

ROLE OF ACOUSTIC AND OPTICAL VIBRATION MODES IN FERROELECTRIC CRYSTAL TECHNOLOGIES: (DEUTERATED TRIGLYCINE SULPHATE CRYSTAL)

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Abstract: A modified Green's function theory with pseudo vibration theory of ferroelectrics has been applied to deuterated triglycine sulphate crystal to predict the applications of the ferroelectric crystal in computing technology.

Keywords: phase transition, quantum states, switching.

1. INTRODUCTION

Ferroelectrics is a special class of condensed matter physics which has a broad application in different technologies such as computing, sensor, display, thermal image technology etc. In computing technology, it has an important role in memory device and quantum capacitor etc. Due to switching process and other physical constants of crystal-like local mode frequency, electric polarisation, micro wave absorption, quality factor, acoustic mode frequency, relaxation time, electric resistivity, differentiability, IR sensitivity etc., these properties may be used directly or indirectly in computing technology. The first mention of the idea of ferroelectrics FETs was in US patent of Ross (1957) and the first realization was by Moll and Tarui (1963) while the first attempt to fabricate one ferroelectric on silicon was by Wu (1974). Early ferroelectrics FETs utilized gate of the lithium niobate (Rice University; Rabson et al 1995) or BaMgF₄ (Westinghouse, Sinharoy et al 1991,92,93). An example of ferroelectrics FET device was fabricated by Mathews et al (1997). The optimum parameters for such a ferroelectrics-gate material are extremely different from those for pass-gate-switched capacitor arrays, in particular, the latter require a remanent polarisation ($\sim 10 \mu\text{C}/\text{cm}^2$), whereas the ferroelectric-gated FETs can function well with 50 times less ($\sim 0.2 \mu\text{C}/\text{cm}^2$). However, the switching array (FRAMs) is very tolerant of surface traps in the ferroelectric (which may be 10^{20}cm^{-3}) in the interface region near electrodes.

1.1. Crystal Study

Triglycine Sulphate (TGS) Crystal was a first crystal to be discovered of all $(\text{NH}_2\text{CH}_2\text{COOH})_3\text{H}_2\text{SO}_4$ type crystals in 1956 by Matthias et al [1]. TGS crystal exhibits a phase transition at 49°C from ferroelectric phase to paraelectric phase which means polar to non-polar form. Triglycine Sulphate (TGS) crystal is a monoclinic type crystal with space group points 2m and 2 which disappears after phase transition. In Triglycine Sulphate (TGS) crystal, there are three different glycine ions with plane mirror symmetry. This plane mirror symmetry produces a double potential well barrier in the crystal and this potential barrier condition is solved by quantum mechanics. Thus we came to know about pseudo spin character of proton between two adjacent potential wells. Some authors have previously carried out study of ferroelectric Triglycine sulphate crystal [2–4]. Its deuterated form is deuterated triglycine sulphate crystal whose phase transition is 333.89 K while other behaviour in terms of physics is similar. Crystal growths and its characteristics with doped condition were studied by Batra et al [5]. DTGS is a successful high sensitive detector type used as infrared spectrometers which is used to take measurements in the mid-infrared (mid IR) range. Domain structure of DTGS crystal has been investigated by Drozhdin et al [6]. J. Bjorkstam et al [7] have shown a phase transition in deuterated triglycine sulphate crystal by deuteron nuclear-magnetic-resonance method. Ferroelectric properties of different solid

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solution of DTGS crystal with different concentration were studied by B. Brezina et al [8]. Optical properties of deuterated triglycine sulphate have

been investigated by O. S. Kushnir et al [9]. Dielectric properties of DTGS were proposed by A. Camnasio and J. A. Gonzalo et al [10].

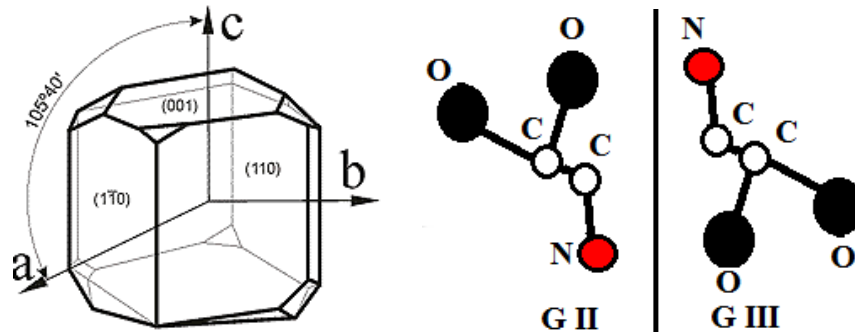


Figure 1. Lattice structure of triglycine sulphate (left) [5] and mirror symmetry in triglycine sulphate crystal which develop a double potential well barrier in the crystal lattices which trapped a hydrogen bond in its either well.

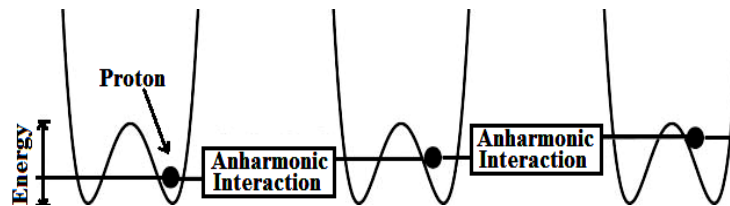


Figure 2. Anharmonic interaction between different lattices of hydrogen bonded ferroelectric crystals.

