THE NUMERICAL ANALYSIS OF ATTENUATED TOTAL REFLECTION (ATR) SPECTROSCOPY OF THE SURFACE MODES IN FERROELECTRIC LATTICE MODEL

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Abstract— In this paper, we discuss the effect of the lattice model in dielectric or ferroelectric materials. The lattice model is used when we study the film configuration which includes the surface effect. Together with effective medium approach, the electric susceptibility is derived. Using this susceptibility, we derived the reflectivity of attenuated total reflection (ATR). Employing this formulation, we calculate numerically ATR reflection spectra by taking parameters appropriate for $BaTiO_3$. We obtain that inhomogeneity in lattice model lead to the existence of the disturbance in ATR spectra. The frequency of the disturbance approach resonance frequency if the number of lattice is increased. The disturbance will disappear when the number of lattice is equivalent to bulk thickness.

Keywords— Lattice model; Ferroelectric; Surface model; Attenuated total reflection (ATR);

I. INTRODUCTION

The Attenuated Total Reflection (ATR) is a non-destructing method to probe the existence of polaritons in a functional material. This method enables sample material to be analysed directly without doing specific preparation. This technique is able to examine both aqueous and solid samples.It is well known, that the method is successfully used in metal surface to show the existence of surface Plasmon polaritons [1], in magnetic system to proof the emergence of magnon polaritons [2], in dielectric system to generate phonon polariton [3], and also in multiferroic system to get the magnon and phonon polaritons [4]. Since this technique is based on total internal reflection phenomena, therefore it requires high index prism which is laid out above the sample. This prism ensures total reflection in the bottom of prism if there is no interaction between initial electromagnetic waves and elementary excitation of the material. When the coupling between electromagnetic waves and elementary excitation of sample are generated lead to the modified electromagnetic waves, the reflectance values will decrease.

In ferroelectrics samples where the elementary excitation is phonon resulted from lattice vibrations, the incoming electromagnetic waves will couple to the phonons around the phonon frequency of the sample. Hence, the ATR reflectance decreases near this frequency illustrating the generation of the phonon polaritons. The sharp dip represents surface modes while the shallow decrease illustrates bulk modes. In numerical calculation of ATR reflectance for ferroelectric sample, the spontaneous polarizations of the ferroelectrics are usually treated as homogeneous parameter.

It was shown that a homogeneous polarization suitable for ferroelectrics in bulk geometry. When the geometry of ferroelectrics is film, the spontaneous polarization becomes inhomogeneous lead to the emergence of disturbance in susceptibility curve. Since the ATR reflection spectra are affected by the susceptibility of the sample, hence the characteristic of the ferroelectric polarization can be observed in ATR spectra. Even though the ATR technique had used to study surface modes in ferroelectric sample, however, as best as our knowledge, the numerical ATR spectra for dielectric lattices model where the effective electric susceptibility is derived using entire-cell effective medium calculation have not yet been discussed. According to the effective medium theory, the lattice or layered model can be treated as a single medium which possess effective permittivity and effective permeability depend on the type of material. Hence, the aim of this paper is to present the ATR spectra in the relation with the effective permittivity of the lattices model offerroelectric.

II. RESEARCH METHOD

The geometry of the study is illustrated in Fig.(1). The lattice model is shown in Fig.(1a). The surface of material is placed in y-z plane while it is sliced along z direction into several lattices. The ATR configuration is explained in Fig.(1b). A high index prism is placed above ferroelectric lattice model with a gap d between the bottom of prism and the surface of ferroelectric as illustrated in Fig.(1). This geometry is well known as Otto configuration. Wefocus the study in transverse magnetic (TM) mode where the magnetic component of electromagnetic waves is perpendicular to the reflection plane. Hence, there are only three components of electromagnetic waves which involve in TM modes. One magnetic component (H_x)and two electriccomponents($E_y$andE_z). In this mode, both the bulk and surface mode are able to be generated in ferroelectrics. Then, the electromagnetic waves can be given as [4]

