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Dielectric And Acoustical Properties Of Triglycine Sulphate Type Crystals In External Electric Field

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Abstract

Green's function theory (time-temperature dependent) have been modified with PLCM (pseudo spin lattice coupled mode) and ISING spin model of ferroelectrics in renormalized boundary condition of polarization with third, fourth and fifth order phonon anharmonic interaction as well as electric field terms for second order phase transition in Triglycine Sulphate (TGS) and Triglycine Selenate (TGSe).

Key words: Green's function, two sub-lattice conditions, normalized wave function, and perturbation theory etc.

1. Introduction

In 1960, at first time zubarev proposed a Green's function [1] theory as a solution of inhomogenouse eigen function and eigen values of the crystal lattice. Afterward V. Ramakrishana et al [2] used Green's function theory in study of Potassium Di-hydrogen Phosphate (KDP) crystal. We also have modified same green function theory and implemented over Triglycine Sulphate (TGS), Triglycine Selenate (TGSe) and their deuterated crystals with PLCM [3,4,5] (pseudo spin lattice coupled mode) and ISING [6] spin model. Substitute model values from different literature and calculate different physical constants of Triglycine Sulphate (TGS), Triglycine Selenate (TGSe) and their deuterated crystal. So during our study, we convert all theoretical properties of crystal into mathematical terms/equations and then solve these mathematical terms/equations and calculate different values. Each derived values gives a theoretical shape of properties of crystal structure and then easily we can predict about crystal behavior. We also check our predictions over experimental verification.

1.1. Crystal Study

Ferroelectric materials has an important role in modern technologies like computing technology, sensor technology, nano technology etc.. Among these ferroelectric material Triglycine Sulphate crystal (TGS), Triglycine Selenate (TGSe) and deuterated crystals are very famous because of its wide range of characteristics suitable for technological purpose. In this we are studying about the properties of Triglycine Sulphate crystal (TGS) type crystals by a theoretical method which is a combination of two different models i.e. PLCM (Pseudo spin lattice coupled mode) and ISING spin model of ferroelectrics. We have extended PLCM model with third, fourth and fifth order and harmonics interaction terms while for better adjustment with ISING spin model, we have diverted pseudo spin values of proton to phase transition condition or polarization changes. Triglycine sulphate $(CH_2NH_2COOH)_3$ H_2SO_4, Deuterated Triglycine sulphate $(CD_2ND_2COOD)_3$ D_2SO_4 and Triglycine Selenate $(CH_2NH_2COOH)_3$ H_2SeO_4, Deuterated Triglycine Selenate $(CD_2ND_2COOD)_3$ D_2SeO_4 crystals are the best pyroelectric materials, whose large crystals can be easily grown from water solution. These two crystals have nearly similar basic characteristics for example these crystals are uniaxial ferroelectric crystal with transition temperature 322K and 295K respectively. Crystals are monoclinic in both polar and non-polar phases. After transition mirror plane disappears and the crystal belongs to isostructural transition. Mathias, Miller and Remeika [7] discovered ferroelectric behaviour of Triglycine Sulphate (TGS), Triglycine Selenate its deuteerated crystals.

Hoshino et al [8] have carried out X-ray diffraction studies on triglycine sulphate crystal. Pasalov et al [9] have made hysteresis loop measurements in triglycine sulphate crystals. Costache et al [10] have made pyroelectric studies on pure and doped triglycine sulphate crystal. Hill and Ichiki [11] have made polarization relaxation studies on triglycine sulphate crystal. Sreekumar and Philips [12] have made ultrasonic attenuation studies on triglycine sulphate crystal. Lal and Batra [13] have characterization studies on pure and doped triglycine sulphate crystal. Bye et al [14] have measured dielectric constant and polarization of triglycine sulphate crystal in presence of electric field. Imai and Ishida [15] have measured polarization of doped triglycine sulphate crystal in Presence of electric field.Later on Tello and Hernandez [16] have applied tunneling model.