We know about domain structure of ferroelectric crystal which may be helpful in memory device. The domain of the crystal is uniaxial, optically distinguished, safe reversible field domain, and the convenient temperature region make it suitable for non-volatile memory device. We have determined that quasi-stable spike-like domains structure in external electric field domain change into regular hexagons domain well are parallel to the facets pulled along the polar axis. The field dependent sideways motion or velocity of these domains is approximately or parallel to the crystal facets. We use this condition in our paper to make a good non-volatile memory structure of crystals and this is possible by one method only, which is real time registration of domain pattern during switching by using electron or optical microscopy. This can be done by measuring the transient current. For memory devices crystal film should be prepared for which polarisation should be any stable thermo-dynamical condition.

It should allow switching between two states with a character of hysteresis loop. So on the bases of these properties of crystals we can form a ferroelectric capacitor which can store information. This is not sufficient for making a non-volatile computer memory.

A pass-gate transistor is required so that a voltage above the coercive voltage is only applied to the capacitor when voltage is applied to both of the word and bit line; how electronics information can be stored in electric polarisation state of ferroelectric materials is a fairly obvious issue, however the realization is not straight forward; the initial barrier in development of ferroelectric memory necessary to make them very thin because the coercive voltage of ferroelectric materials are typically of the order of several kV/cm requiring submicron thick film to make that work on the voltage scale required for computing (all Si device work at ≤ 5 V) with today depositions techniques. This is no longer a problem and high density arrays of non-volatile ferroelectrics memories are commercially available. However reliability remains an issue, a ferroelectric capacitor while capable of storing information is not computational electronic structure theory has increase dramatically giving us new understanding of ferroelectricity. If the capacitor being read is in different state, the difference in current will be quite large where the displacement current associated with for the differences. If capacitor does not switch, it is already in reference state. The difference in current capacitor being read and reference Capacitor is zero.

2. CRYSTAL THEORY

2.1. Inhomogeneous Theory

We consider the Inhomogeneous solution for crystal of hydrogen bonded crystal

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

where $\eta = \pm 1$, $[S_{1i}^z, S_{1j}^z]_{\eta} = S_{1i}^z S_{1j}^z - \eta S_{1j}^z S_{1i}^z$, $\theta(t) = 1$ for $t > 0$, and $\theta(t) = 0$, for $t < 0$.

Angular bracket $\langle \dots \rangle$ denotes ensemble average over a grand canonical ensemble. It follows from the definition that the Green's functions so defined are a function of $t-t'$ only. The Fourier-transformed Green's function is defined by

$$G_{ij}(t-t') = \langle \langle S_{1i}^z | S_{1j}^z \rangle \rangle = \frac{1}{2\pi} \int_{-\infty}^{\infty} G_{ij}(t) e^{i\omega t} dt$$

This Green's function satisfies the equation of motion

$$\omega \langle \langle S_{1i}^z, S_{1j}^z \rangle \rangle_{\omega} = \frac{1}{2\pi} \langle [S_{1i}^z, S_{1j}^z]_{\eta} \rangle + \langle \langle [S_{1i}^z, S_{1j}^z] S_{1j}^z \rangle \rangle_{\omega}$$

The equation for $\langle \langle S_{1i}^z, S_{1j}^z \rangle \rangle_{\omega}$, thus involves and in-homogenous terms and higher-order Green's function. One of the problems of this method is to decouple the higher-order Green's function and ω choose appropriate Green's function so that a closed system of equation is obtained.

In addition we have shown that the poles of the Green function correspond to the energies of the elementary excitation of the system. The average value of the product of two operators can be calculated from the formula.

$$\langle S_{1i}^z, S_{1j}^z \rangle = \lim_{\eta \rightarrow 0} \int_{-\infty}^{\infty} \frac{1}{(e^{i\omega} - \eta)} i \langle \langle S_{1i}^z | S_{1j}^z \rangle \rangle_{\omega+i\epsilon} - \langle \langle S_{1i}^z | S_{1j}^z \rangle \rangle_{\omega-i\epsilon} d\omega$$

The parameter η may be arbitrarily chosen as +1 or -1. If S_{1i}^z and S_{1j}^z are bose operators, η is generally chosen as +1 and if they are Fermi operators, η is chosen to be -1. Sometimes, however, the reverse choice becomes necessary. In the problem of DTGS (Deuterated triglycine Sulphate) crystal, where one deals with spin operators, it would be convenient to chose $\eta = +$. However, it turns out that Green's function for system has a zero frequency pole. Under these consideration, in the calculation for which $\eta = +1$, it cannot be used. Since the integral becomes divergent (efforts to circumvent this problem by the addition of vanishingly small perturbation terms were unsuccessful) on therefore has to resort to fermion Green's function i.e. with $\eta = -1$, to treat the pseudo spin problem.

