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Temperature Effect on Polariton Dispersion in Low Dimensional Systems

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ABSTRACT

The variation of the optical parameters such as the static dielectric constant, high frequency dielectric constant, transverse optical phonon frequency and longitudinal optical phonon frequency are studied for the ferroelectric materials like $LiNbO_3$ and $LiTaO_3$at various temperatures. The behavior of phonon polarities for the quantum well, quantum wire and quantum dot superlattice both at Brillion zone centre and at the edge are discussed at these temperatures. It is found that when the temperature increases the dispersion shifts to new values. The polaritonic gap, within which no electromagnetic radiation can pass through, is almost same at all the temperatures except at the transition region. It is extended to $LiNbO_3/LiTaO_3$quantum well, quantum wire and quantum dot super lattices. The behavior of various modes of the phonon polariton dispersion at various temperatures is investigated systematically.

KEYWORDS: $LiNbO_3/LiTaO_3$quantum well, Phonon polar ton dispersion, Longitudinal optical phonon frequency, Polari tonic gap, Quantum wire and Quantum dot super lattices

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INTRODUCTION

There exist several elementary excitations associated with lattice vibrations, coupled electron density oscillations, spin wave excitations and excitonic excitations (in insulators) inside a crystal. The quanta of these excitations namely phonons, plasmons, magnons and excitons can couple with the propagating electromagnetic radiation inside the medium and exhibit a variety of new coupled excitations, called polaritons [1,2]. There is a rich literature on the study of polaritons, both theoretically and experimentally, with a variety of experimental techniques such as Raman spectroscopy and attenuated total internal reflection [3,4]. After the successful fabrication of superlattice [SL] systems such as quantum well [QWell], quantum wire [QWire] and quantum dot [QDot] systems, the study of polaritons has become more active [5,6,7]. Ferroelectric materials especially $LiNbO_3$ and $LiTaO_3$ are closely related polar materials with high figures of merit for electro optic, nonlinear optic, pyroelectric, piezoelectric and surface acoustic wave applications. They have long been seen in use as highly functional components in optical technologies such as optical communications, signal processing, interconnection, thermal detection and frequency conversion. The various optical properties such as, refractive index, static dielectric constant, high frequency dielectric constant, transverse optical phonon frequency and longitudinal optical phonon frequency of the ferroelectric materials especially $LiNbO_3$ and $LiTaO_3$ are studied. Hence the dielectric function of the material will be analysed with temperature. The behaviour of phonon polariton of these materials can be studied in the case of bulk and superlattices [12]. The external perturbations such as pressure, temperature, electric field, magnetic field and irradiation with electromagnetic radiation brings out appreciable change in the electric and optical properties. Among all these perturbations, the effect of temperature is concentrated in the present work.

THEORY

$LiTaO_3$ and $LiNbO_3$have very attractive combination of electro-optic, piezoelectric and other optical properties that has made it one of the most extensively studied materials in recent years. $LiTaO_3$ and $LiNbO_3$ belong to trigonal crystals of point group 3m, a negative uniaxial crystal, transparent from 0.33 µm to *ca*. 5 µm. When the temperature of the crystals is increased the values of the optical parameters are altered. For the ferroelectric crystals the changes in refractive index with temperature is given by

$$n_{(T)} = n_0(1 + \alpha T) \qquad (1)$$

This equation can be represented in terms of dielectric constants as

$$\varepsilon_{\infty(T)} = \varepsilon_{\infty}(1 + 2\alpha T) \qquad (2)$$

$$\varepsilon_{0(T)} = \varepsilon_0(1 + \beta T) \qquad (3)$$

Where $\alpha = \frac{dn_0}{dT}$ and $\beta = \frac{dk_1^T}{k_1^T dT}$ are the temperature coefficients [8]. The values of α and β are calculated at room temperature.

The changes in transverse optical phonon frequency with temperature is given by [9],

$$\omega_{TO(T)} = A(T - T_c)^{\frac{1}{2}} \quad (4)$$

The corresponding longitudinal optical phonon frequencyat different temperatures can be determined using LST relation.So that the behaviour of polariton dispersion at different temperatures is studied. The dependence of the frequency "ω" on the wave vector k of an electromagnetic wave in a crystal with the dielectric function ε(ω) is determined by a dispersion relation for an infinite isotropic crystal. The dielectric function for the bulk is given by

$$\varepsilon(\omega) = \varepsilon_\infty + \frac{(\varepsilon_0 - \varepsilon_\infty)\omega_{TO}^2}{\omega_{TO}^2 - \omega^2 - i\omega\gamma} \quad (5)$$