While TGSe crystal shows a second order phase transition [17] and specific heat [18, 19] is greater than TGS crystal. Okada and Suzuki [20] have investigated a possible tetracritical point in the crystal at p≈2.3 kbar and x=0.38 (Deuterium Concentration). Many other researchers have studied the characteristics [21, 22, 23, 24, 25, 26] of TGSe crystal but there are quietly different than ours study. All authors have decoupled correlations terms at an early stage in PLCM model. So however, they could not produce better results but we have taken the anharmonic interactions of crystal lattice which goes much closer crystal Hamiltonian. Kwan-Chi Kao et al [32] has discovered that, the density of TGS crystal i.e. 1.69 g/cm^3 and the space group symmetries of the crystal have been studied by Subramanian Balakumar and Hua C.Zeng et al [33]. The existence of hydrogen bond triglycine sulphate is detected by Choudhury, Rajul Ranjan; Chitra et al [34] and Sinha, while B.Vidyanand et al [35] has discovered the phase transition mechanism in TGS crystal. Detection of glycine ions in the triglycine sulpahate crystal done by Santra, A. L. Verma, P. K. Bajpai, B. Hilczer and P. V. Huong,et al [36].

In the present study, we have used a combination form of (PLCM) Pseudospin lattice coupled mode and ISING spin model with Green's function theory in two sub-lattice mode as well as third, fourth and fifth order phonon anharmonic interaction terms and external electric field terms for triglycine sulphate (TGS) type crystals. Expression for shift, width, soft mode frequency, dielectric constant, loss tangent, acoustic attenuation, ratio of figure of merits, electric conductivity, quality factor, smooth function and relaxation time of the crystals even with external D.C. biasing have been derived by Green's function method. Our results have a good agreement with experimental data.

2. Model Hamiltonian

Hamiltonian of TGS and TGSe crystal can be calculated by PLCM and ISING spin model with Green's function theory of ferroelectrics extended with third and fourth order phonon anharmonic interaction terms and electric field terms

$$H = -2\Omega\sum_i \left(S_{1i}^x + S_{2i}^x\right) - \sum_{ij} J_{ij}\left[\left(S_{1i}^z S_{2i}^z\right) + \left(S_{2i}^z S_{2i}^z\right)\right]$$
$$- \sum_{ij} K_{ij}\left(S_{1i}^z S_{2i}^z\right) - 2\mu E\sum_i (S_{1i}^z + S_{2i}^z)$$
$$+ \frac{1}{4}\sum_k \omega_k\left(A_k A_k^+ + B_k B_k^+\right)$$
$$- \sum_{ik} V_{ik} S_{1i}^z A_k - \sum_{ik} V_{ik} S_{2i}^z A_k^+$$
$$+ \sum_{k_1 k_2 k_3} V^{(3)}\left(k_1, k_2, k_3\right) A_{k_1} A_{k_2} A_{k_3}$$
$$+ \sum_{k_1 k_2 k_3 k_4} V^{(4)}\left(k_1, k_2, k_3, k_4\right) A_{k_1} A_{k_2} A_{k_3} A_{k_4}, \qquad \ldots(1)$$

Where, In Eq.(1) above Ω is proton tunneling frequency, S^z and S^x are components of pseudospin variable J_{ij} is interaction between same lattices and K_{ij} is interaction between different lattices. μ is dipole moment of O-H--O bond, E is external electric field V is spin lattice interaction and A_k and B_k are position and momentum operators ω_k is harmonic phonon frequency $V^{(3)}$ and $V^{(4)}$ are third and fourth order atomic force constant[15].

