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Thermal Conductivity of $Ba_xCa_{1-x}TiO_3$

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Abstract: We have discussed the variation of thermal conductivity in the case of $Ba_xCa_{1-x}TiO_3$ ferroelectric perovskites using Silverman Hamiltonian in presence of defect and electric field and Green's Function Technique. The thermal conductivity decreases with the increasing electric field and defect. The results are consistent with previous experimental and theoretical results.

Keywords: Pervoskites • BCT • Thermal Conductivity • Electric Field • Temperature • Defect

Introduction

The discovery of $BaTiO_3$ is of particular scientific and technological importance. It is very well known that $BaTiO_3$ is used in holographic memory, phase conjugate mirror applications, ultrasonic transducers (Mason, 1972), ceramic capacitors (Yoon, 2008) and IR sensor applications (Noh et al, 2008). $BaTiO_3$ has unique combination of photorefractive, piezoelectric and electro-optical properties (Nayak et al, 1999). $BaTiO_3$ has high mechanical strength, heat and moisture resistance, ferroelectricity over a wide temperature range, and is easy to manufacture, which have it preferable over formerly known ferroelectrics. The solid solution of $BaTiO_3$ with other pervoskite materials like $CaTiO_3$, $SrTiO_3$, $PbTiO_3$, $PbSnO_3$, $BaZrO_3$ etc (Mason 1972, Pandey et al 1992, Zhigang and Gang 1990, Kajtoch 1992, Sining and Xiaoli 2006, Qin et al 2007) are interesting materials.

Recently, the Barium Calcium Titanate (BCT) perovskite solid solutions have become an interesting field of study and research (Pandey et al, 1992). BCT is a leading material for under cooled detector fabrication, photo refractive mirrors (Kuper et al 1998, Korneev et al 1999) and as a gate insulator of the oxide superconductor [12]. According to our studies The Curie temperature changes greatly depending on the amount of Ca (Pradeep and Naithani, 2010) and dielectric constant (Pradeep et al, 2010). BCT ceramics [Noh et al 2008, Sining and Xiaoli 2006, Kobayashi and Konayshi 1994, Pradeep and Naithani 2010, Pradeep et al 2010, Xueqin et al 2009) now have increasing demand of dielectric and ferroelectric properties in the area of electronics and communication. That is the reason for inclusion of DRAM, FeRAMs for high charge storage devices, gate dielectrics, microwave applications etc. while other traditional areas are being continuously explored.

Thus it is evident that Barium Calcium Titanate (BCT) is a solid solution between $BaTiO_3$ and $CaTiO_3$, in which the Curie temperature Tc of the ferroelectric varies depending on the value of (x). In this paper solid solutions of $Ba_xC_{1-x}TiO_3$ (for x = 0.5, 0.8, 1) have been widely studied.

Normally $BaTiO_3$ is mixed with $CaTiO_3$ for $Ba_xCa_{1-x}TiO_3$. The aim of the present paper is to find an expression for the defect and field dependent thermal conductivity of $Ba_xCa_{1-x}TiO_3$ by using the approach of reference (Naithani et al, 1977). A current review on $Ba_xCa_{1-x}TiO_3$ is available in the literature (Puli et al 2014, Singh et al 2015, Kadira et al 2016, Silvaa et al 2016, Xu et al 2018, Wang 2022) and references therein. For simplicity the ions are assumed to be non-polarizable.

General Formulation

The thermal conductivity is expressed by Kubo formula as Naithani et al (1977).

$$K = \lim_{\varepsilon\to 0}(k_B\beta/3V)\int_0^\infty dt e^{-\varepsilon t}\int_0^\beta d\lambda < Q(0);Q(t+i\hbar\lambda) > \qquad ...(1)$$

the flux operator Q(t) will be

$$Q(t) = \sum_k \hbar\omega_k^a v_k^a N_k^a(t) + \sum_k{}' \hbar\omega_k^0 v_k^0 N_k^0(t)$$

$$= \sum_{k\lambda}{}' \hbar\omega_k^\lambda v_k^\lambda N_k^\lambda(t) \qquad ...(2)$$

where optical and acoustical modes are represented by o and a respectively. Thus,

K= K^a + K^o = □K□ ; □=o, a;

where,

$$K^\lambda = \lim_{\varepsilon\to 0}(\hbar^2 k_B\beta^2/3V)\sum \omega_k^\lambda\omega_{k'}^\lambda v_k^\lambda v_{k'}^\lambda \int_0^\infty dt e^{-\varepsilon t}\int_0^\beta d\lambda' < N_k^\lambda(0);N_{k'}^\lambda(t+i\hbar\lambda) > \qquad ...(3.1)$$

$$< N_k^\lambda(0);N_{k'}^\lambda(t') > = < a_k^\lambda(0)a_k^{\lambda\dagger}(t) > \qquad ...(3.2)$$

The notation used are the same and in the same sense as used by Naithani et al (1977).