$$\begin{aligned} \omega \langle \langle S_g^+ | S_f^- \rangle \rangle &= \langle S_f^- S_g^+ + \delta_{fg} (1 - 2S_f^- S_g^+) \rangle - 2\Omega \langle \langle S_g^+ | S_f^- \rangle \rangle \\ &+ \frac{1}{2} \sum_m J_{gm} \langle \langle (S_g^+ S_m^+ | S_f^-) \rangle \rangle + \frac{1}{2} \sum_l J_{lg} \langle \langle (S_l^+ S_g^+ | S_f^-) \rangle \rangle \\ \omega \langle \langle S_g^+ | S_f^- \rangle \rangle &= \frac{2 \langle S_f^- S_g^+ \rangle}{2\pi} 2\Omega \langle \langle S_g^+ | S_f^- \rangle \rangle - \frac{1}{2} \sum_m J_{gm} \langle \langle S_g^+ S_m^+ | S_f^- \rangle \rangle \\ &- \frac{1}{2} \sum_l J_{lg} \langle \langle S_l^+ S_g^+ | S_f^- \rangle \rangle \\ \omega \langle \langle S_g^+ | S_f^- \rangle \rangle &= \frac{(1 - \delta_{fg})(S_f^- S_g^+)}{2\pi} - \Omega \langle \langle S_g^+ | S_f^- \rangle \rangle + \Omega \langle \langle S_g^- | S_f^- \rangle \rangle \end{aligned}$$

The above equation can be closed by decoupling the higher order Green's functions. The two decoupling procedure.

In decoupling of pseudospin, one assumes that

$$\begin{aligned} \langle \langle S_g^+ S_m^z | S_f^- \rangle \rangle &= \langle S_m^z \rangle \langle \langle S_g^+ | S_f^- \rangle \rangle \\ \langle \langle S_l^z S_g^+ | S_f^- \rangle \rangle &= \langle S_l^z \rangle \langle \langle S_g^+ | S_f^- \rangle \rangle \end{aligned}$$

Introduce the notation

$$x = \langle S^x \rangle = \langle S^y \rangle, \quad n = \langle S^z \rangle, \quad J_0 = \sum_j J_{ij}$$

Then the above equation of decoupling becomes as, if $f = g$

$$\begin{pmatrix} \omega - J_0 n & 0 & 2\Omega \\ 0 & \omega + J_0 n & -2\Omega \\ \Omega & -\Omega & \omega \end{pmatrix} \begin{pmatrix} \langle \langle + | - \rangle \rangle \\ \langle \langle - | - \rangle \rangle \\ \langle \langle z | - \rangle \rangle \end{pmatrix} = \frac{1}{2\pi} \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}$$

where $\langle \langle + | - \rangle \rangle$, $\langle \langle - | - \rangle \rangle$, $\langle \langle z | - \rangle \rangle$ are aberration of notation for $\langle \langle S_f^+ | S_f^- \rangle \rangle$ etc.

The secular determinant for the system is given by

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

where,

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

From the above mentioned equation

$$\langle \langle + | - \rangle \rangle = \left(\frac{1}{2} \right) [\omega(\omega + J_0 n) - 2\Omega^2]$$

spontaneous polarization in deuterated triglycine Sulphate crystal is

$$P_s = 2N_{\mu} \langle S^z \rangle$$

In two dimensional form of pseudospin in z-directional sum is not zero before T_C (Curie temperature, $T < T_C$):

$$S_1^Z + S_1^Z \neq 0 \text{ and } S_1^Z \neq S_1^Z,$$

but after Curie temperature ($T > T_C$) total spontaneous polarization becomes zero:

$$S_1^Z + S_1^Z = 0.$$

Especially for DTGS crystal (ferroelectric) both spins become zero.

$$S_1^Z = S_1^Z = 0;$$

For Deuterated triglycine sulphate crystal (ferroelectric crystal) at phase transition, while $S_1^Z ; S_1^Z > 0$;

but $P_S \rightarrow 0$ not exactly zero (for second order phase transition).

$$\langle S^x \rangle = \frac{\Omega}{2} \tanh\left(\frac{\beta\tilde{\Omega}}{2}\right)$$

$$\langle S^y \rangle = 0$$

$$\langle S^z \rangle = \frac{(J_0 \langle S^z \rangle + J_0' \langle S^z \rangle^3)}{2\tilde{\Omega}} \tanh\left(\frac{\beta\tilde{\Omega}}{2}\right)$$

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

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

where

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

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

and

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

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

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

The second term of Eq. (6) contains higher order Green's functions which are decoupled by using scheme $\langle abcd \rangle = \langle ab \rangle \langle cd \rangle + \langle ac \rangle \langle bd \rangle + \langle ad \rangle \langle bc \rangle$. Then simpler inhomogeneous 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 $\lim_{m \rightarrow 0} \frac{1}{x + im} = \left(\frac{1}{x}\right) \pm i\pi\delta(x)$. The real part is known as shift $\Delta(\omega)$ and the imaginary part is called width $\Gamma(\omega)$.

These are obtained as follows.

