^2 + 2ikgE_0 - \frac{ik^2 \mu_c n_0 B}{\omega + f\mu_c E_0 k - ifD_n k^2} \right)}{\frac{iq\mu_c n_0}{\omega + f\mu_c E_0 k - ifD_n k^2} - \varepsilon} \quad (26)$$

Equation (26) is the general acoustic dispersion equation including piezoelectric, flexoelectric, electrostriction, and strain-gradient current contributions. Due to the presence of imaginary terms in the dispersion equation, and the possibility to tune the dc electric field E_0 above the Cherenkov condition ($|E_0| > |\omega/(f\mu_c k)|$), allows for phonon amplification in both piezoelectric and flexoelectric materials. Note that flexoelectricity and electrostriction exist in all materials, also in inversion-symmetric crystals! Hence, application of the acoustic Cherenkov effect is not limited to piezoelectric (inversion-asymmetric) materials as considered in earlier works by White et al. and the present authors.^[10–12,14]

In the following, we will consider various cases of physical interest.

2.2. Absence of Piezoelectricity

In inversion-symmetric semiconductors such as silicon, diamond, and graphene, piezoelectric effects vanish, that is, $e = 0$. Then, Equation (26) reduces to

$$\rho\omega^2 = ck^2 + (vk^2 + 2ikgE_0) \left(\frac{vk^2 + 2ikgE_0 - \frac{ik^2 \mu_c n_0 B}{\omega + f\mu_c E_0 k - ifD_n k^2}}{\frac{iq\mu_c n_0}{\omega + f\mu_c E_0 k - ifD_n k^2} - \varepsilon} \right) \quad (27)$$

2.3. Absence of Piezoelectricity, Electrostriction, and Strain-Gradient Current Contributions

If piezoelectricity, electrostriction, and strain-gradient current contributions can be neglected ($e = g = B = 0$), then Equation (26) reduces to

$$\rho\omega^2 = ck^2 + \frac{v^2 k^4}{\frac{iq\mu_c n_0}{\omega + f\mu_c E_0 k - ifD_n k^2} - \varepsilon} \quad (28)$$

2.4. Absence of Flexoelectricity, Electrostriction, and Strain-Gradient Current Contributions

In a piezoelectric semiconductor where flexoelectric, electrostriction, and strain-gradient effects can be neglected, the coefficients v , g , and B vanish. Then, Equation (26) reduces to

$$\rho\omega^2 = ck^2 - \frac{k^2 e^2}{\frac{iq\mu_c n_0}{\omega + f\mu_c E_0 k - ifD_n k^2} - \varepsilon} \quad (29)$$

in agreement with previous results in the literature.^[10–12,14]

3. Numerical Results and Discussions

In this section, we consider barium titanate, BaTiO₃, and examine the importance of piezoelectricity, flexoelectricity, and electrostriction at different frequencies and dc electric fields. Parameters are shown in **Table 1**. We tacitly assume that in all parameters including the permittivity, mobility do not depend significantly on the acoustic frequency. For a detailed discussion of the influence of frequency, in particular at ENZ conditions, on acoustic absorption/gain in GaAs, we refer to our work in ref. [14]. Further, we shall neglect the influence of the strain-gradient current contribution (the term proportional to B in Equation (26)) in the following discussion.

Since the imaginary part of the wave vector k is small compared to its real part, it is possible to simplify the algebraic equation for k versus ω given by the general dispersion equation, Equation (26). First, we write out the numerator of the second term on the right-hand side of Equation (26)

$$(ik\varepsilon + vk^2 + 2ikgE_0)^2 = -(e^2 + 4gE_0 e + 4g^2 E_0^2 - i(2ve + 4vgE_0)k - v^2 k^2) k^2 \quad (30)$$

