P: ISSN No. 2231-0045 RNI No. UPBIL/2012/55438 VOL.-8, ISSUE-4 May -2020

E: ISSN No. 2349-9435 Periodic Research

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

Paper Submission: 10/05/2020, Date of Acceptance: 25/05/2020, Date of Publication: 26/05/2020

Abstract

Using the approach of our previous paper (IJERD, Vol. 4, pp. 61-67, October, 2012) we have discussed the variation of thermal conductivity in the case of $Ba_xSr_{1-x}TiO_3$ ferroelectric perovskites. The thermal conductivity decreases with the increasing electric field and defect. The results are in agreement with previous experimental and theoretical results.

Keywords: Pervoskites, BST, Thermal Conductivity, Electric Field, Temperature Defect.

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Introduction

The most widely used ferroelectric occur in perovskite family which possess the general formula ABO_3. Barium Strontium Titanate $Ba_xSr_{1-x}TiO_3$ is a solid solution between $BaTiO_3$ and $SrTiO_3$ which posses different Ferroelectric Curie temperature. Barium Strontium Titanate (BST) posses an adjustable value of Ferroelectric Curie temperature Tc depending on the value of (*x*). BST used has wide range of applications depending on Curie temperature and Dielectric properties. Among the pervoskites mixed systems BST is an interesting series because of its unique ferroelectric properties which are suitable for various potential applications. BST has been identified as the leading material for under cooled detector fabrication, photorefractive mirrors [1]. BST is used in communications especially in microwave tunable circuits, phase shifter, waveguides, antennas, MOSFET, MLCCs and varactor etc.

We have in [2], discussed the field dependent thermal conductivity of $SrTiO_3$, $BaTiO_3$ and $KTiO_3$ ferroelectric perovskites. Normally $BaTiO_3$ is mixed with $SrTiO_3$ for $Ba_xSr_{1-x}TiO_3$. Naithani and Semwal [3] and Naithani *et al.* [4] have also obtained general expression for thermal conductivity in an anharmonic crystal but did not choose any specific case. The aim of the present paper is to find an expression for the defect and field dependent thermal conductivity of $Ba_xSr_{1-x}TiO_3$ by using the method of double time temperature dependent Green's function in this perovskite using a transformed model hamiltonian for ferroelectric crystal, augmented with an harmonicity up to fourth order and electric dipole moment terms. A current review on $Ba_xSr_{1-x}TiO_3$ is available in the literature [5]-[8]. For simplicity the ions are assumed to be non-polarizable.

General Formulation

Kubo formula expresses the thermal conductivity as

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

where k_B, V, $\hbar$, T and Q(t) are the Boltzmann Constant, volume of the crystal, Plank constant divided by 2□, absolute temperature and the heat current operators of lattice, in the Heisenberg representation and the angular brackets <--> indicate the thermal average over the canonical ensemble described by the Hamiltonian

$<O> = Tr. (e^{-□H}, O) / Tr. (e^{-□H})$

Where Tr. denotes the trace of the expression and H be Hamiltonian of the system.

We write the diagonal part of the flux operator Q as a sum of two operators contributed by optical and acoustical phonons separately, i.e.,

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

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

where o and a are used for optical and acoustical modes respectively. Single index k represents K_S, denoting polarization and v^{λ}_k represents the velocity of sound for optic (k=o) and acoustical (k=a). The diagonal contribution to the thermal conductivity from equation (3), becomes

$K = K^a + K^o = \sum K^{\lambda}$; λ=o, a;

where,

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

… (4.1)

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

… (4.2)

The notation used are the same and in the same sense as used in [2].

