

ICONN 2015 [4th -6th Feb 2015]
International Conference on Nanoscience and Nanotechnology-2015
SRM University, Chennai, India

Analysis of Polariton Dispersion in Dielectric-Ferroelectric superlattices

K.S. Joseph Wilson¹, A. Malarkodi^{1*} and V. Revathy¹

¹Department of Physics, Arul Anandar College (Autonomous),
Karumathur, Madurai – 625 514, India

Abstract: The variation of dielectric constant with temperature of bulk materials like CaTiO₃ & BaTiO₃ are analysed. Hence, the phonon polariton dispersion of the Dielectric-Ferroelectric (CaTiO₃/BaTiO₃) superlattice is studied. The presence of modes in the Polaritonic gap are investigated. It is found that these polariton modes in the forbidden gap are tuned by applying external perturbations.

1. Introduction

Ferroelectric/dielectric superlattices can be designed to control the polarization of their dielectric components using the electrostatic boundary conditions at the interfaces¹. The lattice constant of superlattices is electromechanically coupled to the polarization, and depends on the electrostatic state of the superlattice². The structural and electrical properties of the superlattice at zero external electric field have been well established both experimentally³ and theoretically⁴ based on the electrostatic energy argument. How both the overall polarization and the lattice parameter of the superlattice response to applied electric fields, however, remains an important open question.

The polarization switching process in the superlattice is affected by the electrostatic energy of neighboring domains with differing polarization states. Nano-scale domain can form within superlattices due to the bound charge at interfaces⁵. Polarization switching results in a coupling between the structural properties and the polarization because the lattice distortion is proportional to electric polarization⁶. By probing the structural and electrical properties of a superlattice during polarization switching we obtain insight into how these electrostatic conditions vary in applied electric fields. Here we combine in-situ studies of lattice distortion and electrical displacement current measurements for a ferroelectric/dielectric superlattice capacitor in applied electric fields. A broad distribution of lattice constant was found in electric field region higher than the nominal coercive field.

2. Theory

BaTiO₃ and CaTiO₃ 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. BaTiO₃ and CaTiO₃ belong to trigonal crystals of point group 3m, a negative uniaxial crystal, transparent from 0.33μm to about 5μm. When the temperature of the crystals are increased the values of the optical parameters are altered. For the

ferroelectric crystals the changes in refractive index with temperature is given by $n_{(T)} = n_o(1 + \alpha T)$ -----(1). This equation can be represented in terms of dielectric constants as

$$\epsilon_{\infty(T)} = \epsilon_{\infty}(1 + 2\alpha T) \quad \text{--- (2)} \quad \text{and}$$

$$\epsilon_{0(T)} = \epsilon_0(1 + \beta T) \quad \text{---- (3)}$$

where $\alpha = \frac{dn_o}{dT}$ and $\beta = \frac{dk_1^T}{k_1^T dT}$ are the temperature coefficients⁷. The values of α and β are calculated at room temperature. The changes in transverse optical phonon frequency with temperature is given by $\omega_{TO(T)} = A(T - T_c)^{1/2}$ -----(4). The corresponding longitudinal optical phonon frequency at different temperatures can be determined using LST relation. So that the behavior 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 $\epsilon(\omega)$ is determined by a dispersion relation for an infinite isotropic crystal. The dielectric function for the bulk is given by

$$\epsilon(\omega) = \epsilon_{\infty} + \frac{(\epsilon_0 - \epsilon_{\infty})\omega_{TO}^2}{\omega_{TO}^2 - \omega^2 - i\omega\gamma} \quad \text{-----(5)}$$

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 behavior as a function of frequency is discussed extensively in the literature^{9,10}. However, in the study of polariton behavior, it is required only the real part of $\epsilon(\omega)$. The polariton behavior of the above system can be studied by the following dispersion relation

$$\frac{c^2 k^2}{\omega^2} = \epsilon(\omega) = \epsilon(\infty) + \frac{(\epsilon_0 - \epsilon_{\infty})\omega_{TO}^2}{\omega_{TO}^2 - \omega^2} \quad \text{-----(6)}$$

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 Å. If one constituent, material A, always has thickness d_1 , and the second, material B, always has thickness d_2 , one has built a periodic structure known as a SL. In this work, assuming alternating layers of BaTiO₃ and CaTiO₃ as A and B medium of thickness d_1 and d_2 stacked along the z -direction. Several authors 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:

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

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 $\alpha_i^2 = k_x^2 - \frac{\omega^2}{c^2} \epsilon_i$, where k_x is the component of the wave vector in the X-direction for TM modes.