Where ω_{TO} is the frequency of the transverse optical phonons, ε_∞ and ε_0 are the high frequency and static dielectric constants ,respectively. Here γ is the damping factor. The imaginary part of the dielectric function leads to Frohlich modes which are studied and their behaviour as a function of frequency is discussed extensively in the literature [10,11]. However, in the study of polariton behaviour, it is required only the real part of ε(ω).The polariton behaviour of the above system can be studied by the following dispersion relation

$$\frac{c^2k^2}{\omega^2} = \varepsilon(\omega) = \varepsilon(\infty) + \frac{(\varepsilon_0 - \varepsilon_\infty)\omega_{TO}^2}{\omega_{TO}^2 - \omega^2} \quad (6)$$

where c is the velocity of light in vacuum. There is a polaritonic gap between ω_{TO} and ω_{LO} within which no electromagnetic radiation can pass through. The study of excitations propagating in SL produces new results. Typically the thickness of an individual layer lies in the range 100-5000 A. If one constituent, material A, always has thickness d_1 and the second, material B, always has thicknessd_2, one has built a periodic structure known as a SL. In this work, assuming alternating layers of $LiNbO_3$ and $LiTaO_3$as A and B medium of thickness $d_1$and d_2 stacked along the Z direction. Several authors [5,6,7] have derived the following dispersion relation for TM modes assuming the electromagnetic boundary conditions, namely, the electrostatic potentials and the electric displacement field perpendicular to each interface are continuous:

$$1 - \left(\frac{\varepsilon_B(\omega)\alpha_1}{\varepsilon_A(\omega)\alpha_2}\right)^2 - 2\left(\frac{\varepsilon_B(\omega)\alpha_1}{\varepsilon_A(\omega)\alpha_2}\right)\left(\frac{\cosh(\alpha_1 d_1)\cosh(\alpha_2 d_2) - \cos(qL)}{\sinh(\alpha_1 d_1)\sinh(\alpha_2 d_2)}\right) = 0 \quad (7)$$

For the semiconductor SL ($\mu_v = 1$) consisting of alternating layers of materials A and B. Here $L = d_1 + d_2$ is the SL period and q is the component of the wave vector along the SL axis and for quantum well SL $\alpha_i^2 = k_X^2 - \frac{\omega^2}{c^2}\varepsilon_i$, where k_X is the component of the wave vector in the X-direction for TM modes.

For Quantum wire SL $\alpha_i^2 = \frac{1}{2}(k_x^2 - \frac{\omega^2}{c^2}\varepsilon_i)$

For Quantum Dot SL $\alpha_i^2 = -\frac{1}{3}\varepsilon_i\frac{\omega^2}{c^2}$

RESULTS AND DISCUSSION:

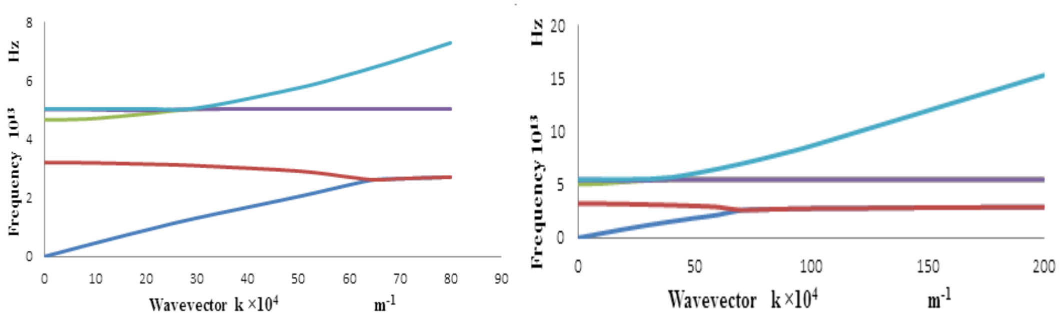
Using the temperature coefficients α andβ the static dielectric constant and high frequency dielectric constant are determined at various temperatures. It is found that the values of dielectric constant increases with temperature. Similarly the transverse and longitudinal optical phonon frequencies are determined. It is found that when the temperature increases, the optical phonon frequency decreases.

Polariton dispersion of quantum well superlattice at room temperature is shown Fig 1(a). Polariton dispersion provides five modes of propagation. The first four modes are the symmetric and anti-symmetric interfacial modes approaching the surface mode frequencies of the $LiNbO_3$ and $LiTaO_3$ materials as $d_1\rightarrow\infty$ and $d_2\rightarrow\infty$.The lower and upper modes of propagation represent the conventional modes of $LiTaO_3$ and $LiNbO_3$.There are three interfacial modes of propagation in the polaritonic gap. One of the interfacial modes starts with 32 THz and ends with ω_{TO} of $LiTaO_3$. The other one starts with ω_{LO} of $LiTaO_3$ and ends with ω_{LO} of $LiNbO_3$.The third mode has a constant frequency value, which is ω_{LO} of $LiNbO_3$ Fig.1(b). Polariton dispersion of quantum well superlattice at 600 K. When the temperature rises to 600 K we get the similar behaviour except the starting point of three upper modes increases. Hence the width of the polaritonic gap increases. Polariton dispersion of quantum wire superlattice at room temperature .

