Phonon Dispersion of Perovskite Protonic Conductor $SrTiO_3$

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Abstract

Phonon dispersion relation of cubic Perovskite $SrTiO_3$ is developed on the basis of lattice dynamical simulation method based on de Launey angular force (DAF) constant model. The two types of force constants, central and angular force constants have been considered up to third neighbours. The calculated zone centre frequencies agree well with available existing results. The phonon dispersion curves of $SrTiO_3$ in cubic phase are also drawn. The calculated results are compared and analyzed with available results.

Keywords: - *Phonon dispersion; proton conductor; perovskite; SrTiO3;*

1. Introduction

$SrTiO_3$ is very interesting compound because of the wide applications ranging from superconducting oxide thin films, ferroelectric to proton conducting materials [1, 2]. So it is very important to understand the physical properties of this compound. Lattice dynamics is one of the important properties to understand the proton conducting nature of any material.

In the present work the phonon dispersion curves of $SrTiO_3$ in cubic phase has been plotted using DAF constant model and compared with available results. The phonon dispersion is helpful to calculate other thermal properties like phonon density of state, specific heat etc.

2. Crystal Structure

$SrTiO_3$ compound shows a cubic perovskite-type crystal structure and belongs to the space group Pm-3m. The Wyckoff positions of the atoms are Sr 1a (0.0, 0.0, 0.0), Ti 1b (0.5, 0.5, 0.5) and O 3c (0.0, 0.5, 0.5).

From the point of view of lattice dynamics, the unit cell contains five atoms give rise to 15 phonons (three acoustics and twelve optic). The symmetry of these phonons at the Γ point (in terms of the O_h representation) is

$$O_h = 4\Gamma_{1u} + \Gamma_{2u}$$

Where Γ_{1u} and Γ_{2u} representing the normal modes with triple degeneracy. One Γ_{1u} mode is acoustic and the rest are optical modes. The Γ_{2u} mode is inactive, while Γ_{1u} modes are only IR active. The compound in cubic phase has no Raman mode.

3. Methodology

A de Launey angular force (DAF) constant model [3] has been used to study the phonons in the $SrTiO_3$. In DAF model [3], the relative displacement of the reference atom and one of the neighbors is considered. The forces due to all neighbors are calculated separately and summed up together. The present calculation involves four central force constants α_1 , α_2, α_3, α_4 and four angular force constants α'_1, α'_2, $\alpha'_3$and α'_4 between Ti-O, Sr-O, Sr-Ti and O-O atoms respectively up to third nearest neighbor. In the present calculation the interatomic force constants are obtained by fitting the calculated results of Zamkova et.al [4] at the ZC for transverse infrared active phonon frequencies. The force constants thus calculated are listed in Table 1. Taking these force constants as input parameters, the dynamical matrix is solved at the zone center (ZC) as well as along three symmetric directions [k00], [kk0] and [kkk]. The ZC phonons and phonon dispersion relations in three symmetric directions are plotted and discussed.

4. Results and Discussion

Table 1 presents the calculated inter-atomic force constants of $SrTiO_3$. It is observed that

Force constant α_1 between (Ti-O) is strongest among all other interatomic interactions. Followed by α'_1 between (Ti–O). This suggests that the covalent

bonding between (Ti-O) is strongest than that of others. The larger force constant corresponds to stronger bond give rise to larger value of frequency. One of the central force constant α_2 between (Sr–O) is negative. The negative force constant corresponds to motion along modes that lead to energy lowering. The zone centre phonons frequencies are in good agreement with the result of Zamkova et.al [4].

The phonon dispersion relations of $SrTiO_3$, calculated along symmetry directions in the Brillouin zone are shown in Figure 1. Obtained results of $SrTiO_3$ are in agreement with experimental results [4, 7].