The value of the parameters are the same and used in the same sense as by Naithani et al (1977).

$$K = \left(\frac{\hbar^2 K_B\beta^2}{3V}\right)\sum_{k\lambda}(\bar{\omega}_k^\lambda)^2(\upsilon_k^\lambda)^2\frac{\exp(\beta\hbar\bar{\omega}_k^\lambda\lambda)}{\{\exp(\beta\hbar\bar{\omega}_k^\lambda)-1\}^2}\cdot\frac{1}{\bar{\Gamma}_k^\lambda(\omega)} \qquad ...(4)$$

Results and Discussion

$\bar{\Gamma}_k^\lambda(\omega) =$ A + BT + CT^2 + DE^2T, coefficient A is temperature independent of temperature and depend only on impurity. Coefficients B is the coefficient of T and and C is the coefficient T^2. B and C are anharmonic terms. Coefficient D is a cross term of defect and electric field. Solving this equation thermal conductivity is given as,

$$K = \frac{G'(E^2+1)(T-T_C')}{T(1+G''E^2)(T-T_C)}$$

Where G''□ D/B, and G' = D, where D is a constant. The values of D were calculated according to Landolt Bornstein series (1981) by best fit of data. We have calculated the thermal conductivity of pure anharmonic $Ba_xCa_{1-x}TiO_3$ crystals in their Paraelectric phase. These calculated values are displayed as shown in Figures 1-3 respectively for different values of *x* and the electric field. Figures 1–3 show the variation of thermal conductivity with temperature and electric field strength for different values of *x* in the paraelectric phase.

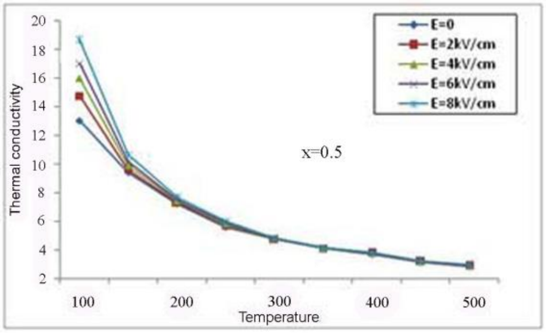

Fig. 1 : Variation between Thermal Conductivity and Temperature (in K) for $Ba_{0.5}Ca_{0.5}TiO_3$ at different electric fields.

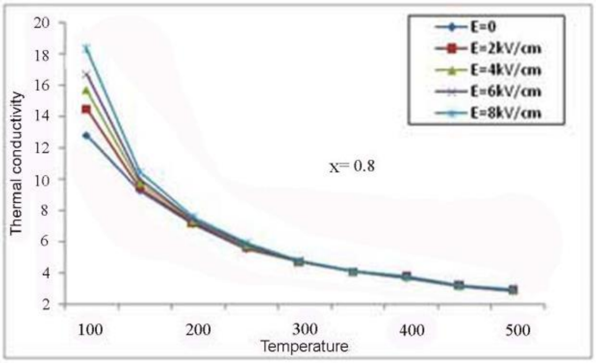

Fig. 2 : Variation between Thermal Conductivity and Temperature (in K) for $Ba_{0.8}Ca_{0.2}TiO_3$ at different electric fields.

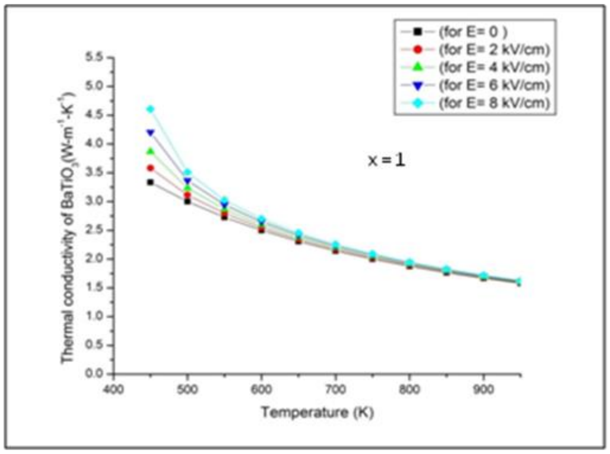

Fig. 3 : Variation between Thermal Conductivity and Temperature (in K) for $BaTiO_3$ at different electric fields.

Conclusion

It is clear from the above figures that with the increase of temperature thermal conductivity decreases in $Ba_xCa_{1-x}TiO_3$. This decrease is larger at low temperatures and smaller at higher temperatures (Yamshita et al 1997, Sharma and Bagadur 1975, Chung et al 2001, Pohl 1968, Pathak 1965). These results are in accordance with those of other workers. It is clear from the figures 1–3 that thermal conductivity decreases with electric field and temperature when defect is present (Steigmeir, 1968). This decrease in thermal conductivity becomes very small at high temperatures. Figures 1 to 3 also show the dependence of the thermal conductivity on the electric field in the paraelectric phase in $Ba_xCa_{1-x}TiO_3$. This disparity is similar to the result of other workers (Landolt Bornstein Series 1981, Pohl 1968, Steigmeir 1968).

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