Spin shift is

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

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

Spin width is

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

$$+ \frac{b^2 c^2}{4\Omega\tilde{\Omega}} [\delta(\omega - \tilde{\Omega}) - \delta(\omega + \tilde{\Omega})] \quad (11)$$

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

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

Spin Phonon width is

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

In Eq.(10) and (12) $\tilde{\omega}_k$ is renormalized phonon frequency and $\Gamma_k(\omega)$ is phonon width in the Green's function $G_{kk'}(t-t') = \langle \langle A_k(t); A_{k'}(t') \rangle \rangle$ which are obtained as

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

$$\tilde{\omega}_k^2 = \tilde{\omega}_k^2 + 2\omega_k \Delta_k(\omega), \quad (14.1)$$

Phonon shift is given as

$$\Delta_k(\omega) = \text{Re } P_k(\omega) = 18P \sum_{k_1 k_2} |V^{(3)}(k_1, k_2, -k)|^2 \times \times \frac{\omega_{k_1} \omega_{k_2}}{\tilde{\omega}_{k_1} \tilde{\omega}_{k_2}} \left\{ (n_{k_1} + n_{k_2}) \frac{\tilde{\omega}_{k_1} + \tilde{\omega}_{k_2}}{\omega^2 - (\tilde{\omega}_{k_1} + \tilde{\omega}_{k_2})^2} + (n_{k_2} - n_{k_1}) \frac{\tilde{\omega}_{k_1} - \tilde{\omega}_{k_2}}{\omega^2 - (\tilde{\omega}_{k_1} - \tilde{\omega}_{k_2})^2} \right\} +$$

$$+ 48P \sum_{k_1 k_2 k_3} |V^{(4)}(k_1, k_2, k_3, -k)|^2 \frac{\omega_{k_1} \omega_{k_2} \omega_{k_3}}{\tilde{\omega}_{k_1} \tilde{\omega}_{k_2} \tilde{\omega}_{k_3}} \times \quad (14.2)$$

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

And, phonon width is given as

$$\Gamma_k(\omega) = \text{Im } P_k(\omega) = 9\pi \sum_{k_1 k_2} |V^{(3)}(k_1, k_2, -k)|^2 \times \times \frac{\omega_{k_1} \omega_{k_2}}{\tilde{\omega}_{k_1} \tilde{\omega}_{k_2}} \left\{ (n_{k_1} + n_{k_2}) \delta(\omega + \tilde{\omega}_{k_1} + \tilde{\omega}_{k_2}) - \delta(\omega - \tilde{\omega}_{k_1} - \tilde{\omega}_{k_2}) + (n_{k_2} - n_{k_1}) [\delta(\omega + \tilde{\omega}_{k_1} + \tilde{\omega}_{k_2}) - \delta(\omega + \tilde{\omega}_{k_1} + \tilde{\omega}_{k_2})] \right\} + 48\pi \sum_{k_1 k_2 k_3} |V^{(4)}(k_1, k_2, k_3, -k)|^2 \frac{\omega_{k_1} \omega_{k_2} \omega_{k_3}}{\tilde{\omega}_{k_1} \tilde{\omega}_{k_2} \tilde{\omega}_{k_3}} + \quad (14.3)$$

$$+ X \left\{ (1 + n_{k_1} n_{k_2} + n_{k_2} n_{k_3} + n_{k_3} n_{k_4}) + X [\delta(\omega + \tilde{\omega}_{k_1} + \tilde{\omega}_{k_2} + \tilde{\omega}_{k_3}) - \delta(\omega - \tilde{\omega}_{k_1} - \tilde{\omega}_{k_2} - \tilde{\omega}_{k_3})] + 3(n_{k_1} n_{k_2} + n_{k_2} n_{k_3} - n_{k_3} n_{k_4}) + 3(n_{k_1} n_{k_2} + n_{k_2} n_{k_3} - n_{k_3} n_{k_4}) + X [\delta(\omega + \tilde{\omega}_{k_1} - \tilde{\omega}_{k_2} - \tilde{\omega}_{k_3}) - \delta(\omega - \tilde{\omega}_{k_1} + \tilde{\omega}_{k_2} + \tilde{\omega}_{k_3})] \right\}$$

$$\tilde{\omega}_k^2 = \tilde{\omega}_k^2 + A_k(T), \quad (14.4)$$

The Green's function (2) finally becomes

$$G_{ij}(\omega) = \frac{\Omega \langle S_{li}^x \rangle \delta_{ij}}{\pi(\omega^2 - \hat{\Omega}^2 - P(\omega))} \quad (15)$$

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

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

$$\tilde{\Omega}^2 = 4\Omega^2 + \frac{1}{\Omega \langle S_{li}^x \rangle} \langle [F, S_{ij}^y] \rangle, \quad (18)$$

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

$$\frac{\langle S_{li}^z \rangle}{a} = \frac{\langle S_{li}^x \rangle}{b} = \frac{1}{2\tilde{\Omega}} \tanh \beta \frac{\tilde{\Omega}}{2} \quad (19)$$

which gives

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

where

$$a = 2J \langle S_1^z \rangle + K \langle S_2^z \rangle + 2\mu E \quad (21)$$

$$b = 2\Omega;$$

and

$$c = 2J \langle S_1^x \rangle + K \langle S_2^x \rangle \quad (22)$$

Solving, Eq.(16)

$$\hat{\Omega}_\pm^2 = \frac{1}{2}(\tilde{\omega}_k^2 + \tilde{\Omega}^2) \pm \frac{1}{2} \left[(\tilde{\omega}_k^2 - \tilde{\Omega}^2)^2 + 8V_{ik}^2 \langle S_{li}^x \rangle \Omega \right]^{1/2} \quad (23)$$

$$T_c = \frac{\eta}{2k_B \tanh^{-1} \left(\frac{\eta^3}{4\Omega^2 J^*} \right)} \quad (24)$$

where

$$\eta^2 = (2J - K)^2 \sigma^2 + 4\Omega^2 + (2\mu E)^2 \quad (25)$$

and

$$(J + K)^* = (2J + K) + \frac{2V_{ik}^2 \tilde{\omega}_k^2}{\tilde{\omega}_k^4 + 4\omega_k \Gamma_k^2} \quad (26)$$

J^* is renormalized exchange interaction constant.