2.1. Green's function, Width, Shift and Soft mode Frequency

We consider the Green's function

$$G_{ij}(t-t') = \left\langle\left\langle S_{1i}^z(t); S_{1j}^z(t')\right\rangle\right\rangle$$
$$= -i\theta(t-t')\left\langle\left[S_{1i}^z(t); S_{1j}^z(t')\right]\right\rangle, \qquad \ldots(2)$$

Where $\eta = \pm 1$, $[S^Z_{1i,} S^Z_{1j}]_\eta = S^Z_{1i} S^Z_{1j} - \eta S^Z_{1i} S^Z_{1j}]$

$\theta(t) = 1$ for $t > 0$

$= 0$ for $t < 0$

The secular determinant for the system is given by

$$\Delta = \omega(\omega^2 - \omega_p^2)$$

Where,

$$\omega_p = [((J_0 m)^2 + (2\Omega)^2)]^{1/2}$$

From above mentioned equation

$$<< + | - >> = (\frac{1}{2})[\omega(\omega + J_0 n) - 2\Omega^2]$$

Spontaneous polarization in TGS crystal is

$P_s = 2N_\mu <s^z>$

In two dimensional form of pseudo spin in z-directional sum is not zero before T_C (Curie temperature).

$S_1^Z + S_1^Z \neq 0$;

And $S_1^Z \neq S_1^Z$; For $T<T_C$,

But after curie's temperature total spontaneous polarization become zero.

$S_1^Z + S_1^Z = 0$; For $T>T_C$,

Specially, for TGS, TGSe and deuterated crystals both spin become zero.

$S_1^Z = S_1^Z = 0$; For TGS, TGSe and deuteraed crystals at phase transition,

while S_1^Z ; $S_1^Z > 0$; but $P_S \to 0$ not exactly zero (for second order phase transition).

$$< S^x >= \frac{\Omega}{\tilde{\Omega}} \tanh(\frac{\beta\tilde{\Omega}}{2})$$

$$< S^y >= 0$$

$$< S^z >= \frac{(J_0 < S^Z > + J_0^{'} < S^Z >^3)}{2\tilde{\Omega}} \tanh(\frac{\beta\tilde{\Omega}}{2})$$

Differentiated twice GF (2) first with respect to time (t) and then with respect to time (t') using model Hamiltonian (Eq.1) taking Fourier transformation and setting it into Dyson's equation from

$$G_{ij}(\omega) = G_{ij}^0(\omega) + G_{ij}^0(\omega) P(\omega) G_{ij}^0(\omega) \quad \ldots(3)$$

Where,

$$G_{ij}^0(\omega) = \frac{\Omega \langle S_{1i}^x \rangle \delta_{ij}}{\pi(\omega^2 - 4\Omega^2)} \quad \ldots(4)$$

$$G_{ij}(\omega) = \frac{\Omega \langle S_{1i}^x \rangle}{\pi(\omega^2 - 4\Omega^2 - P(\omega))} \quad \ldots(5)$$

Where,

$$P(\omega) = \tilde{P}(\omega) + \tilde{\tilde{P}}(\omega), \quad \ldots(6)$$

$$\tilde{P}(\omega) = \frac{\pi i}{\Omega \langle S_{1i}^x \rangle^2} \langle F_i^{(t)}; S_{ij}^y \rangle \quad \ldots(7)$$

and, $$\tilde{\tilde{P}}(\omega) = \frac{\pi^2}{\Omega^2 \langle S_{1i}^x \rangle^2} \langle\langle F_i, F_j \rangle\rangle \quad \ldots(8)$$

The second term of Eq. (6) contains higher order Green's functions which are decoupled by using scheme

<abcd>=<ab><cd>+<ac><bd>+<ad><bc>.

Then simpler Green's functions are solved in the zeroth order approximation i.e. higher order terms are neglected from $P(\omega)$ type terms. In Eq.(8) $\tilde{\tilde{P}}(\omega)$ is resolved into its real and imaginary parts using formula $\lim_{m\to 0} \frac{1}{x + im} = \left(\frac{1}{x}\right) \pm i\pi\delta(x)$. The real part is known as shift $\Delta(\omega)$ and the imaginary part is called width $\Gamma(\omega)$.