The expression for thermal conductivity as used by us in equation (15) of reference [2] is now modified in presence of defect (*x*). The value of the parameters are the same and used in the same sense as in [2].

$$K = \left(\frac{\hbar^2 K_B \beta^2}{3V} \right) \sum_{k\lambda} (\overline{\omega}_k^{\lambda})^2 (\upsilon_k^{\lambda})^2 \frac{\exp(\beta\hbar\overline{\omega}_k^{\lambda}\lambda)}{\{\exp(\beta\hbar\overline{\omega}_k^{\lambda}) - 1\}^2} \cdot \frac{1}{\overline{\Gamma}_k^{\lambda}(\omega)} \quad \text{. . . (5)}$$

Results and Discussion

$\overline{\Gamma}_k^{\lambda}(\omega)$ = A + BT + CT^2 + DE^2T where the coefficients A is independent of temperature and depends upon impurity only. Coefficients B and C are the coefficients of T and T^2 respectively. B and C depend upon third- and fourth order anharmonic coefficients in the potential energy expressions. Coefficient D is a cross term of defect and electric field.

Now using eqns. 20 of [2]

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

Where G'' □ D/B , and G' = D, also D is a constant.

The values of D for $SrTiO_3$ (3132 N/m), for $Ba_{0.5}Sr_{0.5}TiO_3$ (2529 N/m), $Ba_{0.8}Sr_{0.2}TiO_3$ (2017 N/m) and $BaTiO_3$ (1200 N/m) have been calculated by reference [15] by best fit of data. With the help of equation (20) of [2], we have calculated the thermal conductivity of pure anharmonic $Ba_xSr_{1-x}TiO_3$ crystals in their Paraelectric phase. These calculated values are plotted as given in figures 1 to 4 respectively for different values of *x* and the electric field. Figures 1 to 4 show the variation of thermal conductivity with temperature in presence of applied electric field strengths for different values of *x* in the paraelectric phase.

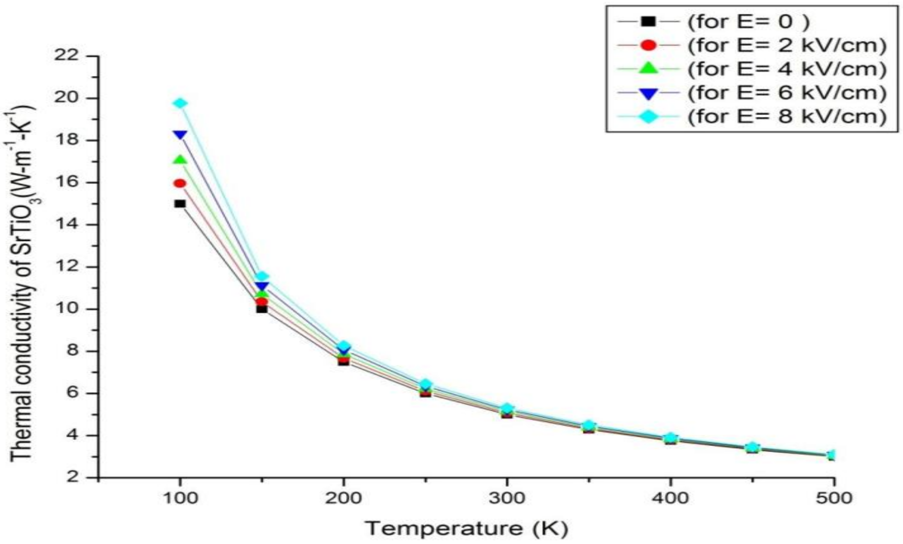

Fig. 1 Thermal Conductivity versus temperature (in K) for $SrTiO_3$ at different Electric Fields