Results and Discussions:

Using the temperature coefficients α and β [8], the static dielectric constant and high frequency dielectric constants 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. Here when the temperature increases, the optical phonon frequencies decreases. In Fig.1 we have plotted the polariton dispersion at temperature $T = 294$ K assuming $d_1=50\text{Å}$ and $d_2=50\text{Å}$. We found five

branches. The first four modes are the symmetric and antisymmetric interfacial modes approaching the surface mode frequencies of the BaTiO₃ and CaTiO₃ materials as $k \rightarrow \infty$. However, the top most mode having frequency in the range of 10^{15} cps, (which is not shown in Fig) behaves as the normal upper mode behavior of polariton dispersion. The frequency of this mode, however, reduces by about two orders when temperature increases as shown in Fig.2.

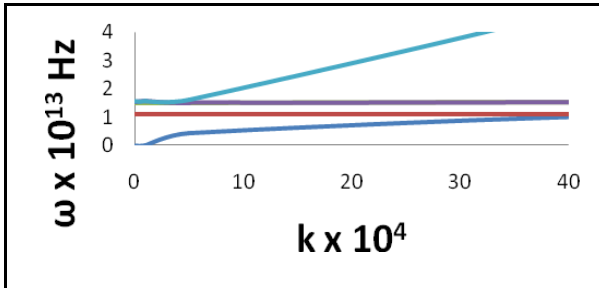


Fig.1.Polariton dispersion at temperature T= 294 K

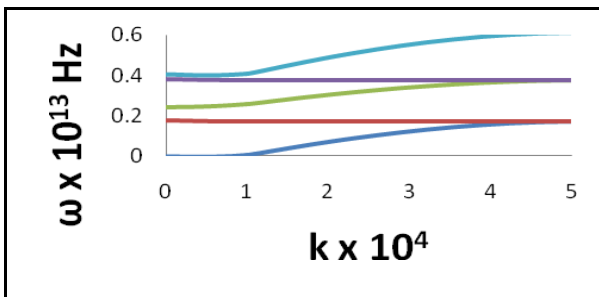


Fig.2 .Polariton dispersion at temperature T=300 K

Conclusions:

The dielectric constant of Bulk materials like CaTiO₃ & BaTiO₃ are analysed. It is found that the dielectric constant increases with temperature while the optical phonon frequency decreases. The polariton dispersion is found to be as usual with other ferroelectric materials. The phonon polariton dispersion of Dielectric-Ferroelectric (CaTiO₃/ BaTiO₃) superlattice at various temperatures is also studied. The dispersion is shifted to lower values with increase of temperature.

References

1. J. B. Neaton and K. M. Rabe, Appl. Phys. Lett. 82, 1586 (2003).
2. H. N. Lee, H. M. Christen, M. F. Chishlom, C. M. Rouleau and D. H. Lowndes, Nature 433,395 (2005).
3. W. Tian, J. C. Jiang, X. Q. Pan, J. H. Haeni, Y. L. Li, L. Q. Chen, D. G. Schlom, J. B. Neaton, K. M. Rabe and Q. X. Jia, Appl. Phys. Lett. 89, 092905 (2006).
4. V. A. Stephanovich, I. A. Lukyanchuk and M. G. Karkut, Phys. Rev. Lett. 94, 047601 (2005).
5. S. Lisenkov, I. Ponomareva and L. Bellaiche, Phys. Rev. B 79, 024101 (2009).
6. A. Grigoriev, R. Sichel, H. N. Lee, E. C. Landahl, B. Adams, E. M. Dufresne and P. G Evans, Phys. Rev. Lett. 100, 027604 (2008).
7. Landolt Bornstein, New Series 111,6 Springer Berlin,Heidelberg (1971).
8. Introduction to Solid State Physics John Wiley &sons Singapore(2005) C. Kittel.
9. V.V.Ursaki, F.J.Manjon, K.Syassen, I.M.Tiginyannu, G.Irmer, and J.Monecke J.Phys.: Condens. Matter 14, 13879 (2002)
10. A.Sarua, J.Monecke, G. Irmer, I.M.Tiginyannu G.Gartner and H.L.Hartnagel J.Phys. Condens. Matter 13, 6687 (2001).