These are obtained as following

Spin shift is

$$\Delta_s(\omega) = \frac{a^4}{2\Omega(\omega^2 - \tilde{\Omega}^2)} + \frac{b^2c^2}{4\Omega\tilde{\Omega}} + \frac{V_{ik}^2 N_k a^2}{2\Omega(\omega^2 - \tilde{\Omega}^2)} + \frac{4\mu^2 E^2 a^2}{2\Omega(\omega^2 - \tilde{\Omega}^2)} \quad \ldots(9)$$

$$\Delta_{s-p}(\omega) = \frac{2V_{ik}^2 \langle S_{1i}^x \rangle \omega_k \delta_{kk^i} \left(\omega^2 - \tilde{\tilde{\omega}}_k^2\right)}{\left[\left(\omega^2 - \tilde{\tilde{\Omega}}_k^2\right)^2 + 4\omega_k^2 \Gamma_k^2(\omega)\right]} \quad \ldots(10)$$

Spin width is

$$\Gamma(\omega) = \frac{\pi a^4}{4\Omega\tilde{\Omega}} \left[\delta(\omega - \tilde{\Omega}) - \delta(\omega + \tilde{\Omega})\right]$$

$$+ \frac{b^2c^2}{4\Omega\tilde{\Omega}} \left[\delta(\omega - \tilde{\Omega}) - (\omega + \tilde{\Omega})\right]$$

$$+ \frac{V_{ik}^2 N_k a^2}{4\Omega\tilde{\Omega}} \left[\delta(\omega - \tilde{\Omega}) - \delta(\omega + \tilde{\Omega})\right]$$

$$+ \frac{2\pi\mu^2 E^2 a^2}{4\Omega\tilde{\Omega}} \left[\delta(\omega - \tilde{\Omega}) - \delta(\omega + \tilde{\Omega})\right], \quad \ldots(11)$$

Spin Phonon width is

$$\Gamma_{s-p}(\omega) = \frac{4V_{ik}^2 \langle S_{1i}^x \rangle \omega_k \left(\omega^2 - \tilde{\tilde{\omega}}_k^2\right)}{\left[\left(\omega^2 - \tilde{\tilde{\omega}}_k^2\right)^2 + 4\omega_k^2 \Gamma_k^2(\omega)\right]} \quad \ldots(12)$$

In Eq.(10) and (12) $\tilde{\tilde{\omega}}_k$ is renormalized phonon frequency and $\Gamma_k(\omega)$ is phonon width in the Green's function

$G_{kk'}(t-t') = << A_k(t); A_{k^1}(t') >>$ which are obtained as

$$G_{ij'}(\omega) = \frac{\omega_k \delta_{kk'}}{\pi\left[\omega^2 - \tilde{\tilde{\omega}}_k^2 - 2\omega_k \{\Delta_k(\omega) + i\Gamma(\omega)\right]} \quad \ldots(13)$$

$$\tilde{\tilde{\omega}}_k^2 = \tilde{\omega}_k^2 + 2\omega_k \Delta_k(\omega), \quad \ldots(14a)$$

Phonon shift is given as

$$\Delta_k(\omega) = \mathrm{Re}\, P_k(\omega)$$

$$= 18P \sum_{k_1 k 2} \left| V^{(3)}(k_1, k_2, -k) \right|^2$$

$$\frac{\omega_{k1}\omega_{k2}}{\tilde{\omega}_{k1}\tilde{\omega}_{k2}} \left\{ \left(n_{k1} + n_{k2}\right) \frac{\tilde{\omega}_{k1} + \tilde{\omega}_{k2}}{\omega^2 - \left(\tilde{\omega}_{k1} + \tilde{\omega}_{k2}\right)^2} + \left(n_{k_2} - n_{k_1}\right) \frac{\tilde{\omega}_{k1} + \tilde{\omega}_{k2}}{\omega^2 - \left(\tilde{\omega}_{k1} + \tilde{\omega}_{k2}\right)^2} \right\}$$