Polariton dispersion of quantum wire superlattice at 600K. In case of quantum wire, there is no appreciable change in the polariton dispersion at 600 K when compare to room temperature except the changes observed in the upper modes at 600 K. Hence the polaritonic gap increases with temperature. Fig 2(a) and Fig. 2(b), explain polariton dispersion of quantum dot SL at room temperature and at 600 k respectively. There are three modes of propagation. The interfacial modes starts with 32 THz and becomes constant (ω_{TO} of $LiTaO_3$).When temperature increases , the dispersion shift towards the higher wavevector region. Polariton dispersion of quantum well superlattice at room temperature at the brillouin zone edge is shown in Fig 3(a) and Fig 3(b); represent the same at 600K. Five modes of propagation as suggested in the literature. At the long wave vector, the first four modes merge as shown in the figures and give two surface modes ω_{LC1} andω_{LC2} .However, the top most mode having frequency in the range of 10^{15} cps, (which is not shown in figure) behaves as the normal upper mode behaviour of polariton dispersion. This mode at qL = π *i.e.*, at the Brillouin zone edge of the SL has a frequency,$\omega = \frac{cq}{\sqrt{\varepsilon_\infty}} \approx 10^{15}$ where is the dielectric constant at optical frequencies corresponding to that of a composite medium defined by

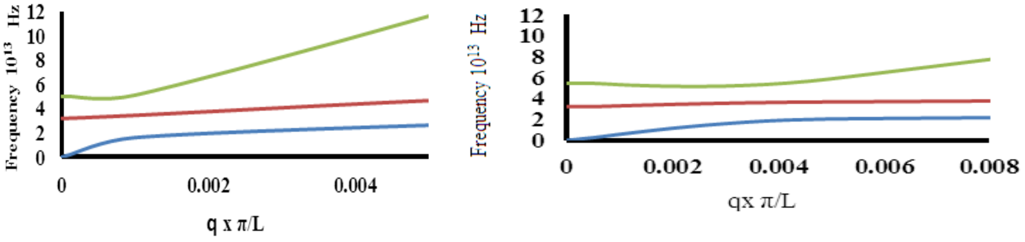
$$\varepsilon_\infty = \frac{\varepsilon_A(\omega)\varepsilon_B(\omega)}{\varepsilon_A(\omega)+\varepsilon_B(\omega)} \qquad (8)$$

The frequency of this mode, however, reduces by about two orders when qL = 0 *i.e.*, at the Brillion zone centre. When the temperature increases, the value of ω_{LC1} increases and the top mode frequency decreases. The temperature effect of the quantum wire and quantum dot is also similar to quantum well system.



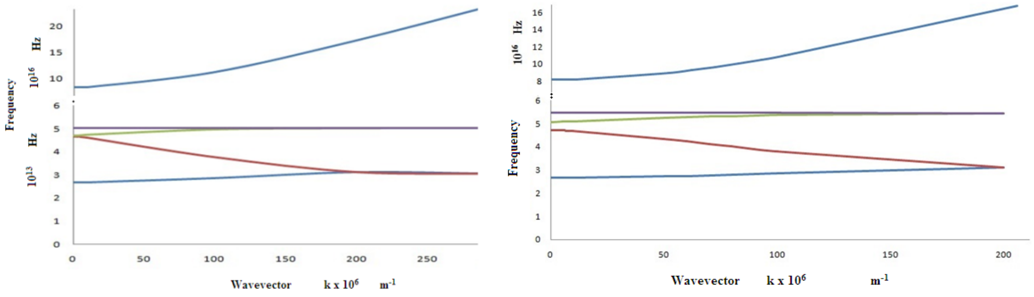
(a) (b)

Fig. 1- Polariton dispersion of quantum well super lattice at (a) room temperature (b) 600 K (qL=0)



(a) (b)

Fig. 2-Polariton dispersion of quantum dot at (a) room temperature (b) 600 K (qL=0).



(a) (b)

Fig. 3- Polariton dispersion of quantum well superlattice at (a) room temperature (b) 600 K (q=π/L).

CONCLUSION:

The behavior of various modes of the phonon polariton dispersion at various temperatures is investigated systematically. The polar tonic gap, with in which no electromagnetic radiation can pass through is almost same at all the temperature except at the transition region. It is found that when the temperature increase the dispersion shifts to new values. It is extended to LiNbO3/LiTaO3 quantum well, quantum wire and quantum dot super lattices. It is found that there is no appreciable change occurs in the polaritonic dispersion except a shift towards higher frequency region.

CONFLICT OF INTEREST

Authors don't have any conflict of interest related to the manuscript.

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