$$\vec{H} = \begin{cases} \hat{x}H_m \exp(\beta z)\exp\left[i\left(k_y y - \omega t\right)\right] \text{in sample medium,} \\ \hat{x}[H_{oi}\exp(\beta_0 z) + H_{or}\exp(-\beta_0 z)]\exp\left[i\left(k_y y - \omega t\right)\right] \text{ in gap, and} \\ \hat{x}\left[H_{pi}\exp(-ik_z z) + H_{pr}\exp(ik_z z)\right]\exp\left[i\left(k_y y - \omega t\right)\right] \text{in prism} \end{cases} \quad (1)$$

where$\beta_0 = \left(k_y^2 - \frac{\omega^2}{c^2}\right)^{1/2}$ represents the attenuation constant of vacuum while the attenuation constant of ferroelectric is given as

$$\beta = \left(k_y^2 - \varepsilon\frac{\omega^2}{c^2}\right)^{1/2}. \quad (2)$$

Here, $\varepsilon = I + 4\pi\chi_e$ is permittivity of ferroelectrics.

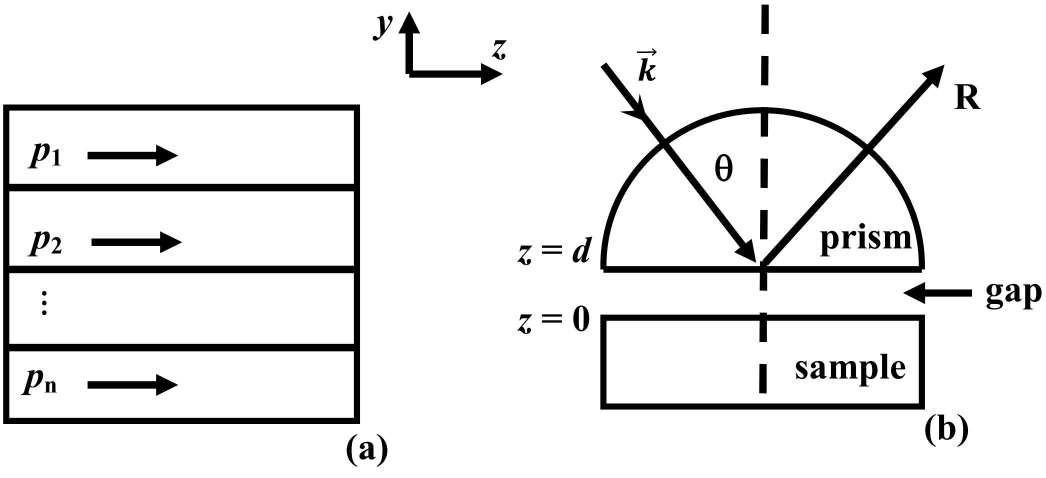

Figure 1.The geometry of the study. In (a) is illustration of the lattice model of ferroelectric. The configuration of the ATR is shown in (b). The surface of material is placed at z = 0 while the bottom of the prism is located at z = d above the sample material.

Using Maxwell's equation together with the constitutive equations to the Eq.(1), it is easy to derive the induced magnetic fields $\vec{B}$, the electric fields $\vec{E}$ and the electric displacement fields $\vec{D}$.

After that, using the continuity of fields which are continuity of tangential $\vec{E}$, normal $\vec{D}$, tangential $\vec{H}$ and normal $\vec{B}$ in the involved surfaces, the ATR reflectance can be derived as

$$R = \left|\frac{k_z[1+r\exp(-2\beta_0 d)]-i\varepsilon_p\beta_0[1-r\exp(-2\beta_0 d)]}{k_z[1+r\exp(-2\beta_0 d)]+i\varepsilon_p\beta_0[1-r\exp(-2\beta_0 d)]}\right| \quad (3)$$

Where d is the gap between prism and sample, ε_p represents the permittivity of the prism and r is reflectance in the surface of the material at z = 0. This reflectance is determined as

$$r = \frac{\varepsilon\beta_0-\beta}{\varepsilon\beta_0+\beta} \quad (4)$$

where ε is permittivity of the sample.

