New Type of Polariton in a Piezoelectric Superlattice

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We studied the propagation of an electromagnetic (EM) wave in a piezoelectric superlattice. Because of the piezoelectric effect, a transverse polarization can be induced by a longitudinal wave which couples strongly to the EM wave in some particular frequency regions, resulting in the creation of a new type of polariton that does not exist in ionic crystals. The forbidden band associated with the polariton is not due to the Bragg reflection, but rather to the coupling.

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Study of the periodic medium has long been a topic of interest. In a crystal, the periodic potential causes the energy structure of electrons to form a band structure with only those electrons in passbands that are capable of moving freely. In artificial composites such as superlattices, the periodic modulation of the related physical parameters may also result in band structure. Associated with the variation of dielectric constants is the photonic crystal [1,2], which is important for applications such as suppressing spontaneous emission, manipulating light in a specific path, and creating novel laser geometries [1–3]. The modulation of nonlinear optical coefficients results in a quasi-phase-matched frequency conversion that is more efficient than that with a birefringence phase-matching method [4–6]. Recently, interest in phononic crystal, a periodic elastic composite, has grown [7–10]. The structure modulation may be extended to quasiperiodic or aperiodic or two-dimensional structures [11–14], and the modulation parameters may be more complicated. For example, objects such as the ferroelectric domain or piezoelectric coefficient may be modulated. Even two or more parameters may be modulated together, which could result in some coupling effects.

In a real crystal, various couplings exist between the motions of electrons, photons, and phonons. For example, infrared absorption and polariton excitation results from the coupling between lattice vibrations (transverse optical phonons) and electromagnetic (EM) waves (photons) in an ionic crystal [15]. If the ferroelectric domain or piezoelectric coefficient is modulated in a superlattice, the coupling between the superlattice vibrations and the EM wave may be established. Similar effects such as polariton excitation can be expected in such an artificial medium. The above idea has been verified for the coupling between the transverse superlattice vibrations and the photons [16].

Then can an EM wave couple with a longitudinal lattice vibration? The problem is treated theoretically for a piezoelectric superlattice (PSL) in this Letter. A piezoelectric material is a material that becomes electrically polarized when it is strained or that becomes strained when placed in an electric field [17], which can be a result of propagation of an electromagnetic wave. That is, superlattice vibration can be excited by an EM wave. On the other hand, the superlattice vibrations will induce electrical polarization either longitudinally or transversely depending on the configuration of the PSL due to the piezoelectric effect. The lateral polarization in turn will emit EM waves that interfere with the original EM wave. In such a case, a longitudinal lattice vibration will couple strongly with the EM wave through the piezoelectric effect, resulting in polariton excitation, dielectric abnormality, etc., at microwave range.

In order to elucidate the above idea, let us consider the following case. Here we assume that the PSL is made of a periodically poled ferroelectric crystal [4–6] (taking a periodically poled $LiNbO_3$ as an example; a ferroelectric material is piezoelectric) arranged along the x axis and that the domain walls lie in the yz plane. The thicknesses of the positive and negative domains are the same (d). Figure 1 is a schematic diagram of the case. Here only three periods of the PSL have been shown. The direction of the spontaneous polarization is along the z axis, perpendicular to the sheet. Also we assume that the transverse dimensions are very large compared with an acoustic wavelength so that a one-dimensional model is applicable and that the EM wave propagates along the x direction. Under these conditions, a longitudinal acoustic wave (LAW) propagating along the x axis will be excited. The piezoelectric equations pertaining to this case are [17]

$$\begin{aligned} T_1 &= C_{11}^E S_1 + e_{22}(x)E_2, \\ P_2 &= -e_{22}(x)S_1 + \varepsilon_0(\varepsilon_{11}^S - 1)E_2, \end{aligned} \tag{1}$$

with

$$e_{22}(x) = \begin{cases} +e_{22}, & \text{in positive domains} \quad (0 \le x < \frac{\Lambda}{2} = d), \\ -e_{22}, & \text{in negative domains} \quad (\frac{\Lambda}{2} \le x < \Lambda = 2d), \end{cases}$$

where T_1, S_1, E_2, and P_2 are the stress, strain, electric field, and polarization, respectively. C_{11}^E, $e_{22}(x)$, and ε_{11}^S are the elastic, piezoelectric, and dielectric coefficients, respectively.