2.2. Crystal energy

Hamiltonian of hydrogen bonded ferroelectric crystal can be calculated by pseudo vibration [11-17] and Ising spin [16] model with Inhomogeneous function theory of ferroelectrics extended with third and fourth order phonon anharmonic interaction terms and electric field terms

$$H = -2\Omega \sum_i (S_{li}^x + S_{2i}^x) - \sum_{ij} J_{ij} [(S_{li}^z S_{2i}^z) + (S_{2i}^z S_{li}^z)] \\ - \sum_{ij} K_{ij} (S_{li}^z S_{2i}^z) - 2\mu E \sum_i (S_{li}^z + S_{2i}^z) + \\ + \frac{1}{4} \sum_k \omega_k (A_k^+ A_k^+ + B_k^+ B_k^+)$$

$$- \sum_{ik} V_{ik} S_{li}^z A_k - \sum_{ik} V_{ik} S_{2i}^z A_k^+ + \quad (27)$$

$$+ \sum V^{(3)}(k_1, k_2, k_3) A_{k_1} A_{k_2} A_{k_3}$$

$$+ \sum V^{(4)}(k_1, k_2, k_3, k_4) A_{k_1} A_{k_2} A_{k_3} A_{k_4},$$

Where, in Eq.(27) above Ω is proton tunneling frequency, S^z and S^x are components of pseudo-spin variable J_{ij} is interaction between the 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 constant¹⁵.

2.3. Dielectric Constant

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

$$\chi(\omega) = -\lim_{X \rightarrow 0} 2\pi N \mu^2 G_{ij}(\omega + iX) \quad (28)$$

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

$$\varepsilon = 1 + 4\pi\chi \quad (29)$$

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

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

$\varepsilon(\omega) \gg 1$ in the ferroelectric crystal.

2.4. Microwave Absorption

The power lost in dielectric when exposed to electromagnetic field is conveniently shown as dielectric microwave absorption which is expressed as

$$\tan \delta = \frac{\varepsilon''}{\varepsilon'} \quad (31)$$

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

$$\tan \delta = -\frac{2\Omega \Gamma(\omega)}{(\omega^2 - \hat{\Omega}^2)} \quad (32)$$

2.5. Ultrasonic Reflection

The acoustic attenuation is given as

$$\alpha = \frac{\Gamma(\omega)}{\nu} \quad (33)$$

where $\Gamma(\omega)$ is width and ν is sound velocity.

2.6. Ratio of Figure of Merits

We know that dielectric permittivity can be written as

$$\varepsilon = \varepsilon' \pm i\varepsilon'' \quad (34)$$

where ε' is real part of permittivity, ε'' imaginary part of permittivity and magnitude of this complex number will be

$$\varepsilon = \sqrt{\varepsilon'^2 + \varepsilon''^2} \quad (35)$$

Solve eq.(35) and eq.(31) we have

$$\varepsilon' = \sqrt{\frac{\varepsilon^2}{1 + \tan^2 \delta}} \quad (36)$$

and

$$\varepsilon'' = \sqrt{\frac{\varepsilon^2 \tan^2 \delta}{1 + \tan^2 \delta}} \quad (37)$$

in IR detection we can write the figure of merit can be written as

$$M_1 = \frac{\rho}{\varepsilon'}$$

High current responsivity

$$M_2 = \frac{\rho}{\sqrt{\varepsilon''}}$$

And vidicons application

$$M_3 = \frac{\rho}{\sqrt{\varepsilon'}}$$

Then relative figure of merits will be

$$\frac{M_2}{M_1} = \sqrt{\varepsilon''}; \quad \frac{M_3}{M_2} = \sqrt{\frac{\varepsilon''}{\varepsilon'}}; \quad \frac{M_3}{M_1} = \frac{\varepsilon''}{\sqrt{\varepsilon'}}$$

2.7. Quality-Factor

$$Q\text{-Factor} = 1/\tan\delta$$

where $\tan\delta$ = tangent loss.

2.8. Electric Conductivity

$$\sigma = \omega\varepsilon_0\varepsilon'' \quad (38)$$

where, σ = electric conductivity
 ω = phonon frequency.

2.9. Relaxation Time (Minimum)

Relaxation time (minimum) is,

$$\tau = \frac{\exp\left(-\frac{\pi}{2}\tan\delta\right)}{\omega} \quad (39)$$

2.10. Differentiability

$$S.F. = \frac{2\varepsilon''}{\pi\varepsilon} \quad (40)$$

3. CALCULATION

We have derived different relations for different physical constants used from different literatures as given below in table 1 and table 2.

Table 1. Crystal constants of deuterated triglycine sulphate crystal.