$$+ 48P \sum_{k1_1 k_{2k_3}} \left| V^{(4)}(k_1 k_2, k_{3,} - k) \right|^2 \frac{\omega_{k_1}\omega_{k2}\omega_{k3}}{\tilde{\omega}_{k_1}\tilde{\omega}_{k_2}\tilde{\omega}_{k3}}$$

$$\left\{\left(1+n_{k_1}n_{k_2}+n_{k_2}n_{k_3}+n_{k_3}n_{k_1}\right)\frac{\tilde{\omega}_{k_1}+\tilde{\omega}_{k2}+\tilde{\omega}_{k3}}{\omega^2-(\tilde{\omega}_{k_1}+\tilde{\omega}_{k_2}+\tilde{\omega}_{k3})^2}\right.$$

$$\left.+3\left(1-n_{k_2}n_{k_1}+n_{k2}n_{k_3}-n_{k_3}n_{k_1}\right)\frac{\tilde{\omega}_{k_1}+\tilde{\omega}_{k2}+\tilde{\omega}_{k3}}{\omega^2-(\tilde{\omega}_{k_1}+\tilde{\omega}_{k_2}+\tilde{\omega}_{k3})^2}\right\}$$

And, phonon width is given as

$$\Gamma_k(\omega)=\mathrm{Im}\,P_k(\omega)$$

$$=9\pi\sum_{k_1k_2}\left|V^{(3)}(k_1,k_2,-k)\right|^2\frac{\omega_{k_1}\omega_{k_2}}{\tilde{\omega}_{k_1}\tilde{\omega}_{k_2}}$$

$$\left\{\left(n_{k_1}+n_{k_2}\right)\left[\delta\left(\omega+\tilde{\omega}_{k_1}+\tilde{\omega}_{k_1}\right)\right.\right.$$

$$\left.-\delta\left(\omega-\tilde{\omega}_{k_1}-\tilde{\omega}_{k_1}\right)+\textit{(higher terms)}\right.$$

$$\left.+\left(n_{k_2}-n_{k_1}\right)\left[\delta\left(\omega+\tilde{\omega}_{k_1}+\tilde{\omega}_{k_2}\right)-\delta\left(\omega+\tilde{\omega}_{k_1}+\tilde{\omega}_{k_2}\right)\right]\right\}$$

$$+48\pi\sum_{k_1k_2k_3}\left|V^{(4)}\left(k_1,k_2,k_3,-k_4\right)\right|^2\frac{\omega_{k_1}\omega_{k_2}\omega_{k_3}}{\tilde{\omega}_{k_1}\tilde{\omega}_{k_2}\tilde{\omega}_{k_3}}$$

$$X\left\{\left(1+n_{k_1}n_{k_2}+n_{k_2}n_{k_3}+n_{k_3}n_{k_4}\right)\right.$$

$$X\left[\delta\left(\omega+\tilde{\omega}_{k_1}+\tilde{\omega}_{k_2}+\tilde{\omega}_{k_3}\right)-\delta(\omega-\tilde{\omega}_{k_1}-\tilde{\omega}_{k_2}-\tilde{\omega}_{k_3})\right]$$

$$+3\left(n_{k_1}n_{k_2}+n_{k_2}n_{k_3}-n_{k_3}n_{k_4}\right)+3\left(n_{k_1}n_{k_2}+n_{k_2}n_{k_3}-n_{k_3}n_{k_4}\right)$$

$$\left.X\left[\delta\left(\omega+\tilde{\omega}_{k_1}-\tilde{\omega}_{k_2}-\tilde{\omega}_{k_3}\right)-\delta(\omega-\tilde{\omega}_{k_1}+\tilde{\omega}_{k_2}+\tilde{\omega}_{k_3})\right]\right\}$$