Then approximative solutions k_1, k_2 are now determined from the second-degree polynomial equation

$$\rho\omega^2 = ck_1^2 - \frac{(e^2 + 4gE_0 e + 4g^2 E_0^2 - i(2ve + 4vgE_0)k_{0,1} - v^2 k_{0,1}^2) k_1^2}{\frac{iq\mu_c n_0}{\omega + f\mu_c E_0 k_{0,1} - ifD_n k_{0,1}^2} - \varepsilon} \quad (31)$$

$$\rho\omega^2 = ck_2^2 - \frac{(e^2 + 4gE_0 e + 4g^2 E_0^2 - i(2ve + 4vgE_0)k_{0,2} - v^2 k_{0,2}^2) k_2^2}{\frac{iq\mu_c n_0}{\omega + f\mu_c E_0 k_{0,2} - ifD_n k_{0,2}^2} - \varepsilon} \quad (32)$$

where

$$k_{0,1} = -k_{0,2} = \sqrt{\frac{\rho\omega^2}{c}} \quad (33)$$

In **Figure 2**, 2D plots of the wave vector k_1 as a function of the dc electric field E_0 and the frequency $f = \omega/(2\pi)$ are shown. The four panels correspond to cases with piezoelectricity only (upper left), flexoelectricity only (upper right), electrostriction

Table 1. Physical properties. Note that the electrostriction constant g is given by $g = cM = c\epsilon^2 Q$. Observe that (GO) are data for graphene oxide.

Parameter	BaTiO ₃	GaAs	Graphene
σ [$\Omega^{-1}\text{m}^{-1}$]	1×10^{-5}	2.69×10^{-7}	1×10^4
μ_c [$\text{m}^2 \text{V}^{-1} \text{s}^{-1}$]	6.9×10^{-5} ($T = 300 \text{ K}$) ^[22]	0.8	1.5
ρ [kg m^{-3}]	6020	5320	
e [C m^{-2}]	$e_{15} = 21.3, e_{31} = -2.7, e_{33} = 3.7$ ^[21]	0.154	
ϵ (ϵ_0)	2000	10.89	$\epsilon_{11} = 4.4, \epsilon_{33} = 1.3$
M [$\text{m}^2 \text{V}^{-2}$]	$Q = 0.05 \text{ m}^4 \text{C}^{-2}$ ^[19]	$M = -1 \times 10^{-22}$ ^[20]	$M = -3 \times 10^{-23}$ (GO) ^[27]
ν [C m^{-1}]	-5×10^{-5} ^[18]	5.1×10^{-12} ^[24]	2.86×10^{-12} ^[23]
c [10^{11}Pa]	$c_{11} = 2.75, c_{33} = 1.65, c_{44} = 0.543, c_{12} = 1.79$	0.855	

only (lower left), and all three together (lower right), that is, according to Equation (31). The left (right) colorbar in the four panels refers to the real part of k_1 : $k_1' = \text{Re}(k_1)$ (the imaginary part of k_1 : $k_1'' = \text{Im}(k_1)$). In the calculations, we use the values $\nu = -5 \times 10^{-5} \text{ C m}^{-1}$ for BaTiO₃ where the minus sign reflects the best compromise between experimental data and density functional theory calculated flexoelectric coefficients for BaTiO₃ from Tables 3.2 and 3.4 in ref. [18]. For the electrostriction constant we used $g = cM = c\epsilon^2 Q$ with $Q = 0.05 \text{ m}^4/\text{C}^2$ taken from ref. [19] and $\epsilon = 2000\epsilon_0$. This yields a value of M equal to $1.6 \times 10^{-17} \text{ m}^2/\text{V}^2$ and $g = 4.3 \times 10^{-6} \text{ Pa} \cdot \text{m}^2/\text{V}^2$. As mentioned earlier, we tacitly assume the dielectric constant is a constant with frequency to focus on the different contributions from piezoelectricity, flexoelectricity, and electrostriction. For the piezoelectric coefficient we have chosen $e = e_{15} = 21.3 \text{ C m}^{-2}$ taken from ref. [21]. We also use $c = 275 \text{ GPa}$, $\sigma = q\mu_c n_0 = 1 \times 10^{-5} \Omega^{-1}\text{m}^{-1}$, and $\mu_c = 6.9 \times 10^{-5} \text{ m}^2 \text{V}^{-1} \text{ s}^{-1}$ ($T = 300 \text{ K}$).^[22]

It is evident that the real part of the wave vector k_1 is several orders of magnitude larger than the imaginary part. The most important isolated contribution to the absorption stems from electrostriction (lower left panel). Flexoelectricity (upper right panel) leads to an absorption contribution about two orders of magnitude smaller than the contribution from electrostriction and one order of magnitude smaller than the piezoelectric contribution (upper left panel). It is very interesting to notice that all three effects combine (lower right panel) to yield a substantially higher absorption coefficient, approximately five orders of magnitude higher than the sum of the isolated contributions shown in the other three panels! This difference is attributed to the coupling of electrostriction and piezoelectricity with flexoelectricity, that is, the terms $-4ivgE_0k_{0,1}$ and $-2ivek_{0,1}$ appearing inside the parentheses in the numerator of Equation (31). The reason these terms have a drastic effect on the absorption is that they are imaginary while all the isolated absorption contributions Equation (31) are real. In other words, our results anticipate the importance of accounting for the full coupling of electrostriction, piezoelectricity, and flexoelectricity to the absorption. This coupling is obviously absent from earlier analyses^[10–12,14] where only piezoelectricity was considered.