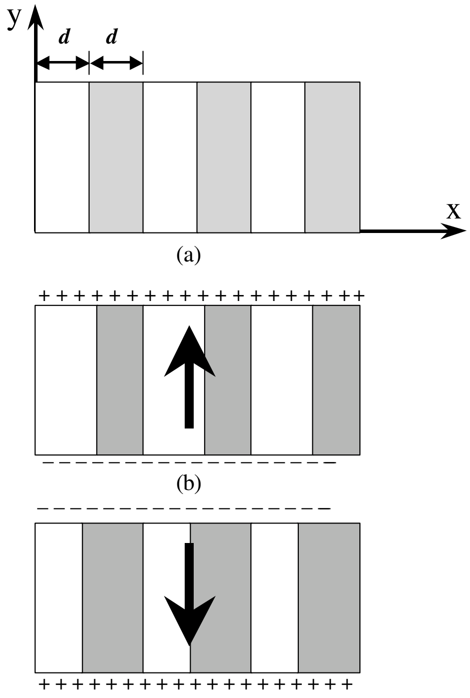

FIG. 1. (a) A schematic diagram of a PSL. The white area represents the positive domain and the gray area the negative domain. (b),(c) At any instant of time under the action of an EM wave, the positive and negative domains act differently. That is, when the positive domains expand, the negative ones contract and vice versa, which results in the appearance of the charges of the same sign (positive or negative) on the same side of the two different domains. The arrow indicates the stress-induced electric polarization.

Previous study shows that under the action of an electric field, the positive and negative domains act differently [18,19]. That is, when the positive domains expand, the negative ones contract and vice versa, which results in the appearance of the charges of the same sign (positive or negative) on the same side of the two different domains [Figs. 1(b) and 1(c)]. That is, the PSL as a whole polarizes electrically synchronously. This fact can be seen in Eq. (1). It tells us that a transverse polarization P_2 can be induced by a longitudinal wave S_1 through the piezoelectric effect. And through Maxwell equation, this transverse polarization P_2 will in turn emit EM waves that interfere with the original EM wave. In other words, it is this transverse polarization P_2 that couples strongly with the EM wave. This resembles the lattice vibrations belonging to the transverse optical branches. In that case, the atoms carrying opposite charges vibrate against each other. This type of vibration can be coupled with an electric field of a light wave, resulting in a so-called polariton excitation [15].

With the use of Newton's law, the equation of motion for a vibrating medium can be obtained

$$\rho\frac{\partial^2 S_1}{\partial t^2}-C_{11}^E\frac{\partial^2 S_1}{\partial x^2}=-\frac{\partial^2[e_{22}(x)E_2]}{\partial x^2}, \tag{2}$$

where ρ is the mass density. Equation (2) indicates that the PSL is a forced oscillator. That is, a LAW propagating along the x axis will be excited by a transverse EM wave. The frequency of the acoustical wave will be that of the EM wave. By using the Fourier transformation

$$\begin{aligned} E_2(x,t)&=\int E(k)e^{i(\omega t-kx)}dk,\\ S_1(x,t)&=\int S(q)e^{i(\omega t-qx)}dq,\\ e_{22}(x)&=\sum_{m\neq 0}\frac{i(1-\cos m\pi)e_{22}}{m\pi}e^{-iG_m x}\qquad\left(G_m=m\frac{2\pi}{\Lambda}\right).\end{aligned} \tag{3}$$

Here different wave numbers for photons and phonons have been used. Equation (2) becomes

$$\int(\rho\omega^2-C_{11}^E q^2)S(q)e^{-iqx}dq=\int-\sum\frac{i(1-\cos m\pi)e_{22}}{m\pi}(G_m^2+2G_m k+k^2)E(k)e^{-i(k+G_m)x}dk, \tag{4}$$

where $e^{i\omega t}$ has been omitted. For photons with very long wavelength, that is $k\to 0$ or $k\ll G_m$, Eq. (4) becomes

$$\int(\rho\omega^2-C_{11}^E q^2)S(q)e^{-iqx}dq=-\sum_m\frac{i(1-\cos m\pi)e_{22}}{m\pi}G_m^2E(k)e^{-i(k+G_m)x}. \tag{5}$$

In order for the two sides to be equal, q must take the form $q=k+G_m=k+m\frac{2\pi}{\Lambda}$. Then we obtain

$$S(q=k+G_m)=-\frac{i(1-\cos m\pi)e_{22}}{m\pi}\frac{G_m^2}{\rho\omega^2-C_{11}^E G_m^2}E(k) \tag{6}$$

and

$$S_1(x,t)=-\sum\frac{i(1-\cos m\pi)e_{22}}{m\pi}\frac{G_m^2}{\rho\omega^2-C_{11}^E G_m^2}e^{iG_m x}E(x,t)=H(x)E(x,t). \tag{7}$$