$$\tilde{\tilde{\omega}}_k^2=\tilde{\omega}_k^2+A_k(T), \qquad \ldots(14d)$$

The Green' function (2) finally becomes

$$G_{ij}(\omega)=\frac{\Omega\left\langle S_{1i}^x\right\rangle\delta_{ij}}{\pi\left(\omega^2-\hat{\Omega}^2-P(\omega)\right)}, \qquad \ldots(15)$$

$$\hat{\Omega}^2=\tilde{\tilde{\Omega}}^2+2\Omega\Delta_{s-p}(\omega), \qquad \ldots(16)$$

$$\tilde{\tilde{\Omega}}^2=\tilde{\Omega}^2+2\Omega\Delta_s(\omega), \qquad \ldots(17)$$

$$\tilde{\Omega}^2=4\Omega^2+\frac{1}{\Omega\left\langle S^x{}_{1i}\right\rangle}\left\langle\left[F,S_{1j}{}^y\right]\right\rangle, \qquad \ldots(18)$$

In Eq.(18) second term is evaluated using mean field approximation i.e.

$$\frac{\left\langle S_{1i}^z\right\rangle}{a}=\frac{\left\langle S_{1i}^x\right\rangle}{b}=\frac{1}{2\tilde{\Omega}}\tanh\beta\frac{\tilde{\Omega}}{2} \qquad \ldots(19)$$

which gives

$$\tilde{\Omega}^2=a^2+b^2+bc \qquad \ldots(20)$$

where

$$a=2J\left\langle S_1^z\right\rangle+K\left\langle S_2^z\right\rangle+2\mu E. \qquad \ldots(14b) \quad \ldots(21)$$

$$b=2\Omega; \qquad \ldots(22)$$

and

$$c=2J\left\langle S_1^x\right\rangle+K\left\langle S_2^x\right\rangle \qquad \ldots(23)$$

Solving,Eq.(16)

$$\hat{\Omega}_{\pm}^2=\frac{1}{2}\left(\tilde{\tilde{\omega}}_k^2+\tilde{\tilde{\Omega}}^2\right)\pm\frac{1}{2}\left[\left(\tilde{\tilde{\omega}}_k^2-\tilde{\tilde{\Omega}}^2\right)^2+8V_{ik}^2\left\langle S_{1i}^x\right\rangle\Omega\right]^{1/2} \qquad \ldots(24)$$

$$T_c=\frac{\eta}{2k_B\tanh^{-1}\left(\frac{\eta^3}{4\Omega^2J^*}\right)} \qquad \ldots(25)$$

where

$$\eta^2=(2J-K)^2\sigma^2+4\Omega^2+(2\mu E)^2 \qquad \ldots(26)$$

and

$$(J+K)^*=(2J+K)+\frac{2V_{ik}^2\tilde{\tilde{\omega}}_k^2}{\left[\tilde{\tilde{\omega}}_k^4+4\omega_k\Gamma_k^2\right]} \qquad \ldots(27)$$

J^* is renormalized exchange interaction constant.

2.2. Dielectric constant and Loss tangent

The response of a dielectric crystal to the external electric field is expressed dielectric susceptibility χ given as

$$\chi(\omega)=-\lim_{X\to0}2\pi N\mu^2G_{ij}(\omega+iX) \qquad \ldots(28)$$

The $\chi(\omega)$ is related to dielectric constant as (14c)

$$\in=1+4\pi\chi \qquad \ldots(29)$$

With the help of Eq.(25) and (26) one obtain expression for dielectric constant as

$$\in(\omega)=\left(-8\pi N\mu^2\right)\frac{\left\langle S_1^x\right\rangle\Omega}{\left[\left(\omega^2-\hat{\Omega}^2\right)^2+4\Omega^2\Gamma^2\right]} \qquad \ldots(30)$$