Our results also reveal that the imaginary part of k_1 changes sign (absorption to gain) as the dc electric field magnitude E_0 crosses the value -2.471 MV m^{-1} (refer to the white dashed line in the lower right panel). This effect reflects the strong coupling of flexoelectricity to both electrostriction and piezoelectricity and *not* due to the acoustic Cherenkov condition being

satisfied. Indeed, the electric field E_0^c required to fulfill the Cherenkov condition is given by $|E_0^c| \geq \frac{\omega}{\beta \mu_{k_1}} \gtrsim 100 \text{ MV m}^{-1}$. The explanation follows from inspection of the second term on the right-hand side of the dispersion relation Equation (26). The flexoelectric term provides a real value: νk^2 while the piezoelectric and electrostrictive terms are imaginary (*ike* and *2ikgE₀*, respectively). In effect, the overall sign of the imaginary term in the dispersion equation is determined not only by the Cherenkov condition. Thus, when flexoelectricity is present and sufficiently large, as it is for BaTiO₃, gain occurs at a much smaller electric field value than that determined by the Cherenkov condition.

We emphasize that the detailed frequency dependence of the dielectric constant and the mobility is not considered in the present work. This choice is made since the isolated consequence of a frequency-dependent dielectric constant and mobility will not affect the relative importance of piezoelectric, flexoelectric, and electrostrictive contributions for the total absorption/gain coefficient nor the obtained five-order enhancement of the total absorption/gain coefficient due to their coupling. The latter conclusion follows from our general dispersion result in Equation (26). Further, frequency-dependent data are scarce for other model parameters such as the piezoelectric e , flexoelectric ν , and electrostriction g constants. Hence, so as to maintain a homogeneous presentation, we have chosen to discard the frequency (as well as the electric field) dependence of all material parameters. It is important to notice, however, that Equation (26) (and other equations) can be directly used also for the case with frequency-dependent material parameters.

Due to the small flexoelectric and electrostrictive coefficients of bulk GaAs, we do not find important coupling contributions from piezoelectricity, flexoelectricity, and electrostriction to the total absorption/gain in bulk GaAs. Indeed, our calculations reveal that only piezoelectricity is important for absorption/gain of bulk GaAs. Hence, we find that the unique combination of large piezoelectric, flexoelectric, and electrostrictive constants makes BaTiO₃ a promising material for tunable acoustic absorption/gain devices.

It should be kept in mind that besides the above effects, there are other mechanisms that contribute to the imaginary part of the acoustic wave vector and lead to acoustic absorption in a solid. These include temperature relaxation phenomena such as phonon absorption due to temperature gradients and mechanical friction from scattering on impurities and dislocations. Note also that a 1D model represents an approximation and relies on parameter estimation based on real