Substituting Eq. (7) into Eq. (1), we have

$$P_2 = \{-e_{22}(x)H(x) + \varepsilon_o(\varepsilon_{11}^S - 1)\}E_2(x,t) = \kappa(x)E_2(x,t), \tag{8}$$

where $\kappa(x)$ is a function of the x coordinate. For EM waves with $k \to 0$ or their wavelength (λ) much larger than the length of the sample, the PSL can be taken to be homogeneous. The space average value of $\kappa(x)$ should be used:

$$\kappa = \overline{\kappa(x)} = \frac{1}{\Lambda}\int_0^\Lambda \kappa(x)dx = \varepsilon_o(\varepsilon_{11}^S - 1) + \frac{1}{\Lambda}\int_0^\Lambda e_{22}(x)H(x)dx$$
$$= \varepsilon_o(\varepsilon_{11}^S - 1) + \frac{1}{\Lambda}\sum \frac{(1-\cos m\pi)e_{22}^2}{m\pi}\frac{G_m}{\rho\omega^2 - C_{11}^E G_m^2}2(e^{-im\pi} - 1). \tag{9}$$

The dielectric function obtained from Eq. (9) is

$$\varepsilon(\omega) = \varepsilon_{11}^S + \frac{4e_{22}^2/(d^2\rho\varepsilon_o)}{\omega_L^2 - \omega^2}, \tag{10}$$

where $\omega_L = m\pi\nu_a/d$ $(m = 1, 3, 5, \ldots)$, the resonance frequency of the LAW due to piezoelectric effect; $\nu_a = \sqrt{C_{11}^E/\rho}$ represents the velocity of the acoustic wave.

The polariton dispersion relation due to the coupling between the lateral polarization induced by a LAW and EM wave can be deduced from Eqs. (9) and (10) and Maxwell's equations

$$\frac{c^2k^2}{\omega^2} = \varepsilon_{11}^S + \frac{4e_{22}^2/(d^2\rho\varepsilon_o)}{\omega_L^2 - \omega^2}, \tag{11}$$

where c is the EM wave velocity in vacuum.

This result resembles the dispersion relation in an ionic crystal where the EM wave couples strongly with the transverse optical phonons [15]. Figure 2(a) shows the coupled modes of photons and longitudinal phonons in the PSL described by Eq. (11). The solid line labeled $\nu_c = \frac{\omega}{k} = c/\sqrt{\varepsilon_{11}^S}$ corresponds to EM waves, but uncoupled to the lattice vibrations, and the dotted line represents the lattice vibration in the absence of coupling to the EM field due to the Brillouin zone folding of the PSL. The wave number of the acoustic wave $q = k + G_m$ is equivalent to $q = k$ [15]. The region of the crossover [marked by A in Fig. 2(a)] of the solid line and the dotted line is the resonance region. By resonance, we mean that the frequency of the EM wave equals the acoustic resonance frequency of the PSL determined by the periodicity. At resonance the photon-phonon coupling entirely changes the character of the propagation. The heavy lines are the dispersion relations in the presence of coupling between the lateral polarization induced by a LAW and the EM wave. In the resonance region the propagation mode is neither a pure photon mode nor a pure longitudinal acoustic mode in a narrow range of k values (unlike the case in the ionic crystal, where the coupling occurs between the photons and the transverse optical phonons). The quantum of the coupled photon-phonon wave field is called a polariton. It is a new type of polariton. One effect of the coupling is to create a frequency gap between ω_o and ω_L. Here ω_o can be obtained by setting $\varepsilon(\omega_o) = 0$ in Eq. (10). Thus, we have

$$\omega_o^2 = \omega_L^2\left(1 + \frac{4}{(m\pi)^2}K^2\right) \tag{12}$$

and

$$\varepsilon(\omega) = \varepsilon_{11}^S\frac{\omega_o^2 - \omega^2}{\omega_L^2 - \omega^2}, \tag{13}$$

where K^2 is an electromechanical coupling coefficient [17],

$$K^2 = \frac{e_{22}^2}{C_{11}^E\varepsilon_o\varepsilon_{11}^S}. \tag{14}$$

For frequencies $\omega_L < \omega < \omega_o$, $\varepsilon(\omega)$ is negative and the corresponding refractive index becomes imaginary as can be seen in Fig. 2(b). The incident radiation with these frequencies will be reflected. However, this gap does not originate from the Bragg reflection due to the periodic structure, but rather originates from the coupling of the photon and the longitudinal phonon. Since K^2 is less than 1, Eq. (12) can be approximated to