$\in(\omega)>>1$ in the ferroelectric crystal. The power lost in dielectric when exposed to electromagnetic field is conveniently shown as dielectric tangent loss which is expressed as

$$\tan\delta=\frac{\in''}{\in'} \qquad \ldots(31)$$

By using Eq. (30) and (31) we obtains expression for loss tangent as

$$\tan\delta=-\frac{2\Omega\Gamma(\omega)}{\left(\omega^2-\hat{\Omega}^2\right)} \qquad \ldots(32)$$

2.3. Acoustic Attenuation

The acoustic attenuation is given as

$$\alpha = \frac{\Gamma(\omega)}{v} \qquad \ldots(33)$$

Where $\Gamma(\omega)$ is width and v is sound velocity.

3. Numerical calculation & Results

By using model values of various quantities in expression form literature (given in table-1) temperature and electric field dependence of width, shift, soft mode frequency dielectric constant, tangent loss, quality factor, ratio of figure of merits and electric conductivity (A.C.) for triglycine sulphate type crystals have been calculated and shown in Fig.1 to 4.

Table 1. Model values of physical parameters for TGS crystal.

Sample	T_c (^0C)	C (^0C)	Ω (cm^{-1})	J (cm^{-1})	V_o (cm^{-1})	$\hbar\omega$ (cm^{-1})	A (cm^{-1})	N_μ ($\mu C/cm^2$)
TGS	49.1	3007	0.1	340	10	0.59	10.20	2.22(323K)
TGSe	22.5	4727	0.4	320	12	0.61	11.15	3.70(285.5K)

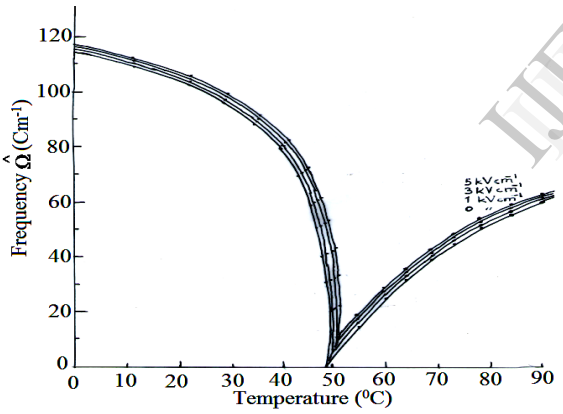

Figure 1. Calculated temperature dependence of ferroelectric mode frequency of TGS type crystal in presence of electric field.

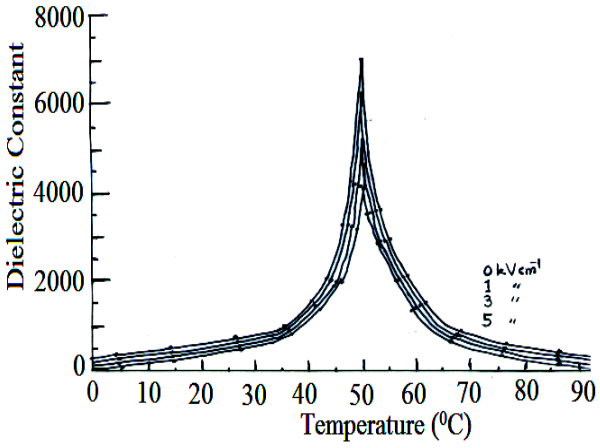

Figure 2. Calculated temperature dependence of dielectric constant of TGS type crystal in presence of electric field.

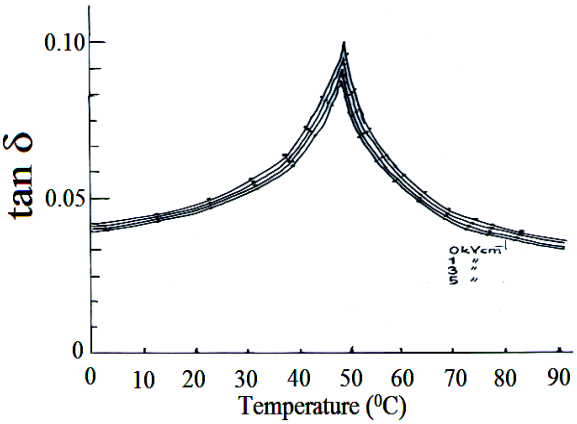

Figure 3. Calculated temperature dependence of loss tangent of TGS type crystal in presence of electric field.