In order to derive the electric susceptibility of the sample ferroelectric, we firstly determine the density energy of the system. In ferroelectric lattice model, we set the density energy as [5]

$$F = \sum_{i=1}^{n}\left\{\frac{a_0}{2}[T-T_C]P_i^2+\frac{\beta}{4}P_i^4+\frac{K}{2}[P_i-P_{i-1}]^2-E_iP_i\right\}. \quad (5)$$

Here, P_i represents lattice's polarization, $T_C$is Curie's Temperature. Parameters $a_0$and β are ferroelectric stiffness constant while K is lattice's interaction constant. In this study, we set the direction of external electric field E_i parallel to the electric polarization. The susceptibility can be derived by using Landau-Khalatnikov equation of motion as:

$$\frac{\partial^2 P_i}{\partial t^2} = -f\frac{\partial F}{\partial P_i} \quad (6)$$

Where f is inverse of phonon mass. Here, we assume that polarization and external electric field comprise of static and dynamic terms such as $P_i = P_i^s + p_i$ and $E_i = E_i^s + e_i$ where the dynamic terms (p_i; e_i) are much smaller than static terms (P_i^s; E_i^s). In this calculation, the dynamic terms are related to time as $p_i, e_i \propto e^{-i\omega t}$.Then, we use these polarizations and fields together with Eq.(5) into L-K Equation of motion Eq.(6). After linearization and considering only the dynamic terms, we obtain

$$\sum_{i=1}^{n}[(\omega_i^2-\omega^2)p_i - Kfp_i = fe_i] \quad (7)$$

Where the frequency ω_i is defined as

$$\omega_i = \left\{f\left[a_0T_C\left(\frac{T}{T_C}-1\right)+3\beta(P_i^s)^2+3KP_i^s\right]\right\}^{1/2}. \quad (8)$$

Then, using continuity of tangential component of dynamic electric fields e as:

$$e_1 = e_2 = \cdots = e_n = C_z \quad (9)$$

and setting the value of C_z, we can solve Eq.(3) to obtain p_i. Susceptibility is calculated using relation

$$\langle p_i\rangle = \chi_e\langle e_i\rangle \quad (10)$$

with two sets of C_z .

III. RESULT AND DISCUSSION

In the calculation of the ferroelectric permittivity, the values of the parameters used are: $a_0 = 6.65 \times 10^5 Vm/C^{-1}K^{-1}$, $\beta = 3.56\times 10^9 Vm^5/C^3$, $K = 4.51 \times 10^{-9} Vm^3/C$ and Curie temperature T_c = 391 K illustrating ferroelectric material $BaTiO^3$.For the calculation of the ATR reflectance, the prism has an index of refraction, n = 3.4 illustrating silicon prism. Using 5 and 10 lattices for the lattice model of ferroelectric and setting the initial angle at 30^o. If the gap is arranged atd = 0.4 mm, we obtain the ATR spectra which are illustrated in Fig.(2).