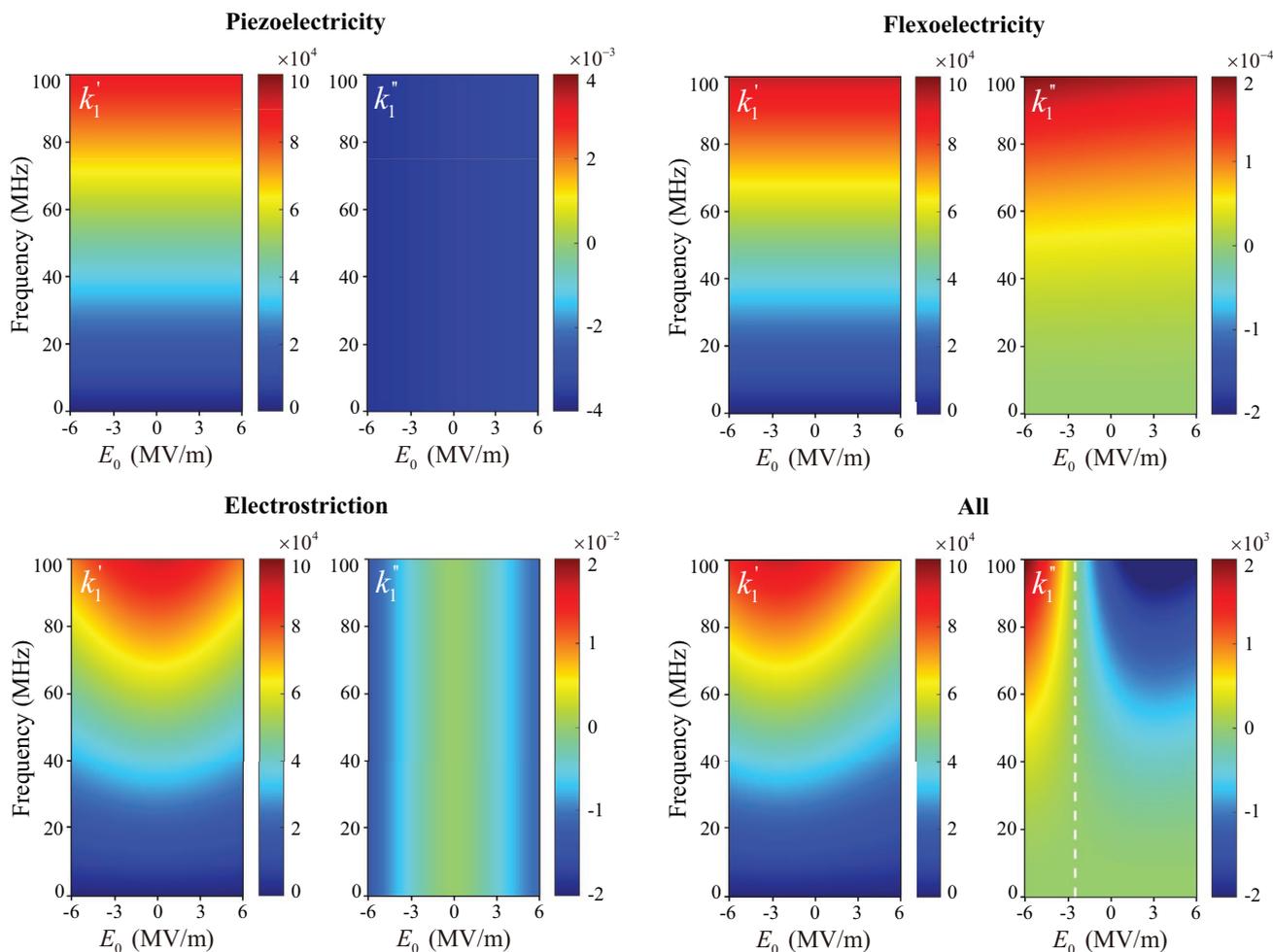


Figure 2. 2D plots of k_1 solutions for bulk BaTiO_3 in the case with piezoelectricity only (upper left plot), flexoelectricity only (upper right plot), electrostriction only (lower left plot), and all (lower right plot). The x axis is the dc electric field E_0 and the y axis is the acoustic frequency $f = \omega/(2\pi)$. The left (right) colorbar in the four panels refers to the real part of k_1 : $k_1' = \text{Re}(k_1)$ (the imaginary part of k_1 : $k_1'' = \text{Im}(k_1)$).

material data. We therefore expect the present analysis to be of a qualitative nature more than strict quantitative. We anticipate that quantitative data for the acoustic absorption/gain in the presence of a dc electric field must be based on detailed experimental investigations.

4. Estimation of Flexoelectricity, Electrostriction, and Strain-Gradient Current Contributions in Other Solids

In this section, we make rough estimations of the importance of electrostriction, flexoelectricity, and strain-gradient current contributions in selected other solids.

4.1. Flexoelectricity

According to a recent review article,^[23] direct flexoelectric constants μ are about 0.001–0.01 nC m^{-1} in 2D materials but there

is substantial variation among the different 2D materials (in MoS_2 the value is as high as 0.03 nC m^{-1}). In bulk GaAs, the flexoelectric coefficient is 5.1×10^{-12} C m^{-1} (see ref. [24]), that is, of the same order of magnitude as for the 2D materials. Therefore, at frequencies near or below 10 MHz, flexoelectricity plays a reduced role. Yet, at frequencies near or above 1 – 10 GHz, by virtue of the k^4 dependence of the flexoelectric term in the numerator of the dispersion equation, flexoelectricity provides a dominant contribution in most solids.