Ω (cm ⁻¹)	J (cm ⁻¹)	K (cm ⁻¹)	V_k (cm ^{-3/2})	T_c (K)	C (K)	μ (10 ¹⁸ esu)	$\hbar\omega$ (cm ⁻¹)
0.01	470	0	15	333.86	4873.16	2.3	1.92

Table 2. Calculated values of $\langle S_1^x \rangle$, $\langle S_2^x \rangle$, $\langle S_1^z \rangle$, $\langle S_2^z \rangle$ for deuterated triglycine sulphate crystal.

T(K)	$\langle S_1^x \rangle$	$\langle S_2^x \rangle$	$\langle S_1^z \rangle$	$\langle S_2^z \rangle$
285	0.0003	-0.08598	0.0134	-0.0156
297	0.00051	-0.08596	0.0118	-0.0171
309	0.00052	-0.0713	0.0083	-0.0193
321	0.00054	-0.0398	0.0071	-0.0206
333	0.000568	-0.004956	0	0
345	0.000513	-0.00138	0	0
357	0.000512	-0.0009101	0	0
369	0.000511	-0.000601	0	0
381	0.000510	-0.000342	0	0
393	0.000509	-0.000521	0	0

4. RESULTS

We have calculated results, which are given in the form of temperature gradient form in Figures 3-15 by using physical constant from table no. 1 and 2.

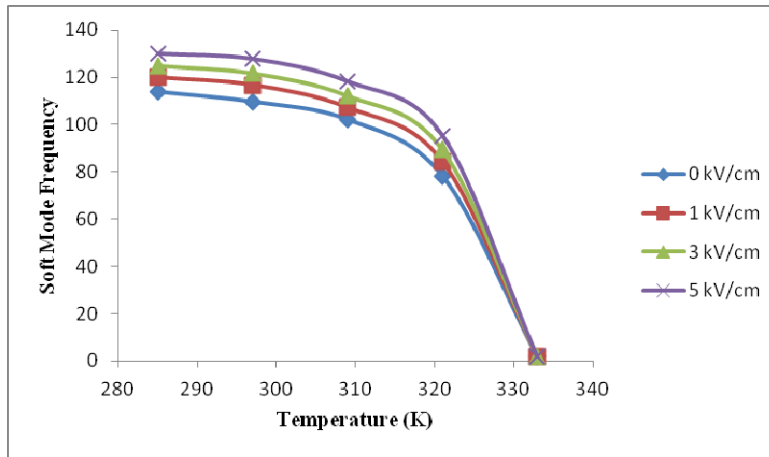


Figure 3. Temperature dependence of soft mode frequency of deuterated triglycine sulphate crystal.

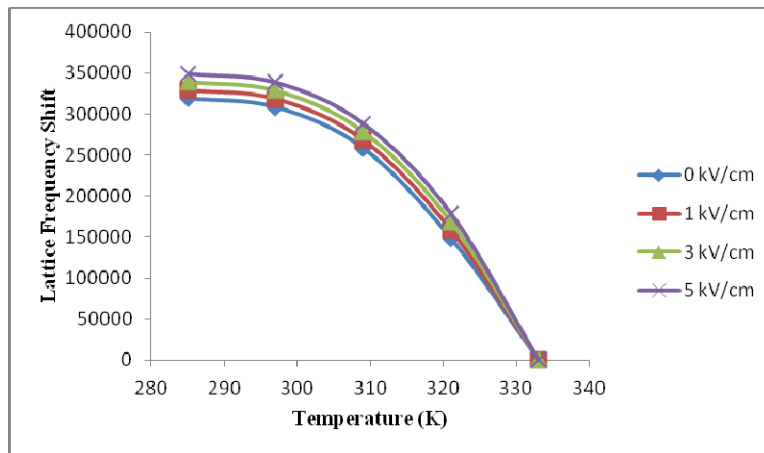


Figure 4. Temperature and electric field dependence of lattice frequency shift of deuterated triglycine sulphate crystal.

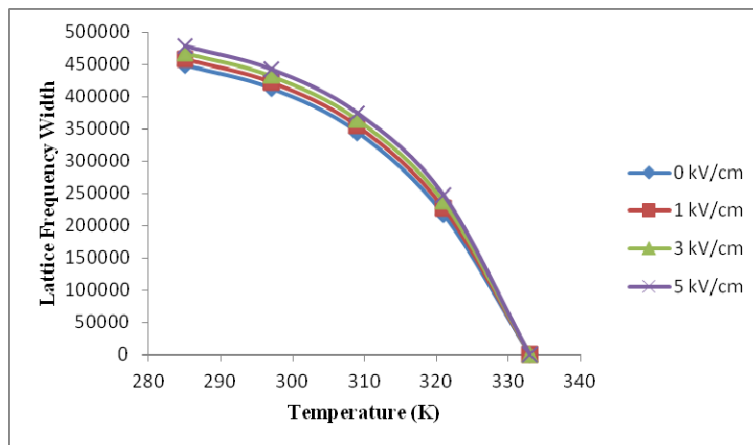


Figure 5. Temperature and electric field dependence of lattice frequency width of deuterated triglycine sulphate crystal.