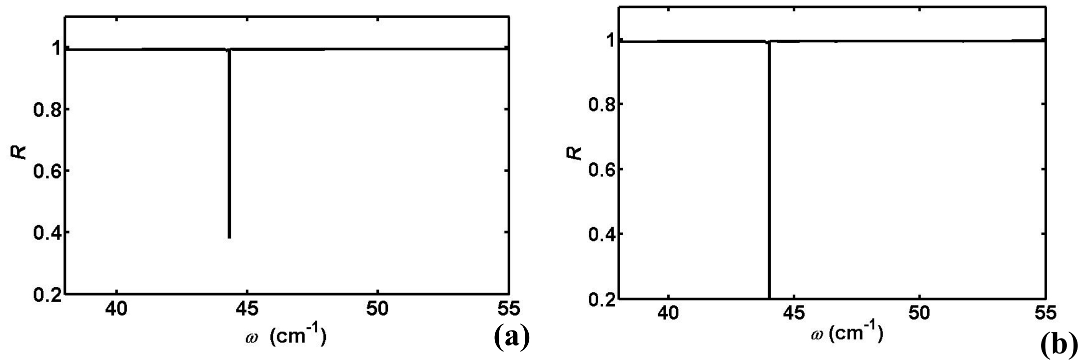

Figure 2.The ATR spectra of ferroelectric lattice model. In (a), the number of lattice is 5 lattices while in (b)is 10 lattices.

It can be seen from ATR reflection spectrum in Fig.(2) above that there are sharp dips around frequency 44 cm^{-1} which are illustrating the generation of surface modes. These surface modes are just above the resonant frequency of BaTiO3 in lattice model (43cm^{-1}) [6]. It is well known that the surface modes can be found in the region between resonant frequency and the zeros of permittivity of the sample. Hence, these results agree with the findings from previous studies.

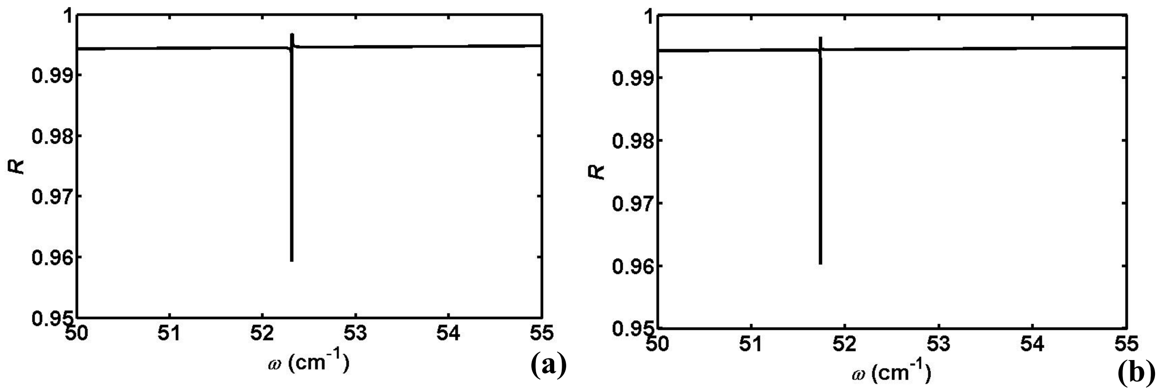

Figure 3.The disturbance of ATR spectra of ferroelectric lattice model. In (a), the number of lattice is 5 lattices while in (b) is 10 lattices. It can be seen that the increase of the number of lattice from 5 lattices to 10 lattices shift the frequency of ATR disturbance approaching resonant frequency.

However, if we decrease the gap from d = 0.4 mm into d = 0.2 mm, we can notice the existence of disturbance of the surface modes around frequency 52 cm^{-1}as illustrated in Fig.(3). The disturbance has only little decrease in ATR reflectance. This surface modes disturbance appears as a result of the inhomogeneity of lattice polarization. The inhomogeneity of the electric polarizations emerges as a result of edge effect. By increasing the number of lattices, the homogeneity of electric polarization of the sample becomes increase lead to the shift of disturbance frequency of the electric susceptibility approaching resonance frequency. Then, this behaviour also initiatesthe frequency shift of the disturbance in ATR reflectance spectrum. In certain number of lattices, the frequency of the disturbance in susceptibility will merge with the resonant condition lead to the disappearance of the disturbance both in susceptibility and ATR reflectance spectra. This condition reflects the bulk behaviour.

IV. CONCLUSIONS

In lattice model which is usually used in film configuration with finite thickness. This configuration leads to the in homogeneity of the electric polarization. Through the electric susceptibility, the in homogeneity of the electric polarization initiate the disturbance in ATR reflectance spectra even though the reduction of the reflectance is very small.

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