Table 1. Values of force constants (in 10^3 dyne cm^{-1})

Compound:	**$SrTiO_3$**
α_1 (Ti-O)	77.90
α'_1 (Ti–O)	18.35
α_2 (Sr–O)	-11.03
α'_2 (Sr–O)	5.0
α_3 (Sr–Ti)	3.0
α'_3 (Sr– Ti)	1.833
α_4 (O– O)	1.5
α'_4 (O– O)	1.0

Table 2. Calculated zone center phonon frequencies in cm^{-1}

ZC-phonon	Present Work	Zamkova et.al.
T_{1u}(TO1)	26.02	26
T_{1u}(TO2)	254.1	260
T_{1u}(TO3)	501	501
T_{2u}	199	199

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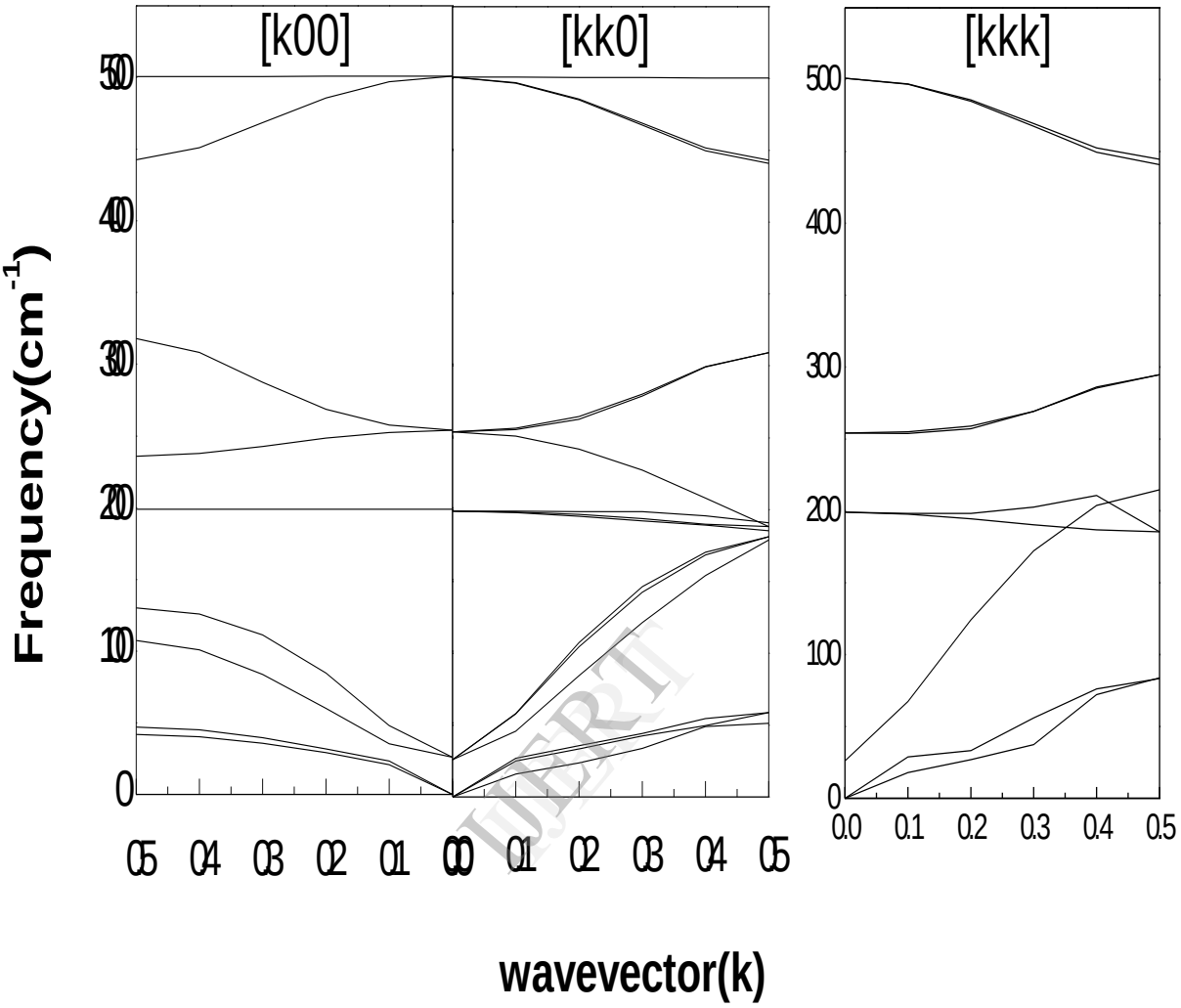

Figure 1: Phonon Dispersion relation of $SrTiO_3$