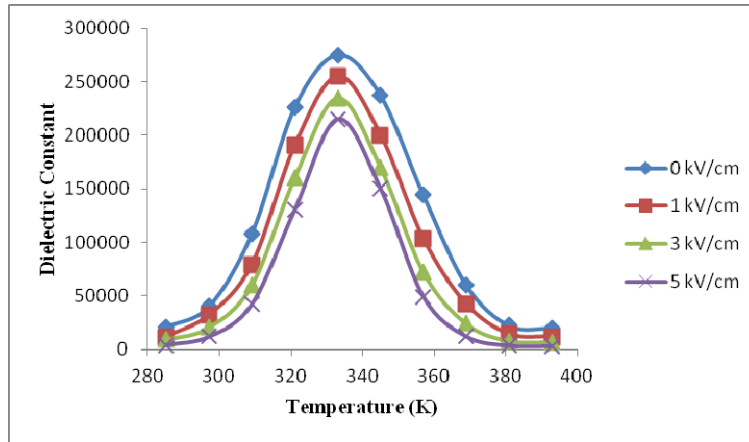


Figure 6. Temperature and electric field dependence of dielectric constant of deuterated triglycine sulphate crystal. (matched with experimental result Bye et al [18])

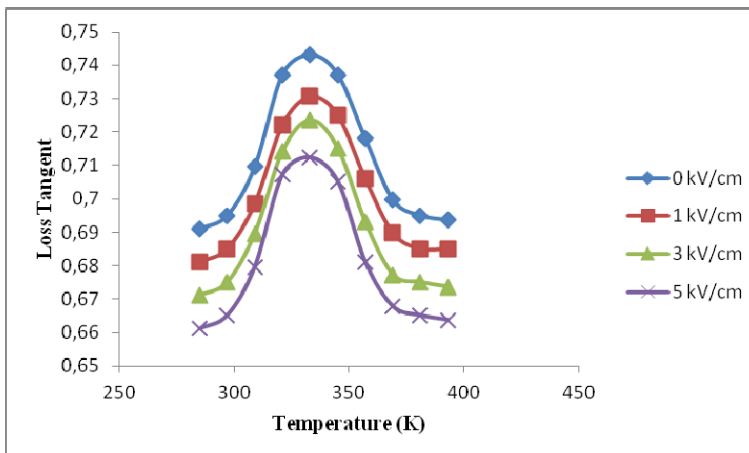


Figure 7. Temperature and electric field dependence of loss tangent of deuterated triglycine sulphate crystal. (matched with experimental result of Hills and Ichiki et al [19])

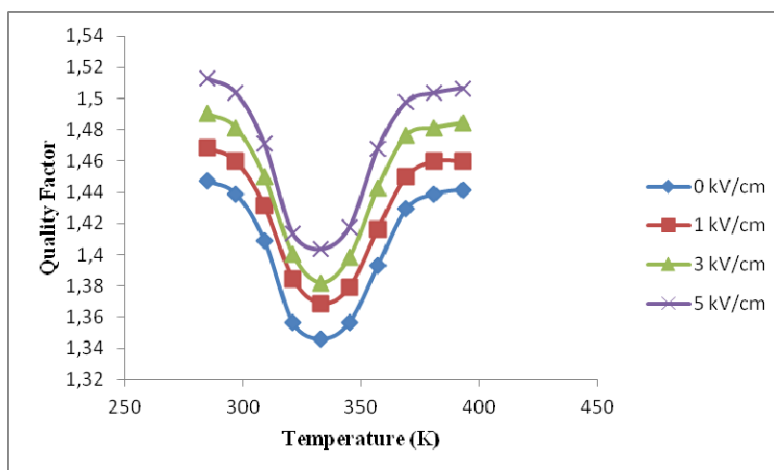


Figure 8. Temperature and electric field dependence of quality factor of deuterated triglycine sulphate crystal. (matched with experimental result of Hills and Ichiki et al [19])

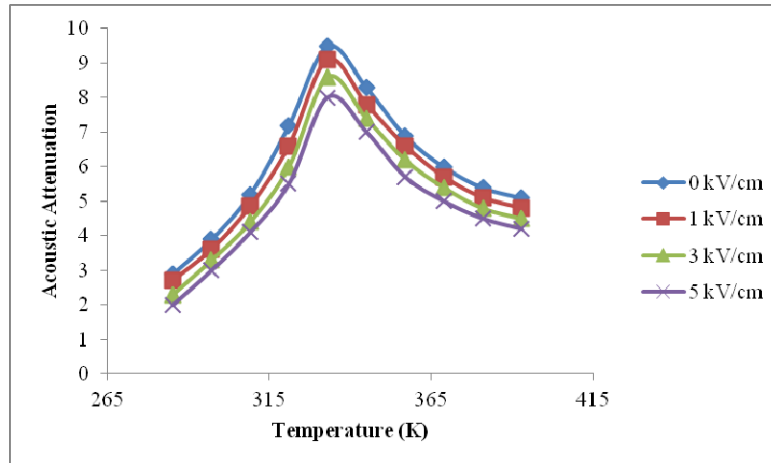


Figure 9. Temperature and electric field dependence of acoustic attenuation of deuterated triglycine sulphate crystal. (matched with experimental result of Shreekumar et al [20])

