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A Theoretical Study of the Variation in the Curie Temperature of the La and Zr Doped $BaTiO_3$when External Electric Field Is Applied.

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Research Article

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ABSTRACT

As Barium Titanate ($BaTiO_3$) is a noble ferroelectric material and has enormous applications in various electrical and electronics applications. Different properties of $BaTiO_3$ depend on the Curie temperature of the material and the Curie temperature varies with the introduction of different impurities and the concentration of that impurity. In the present study an expression has been derived for the variation in the Curie Temperature T_c, by using double time temperature dependent Green's function and a modified Joseph Hamiltonian. In the formalism the fourth order anharmonic phonon-phonon interaction is considered. The variation of the T_c is also studied under the effect of applied electric field and the results are compared with the previous studies achieved by different researchers.

INTRODUCTION

The Perovskite family includes many Titanates used in various electro-ceramic applications, such as electronic, electro-optical, and electromechanical application of ceramics. Barium Titanate, a Perovskite structure is a common ferroelectric material with a high dielectric constant, widely utilized to manufacture electronic components such as multilayer capacitors (MLCs), PTC thermistors, piezoelectric transducers, and a variety of electro-optic devices [1]. Because of the great demand of these non-conducting ceramic materials peoples are going to reduce the size of all the communication devices as small as possible. Because of which materials with high dielectric constant like Barium titanate are very important in ceramic materials. The changes in the physical properties are also remarkable when one system is mixed with the other to form a composite system and their study helps in understanding basic mechanism of mixed crystal formation. For example solid solution of the BT ceramics with the other ferroelectric Perovskites of same class and also with certain compounds which are not themselves ferroelectric materials possess ferroelectric properties and change in the composition of their solid solutions leads to change in the Curie point within the broad range of the temperature.

In the recent year, among all these ferroelectric Perovskites of mixed systems $Ba_{1-x}La_xTiO_3$ (BLT) and $Ba_{1-x}Zr_xTiO_3$ (BZT) has been found an interesting series because of the unique and interesting ferroelectric properties of these ceramic materials which are applicable in various potential applications and also these materials are studied very less so these have large scope in the field of research.The dependence of the Curie temperature on the impurities added in ferroelectric crystals is discussed by many workers[2-5] considering the change in mass and harmonic force constant between the impurity atoms and host lattice atoms. They have obtained a general expression and not taken a specific crystal. But this work is slightly different from their work[2,3] aswe have considered a mixed composite of BT containing La or Zrsubjected toan external electric field.

The aim of the present work is to study theoretically the electric field and defect dependent curie temperature in anharmonic polycrystalline mixture of $Ba_{1-x}La_xTiO_3$ (BLT) and $Ba_{1-x}Zr_xTiO_3$ (BZT) in paraelectric phase by using the double time thermal Green's function technique. Double time thermal green's function is used to obtain thermally averaged correlation function and hence, the observable quantities with the help of modified model Hamiltonian by taking in to account the anharmonic effect upto fourth order with substitutional defects and electric moment terms. The soft mode frequency is held responsible for the anomalous behaviour of the

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ferroelectric at the stage when T approaches T_c. The calculated results compared with the experimental and theoretical results of other researchers [6,7].

General Formulation

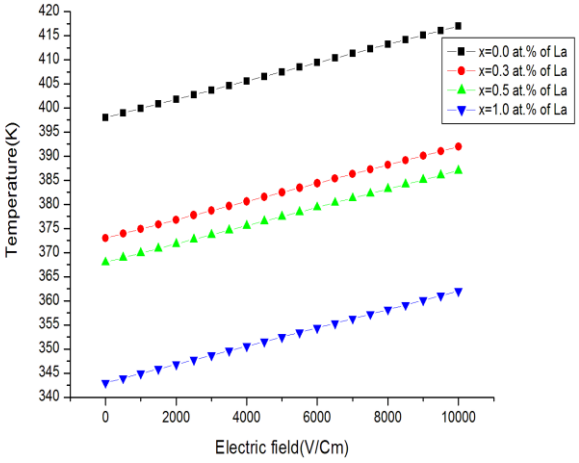

Figure 1(a) Variation of Curie temperature with external applied electric field for La