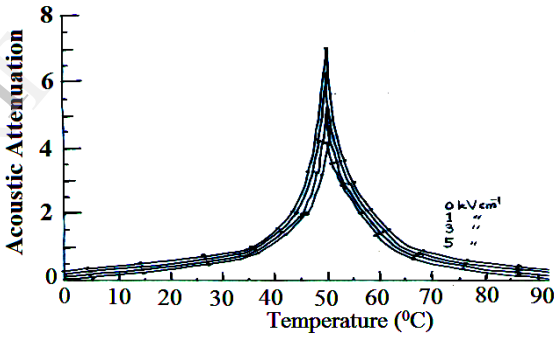

Figure 4. Calculated temperature dependence of loss tangent of TGS type crystal in presence of electric field.

4. Discussion

After solving all the mathematical derivations we have plot different graphs (graphs no. 1 to 4) for different constants of TGS, TGSe and its deuterated crystals. our modified (PLCM) Pseudo spin lattices coupled mode model (two sub lattice mode as well as third, fourth and fifth order phonon anharmonic interaction terms and electric field terms) and ISING spin model with Green's function theory (double time-temperature dependent) for triglycine sulphate (TGS) type crystal gives different expressions for shift, width, soft mode frequency, dielectric constant, loss tangent, acoustic attenuation, quality factor, ratio figure of merits and electric conductivity by using model values, given by Chaudhuri et al [4] and Gonzalo et al [6]. Previous researcher [3,5] have not considered phonon anharmonic interactions, as well as two sublattice model only chaudhuri et al [4] have considered the two sublattice pseudospin lattice coupled mode model with third, fourth and fifth order phonon anharmonic interaction terms but even not in

a convincing way as they have decoupled the correlations at an early stage. As a result, some important interactions disappeared from the calculations and width as well as shift are calculated, if these are neglected from our results, these at once reduce to the results of Chaudhuri et al. Previous researchers have not calculated the effect of electric field on soft mode frequency, dielectric constant, tangent loss, attenuation constant of TGS type crystal. This theoretical study about dielectric, acoustic, thermal and electric behavior of TGS crystal shows very interesting results which have a very balanced relation with experimental data. Theoretically at phase transition in ferroelectrics the soft mode frequency should be zero at transition temperature (T_C), though in external biasing slightly increase. Dielectric constant of these crystals are in order of $>10^4$ which is very high at T_C while in external biasing reduces gradually at T_c and corresponding energy loss increases at T_c and decreases in external biasing. All theoretical data have a good agreement with experimental results. [T Iglesias et al [31], Bye et al [14], Hill and Ichiki et al [11], Shreekumar et al [12]. Although in external biasing the curie's temperature (T_C) slightly decreases.

5. Conclusions

In present study, (PLCM) two sub lattice pseudo spin-lattice coupled mode model and ISING spin model of ferroelectrics with double time-temperature dependent Green's function theory predict a true characteristics of TGS, TGSe and its deuterated crystals and indirectly suggest the technological importance of the crystal like computing technology, sensor technology, nano technology and food technology etc. On the bases of applicability of this method it can be applied over any other hydrogen bonded crystal such that $PbHPO_4$, $C_4O_4H_2$, KDP (KH_2PO_4) and Rochelle salt ($NaKC_4H_4O_6.\ 4H_2O$) etcs.

Future Aspect

We are trying to explain about lattice dynamics in photo sensitive effect and liquid state properties of TGS crystal by the same method.

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