$$\omega_o \approx \omega_L\left(1 + \frac{2}{(m\pi)^2}K^2\right). \tag{15}$$

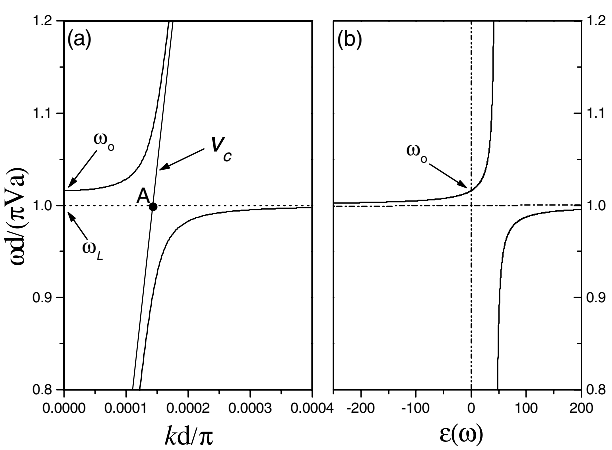

FIG. 2. Calculated polariton dispersion (a) and dielectric abnormality (b). The dielectric constant is negative between ω_o and ω_L where no EM waves will be permitted to propagate in the sample, but will be reflected at the boundary. Thus, a band gap appears.

From it the gap (ω_o-ω_L) can be determined. The larger the K value is, the stronger the coupling and the wider the gap. Here for the coupling between the EM wave and the LAW in $LiNbO_3$, K is about 0.28 [19]. Thus, the gap is about 1.6% for $m = 1$. If the period of the PSL is 6.6 μm, then the polariton will be excited around the resonance frequency 1 GHz (determined by $\omega_L = \pi \nu_a / d$ with $m = 1$) [19], which lies at microwave region. High-order polaritons ($m = 3, 5, \ldots$) can create in higher frequency regions, however, the corresponding gaps are much narrower that are inversely proportional to m^2 as indicated by Eq. (15). Please note that here m is an odd number. For even m, no polariton can be excited. The gap can be widened by use of some materials with larger electromechanical coupling coefficients. For $Pb(ScNb)_{0.5}O_3$:$PbTiO_3$, the K value for the coupling between the EM wave and the LAW can get to 0.48 [20]. Theoretically, the corresponding gap is about 4.67%. An even larger gap can be realized by using the coupling between the EM wave and the transverse lattice vibration. For $LiNbO_3$, K can be as large as 0.76 [19]. In that case, the gap is 11.7%. The above result might have potential applications for microwave reflectors based on polariton excitation.

For piezoelectric materials, there are still two coupled waves even without periodic modulation, each having both EM and acoustic fields [17]. In both cases the relationship between the EM and acoustic fields is given by the dispersion

$$(\rho\omega^2 - C_{11}^E k^2)\left(\frac{\varepsilon_{11}^S \omega^2}{c^2} - k^2\right) = \frac{e_{22}^2 \omega^2 k^2}{\varepsilon_o c^2} \qquad (16)$$

or

$$\left(\frac{\omega}{k}\right)^2 \approx \begin{cases} \nu_c^2 \left(1 + \frac{\nu_a^2 K^2}{\nu_c^2}\right) & \text{quasielectromagnetic} \\ \nu_a^2 \left(1 - \frac{\nu_a^2 K^2}{\nu_c^2}\right) & \text{quasiacoustic} \end{cases} \qquad (17)$$

with $\nu_c^2 = c^2 / \varepsilon_{11}^S$.

Compared with Eq. (11), the dispersion here is quite different. The dispersions represented by Eq. (17) are two straight lines passing through the origin. In the presence of piezoelectric coupling, the quasiacoustic phase velocity shifts to a lower value than the acoustic velocity and the quasielectromagnetic phase velocity shifts to a higher value than the electromagnetic velocity. However, the coupling is so weak that only very small shifts are produced, and no polariton is excited.

In summary, the propagation of an EM wave in a PSL was studied theoretically. A new type of polariton was proposed that comes from the coupling of the EM wave with the LAW. The polariton dispersion and dielectric abnormality were discussed. The origin of the band gap is not due to the Bragg reflection, but rather to the coupling.

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