4.2. Electrostriction

The importance of electrostrictive effects is estimated as follows. According to ref. [25], electrostrictive constants ($M = \frac{g}{c}$) are very small, about 1×10^{-18} $\text{m}^2 \text{V}^{-2}$ in GaN and 10^{-21} $\text{m}^2 \text{V}^{-2}$ in silica.^[26] For the 2D material graphene oxide the electrostriction coefficient is only $M = -3 \times 10^{-23}$ $\text{m}^2 \text{V}^{-2}$ (see ref. [27]). Indeed, density functional theory calculations^[13] give much smaller electrostriction coefficients for GaN and similar materials closer to the values reported by ref. [26] for silica. Hence, the role of

electrostriction is expected to be significantly smaller in typical bulk and 2D solids as compared to BaTiO₃ at dc electric fields of less than or near several MV m⁻¹. Note, however, that at electric fields near or above 0.1 GV m⁻¹, electrostriction will play a significant role in most materials. Such strong electric fields are realized in many nanostructure device applications.^[28,29]

4.3. Strain-Gradient Current Contribution

Let us attempt to determine the importance of the strain-gradient term in Equation (21). By use of Equation (23)

$$u_1 = \frac{\epsilon E_1 - D_1}{ik\epsilon + vk^2 + 2ikgE_0} \quad (34)$$

Equation (21) becomes

$$\left(\omega k - ik^3 fD_n + k^2 \mu_c fE_0 - \frac{\mu_c n_0 Bk^2}{e - ivk + 2gE_0} \right) D_1 = \left(q\mu_c n_0 ik - \frac{\mu_c n_0 Bk^2 \epsilon}{e - ivk + 2gE_0} \right) E_1 = q\mu_c n_0 ik \left(1 + \frac{ikB\epsilon}{q(e - ivk + 2gE_0)} \right) E_1 \quad (35)$$

For GaAs^[14] with $B \sim 5$ eV, $\epsilon \sim 11\epsilon_0$, $e \sim -0.16$ C m⁻², $\mu_c = 0.85$ m² s⁻¹ V⁻¹, $n_0 \sim 2 \times 10^{12}$ m⁻³, $\omega/(2\pi) \sim 15$ MHz, and a sound speed about 4×10^3 m s⁻¹, we have $\left| \frac{kB\epsilon}{qe} \right| \sim 1 \times 10^{-4}$ [SI],

which is negligibly small compared to 1 on the right-hand side. Similarly, on the left-hand side, comparing $\omega k \sim 1 \times 10^8 \times 10^4 = 10^{12}$ [SI] and $\left| \frac{\mu_c n_0 Bk^2}{e} \right| \sim 1 \times 2 \times 10^{12} \times 5 \times 10^8 / 0.16 \sim 10^3$ [SI] so strain-gradient current contributions are typically negligible. The above assertion that the strain-gradient current contribution can be neglected also holds in the case of BaTiO₃.

5. Conclusions

An quantitative discussion of the combined effects of piezoelectricity, flexoelectricity, and electrostriction in solids for the acoustic absorption coefficient was presented. While piezoelectricity occurs in non-centrosymmetric materials only, flexoelectricity and electrostriction exist in all materials. For bulk BaTiO₃, in the presence of a dc electric field of the order of MV m⁻¹, electrostriction is the most important isolated contribution to absorption. At lower electric fields, of the order of kV m⁻¹ or below, piezoelectricity provides the dominant contribution. It is demonstrated that net acoustic gain is introduced at sufficiently high dc electric fields, when the acoustic Cherenkov condition is fulfilled, and the magnitude of the net absorption/gain coefficient is governed by dominant cross-coupling effects between electrostriction, piezoelectricity, and flexoelectricity. The cross-coupling contribution leads to absorption/gain coefficients about five orders of magnitude higher than the isolated contributions from electrostriction, piezoelectricity, and flexoelectricity. Examples were presented for BaTiO₃. Estimation of the importance of flexoelectricity, electrostriction, and strain-gradient effects was also discussed for other typical bulk and 2D semiconductors.

Conflict of Interest

The authors declare no conflict of interest.

Keywords

acoustic gain, Cherenkov effect, electrostriction, flexoelectricity, piezoelectricity

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