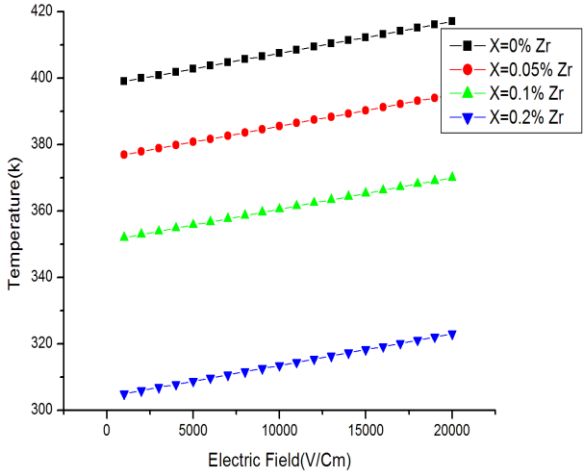

Figure 1(b) Variation of Curie temperature with external applied electric field for Zr

In order to calculate the expression for the various dynamic properties, in the presence of impurity and electric field, we introduced the retarded double time Green's function for the optical phonon as [6],

$$G_0^0(\omega + i\varepsilon) = \ll A_0^0(t)A_0^0(t') \gg_{\omega+i\varepsilon} = G'(\omega) - iG''(\omega), \quad \ldots (1)$$

This gives the real part of dielectric constant as,

$$\varepsilon'(\omega) - 1 = -8\pi^2 M_\mu^2(0) G'(\omega)) \ldots (2)$$

$$\tan\delta(\omega) = G''(\omega)/\, G'(\omega) \ldots (3)$$

where G' (ω) and G" (ω) are real and imaginary parts of the green's function G (ω).

Writing the equation of motion for the Green's function (Eq. (1) with the help of modified Hamiltonian [6], Fourier transforming and writing it in the Dysons Equation, one obtains

$$G_0^0(\omega + i\varepsilon) = \omega_0^0/\pi[\omega^2 - \bar{v}_0^{0^2}(\omega) + i\bar{\Gamma}_0^0(\omega)] \ldots (4)$$

$$\text{where } \bar{v}_0^{0^2}(\omega) = -(\omega_0^0)^2 + 4\omega_0^0 D(0,0) + \omega_0^0 E^2(96g^2V - 24g D_1') + 4\omega_0^0\bar{Q} + \bar{\Delta}_0^0(\omega) \ldots\ldots\ldots\ldots (5)$$

Here $\bar{\Delta}_0^0$is defect, temperature and field dependent shift of soft mode frequency. g and $D'_1$are linearand second order electric moment coefficients respectively. D (0, 0) is defect dependent parameter depending upon harmonic force constant change.

Variation of Curie temperature (T_c) with Electric field (E)

Impurity dependent Curie temperature (T_c) in $Ba_{1-x}La_xTiO_3$ (BLT) and $Ba_{1-x}Zr_xTiO_3$ (BZT) (BZT) for different concentrations have been taken from the best fit of the data from the study of Wei Cai et.al. [2] and Binhayeeniyi et.al.[3] respectively. Using Equation ($T_c' = T_c + (1.9*10^{-3})E$) (V/cm) we have calculated the field dependent Curie temperature in BZT and BLT. Figure 1(a), shows the variation of Curie temperature with the external electric field as a parameter for $Ba_{1-x}La_xTiO_3$ (BLT) for different concentrations of La. Figure 1(b) shows the variation of Curie temperature with the external electric field as a parameter for $Ba_{1-x}Zr_xTiO_3$ (BZT) for different concentrations of Zr

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RESULTS AND DISCUSSION

The calculated value shows the comparative variation of the Curie temperature (T_c) and Electric field (E) in $Ba_xLa_{1-x}TiO_3$ and $Ba_xZr_{1-x}TiO_3$. Figure 1(a) and Figure 1(b) are showing the variation of Curie temperature (T_c) and electric field (E) for $Ba_{1-x}La_xTiO_3$ and $Ba_{1-x}Zr_xTiO_3$ respectively. It is clear from the both the figures(a) and 1(b) that taking any impurity concentration of La and Zr the Curie temperature increases linearly increasing external electric field strength. The variation is same for all the values of the 'x' as shown in both the figures. The results obtain are in good agreement with the previous experimental results [6, 7].Kanzig and Maikoff[8] had discussed the effect of electric field on the Curie temperature and investigated that the Curie temperature $T_c$in $BaTiO_3$ shift to a higher value by an amount proportional to the strength of electric field applied. So from this it can be concluded that the at sufficiently high field strength the crystal may became ferroelectric at temperature above its zero field Curie temperature.

The La or Zr doped barium titanate is a family which covers wide range of Curie temperature. When these impurity atoms are introduced to barium Titanate'sPerovskite crystal structure the ferroelectric to paraelectric phase transition temperature decreases and on application of external electric field this phase transition Curie temperature increases.

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