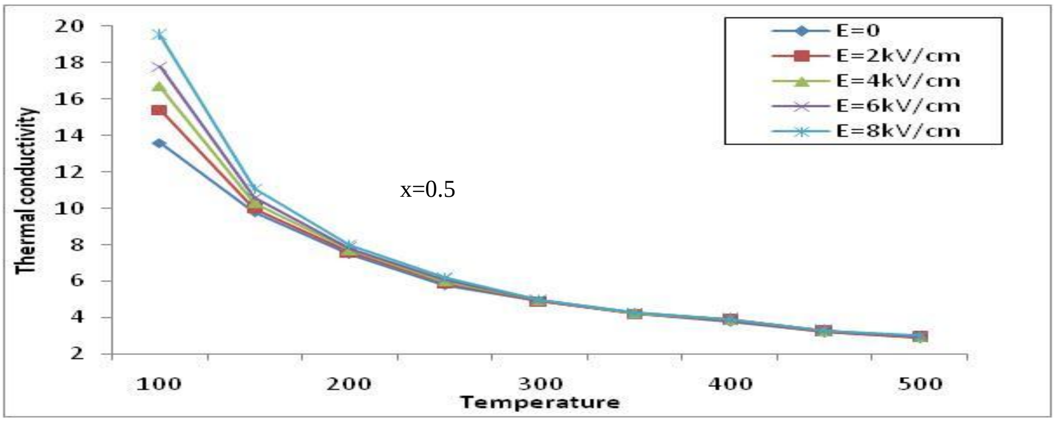

Fig. 2 Thermal Conductivity versus temperature (in K) for $Ba_{0.5}Sr_{0.5}TiO_3$ at different Electric Fields

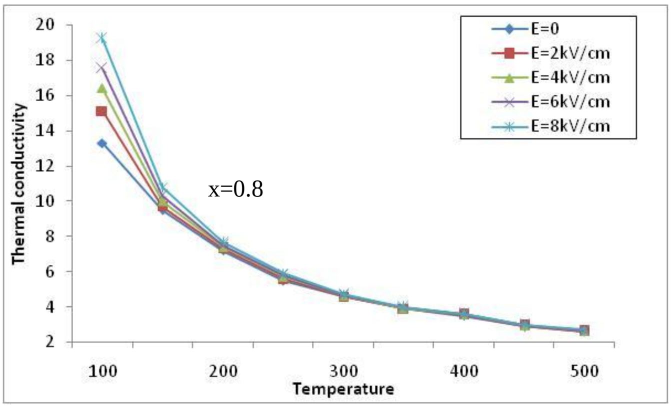

Fig. 3 Thermal Conductivity versus temperature (in K) for $Ba_{0.8}Sr_{0.2}TiO_3$ at different Electric Fields

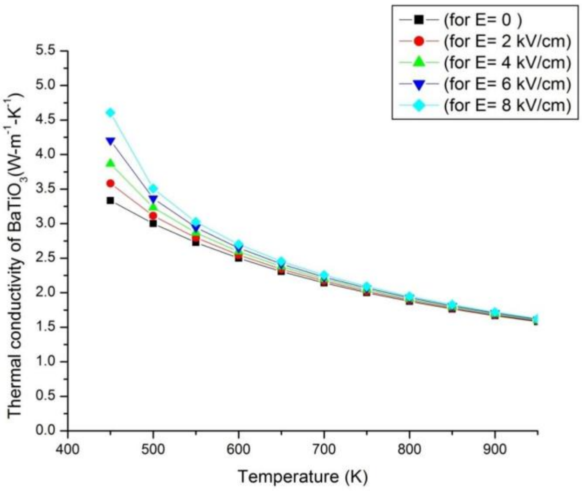

Fig. 4 Thermal Conductivity versus temperature (in K) for $BaTiO_3$ at different Electric Fields

Conclusion

It is evident from these figures that thermal conductivity decreases with increase of temperature in $Ba_xSr_{1-x}TiO_3$. This decrement is large in low temperature case but small in high temperature case [9-13]. These results are in good agreement with the results of other workers. Soft mode is held responsible for this variation of thermal conductivity. The effect of a decreasing electric field is to decrease the total thermal conductivity. It is evident from the figures 1 to 4 that thermal conductivity decreases with electric field and temperature in presence of defect[14]. This decrement in thermal conductivity becomes very small in higher temperature range. Fig. 1 to 4 also show the electric field dependence of thermal conductivity in paraelectric phase in $Ba_xSr_{1-x}TiO_3$. This variation is similar to the result of others [3-4], [12], [14-15]. Recently [16] we have applied double time thermal Green's function technique in obtaining expression for electric field dependent inelastic scattering cross section of neutrons in $Ba_xSr_{1-x}TiO_3$ displacive ferroelectric perovskites.

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