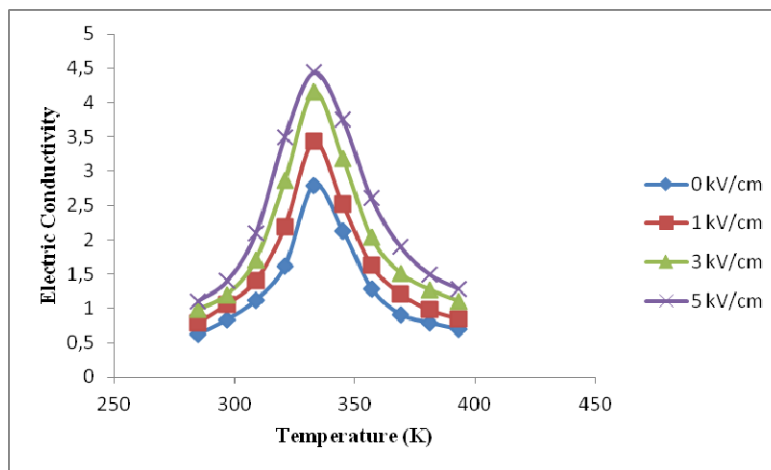


Figure 10. Temperature and electric field dependence of electric conductivity of deuterated triglycine sulphate crystal. (matched with experimental result of Gaffers et al [21])

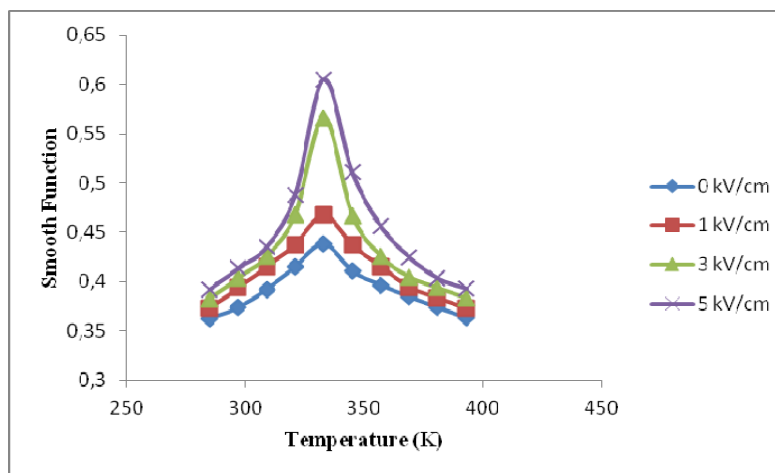


Figure 11. Temperature and electric field dependence of smooth function of deuterated triglycine sulphate crystal.

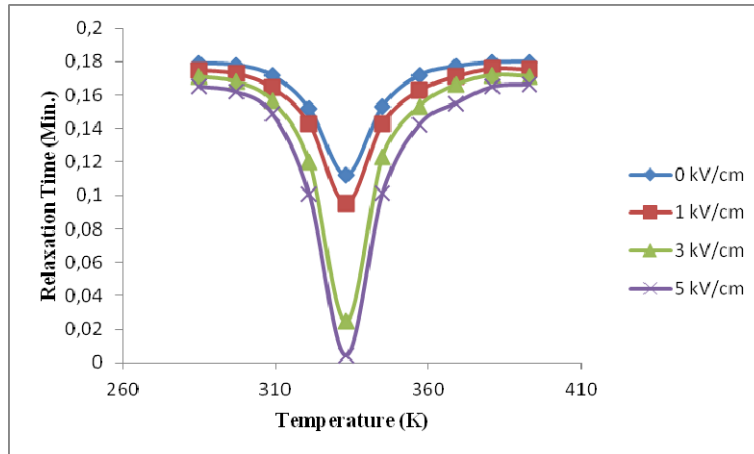


Figure 12. Temperature and electric field dependence of relaxation time of deuterated triglycine sulphate crystal (matched with experimental result of Drozhdin et al [6-9, 21-23])

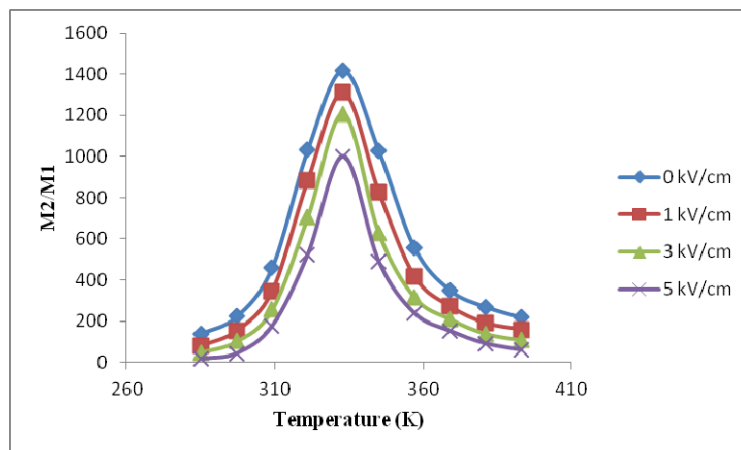


Figure 13. Temperature and electric field dependence of ratio of figure of merits ($M2/M1$) of deuterated triglycine sulphate crystal. (matched with experimental result of Banan et al [23] and Kushnir et al [9])

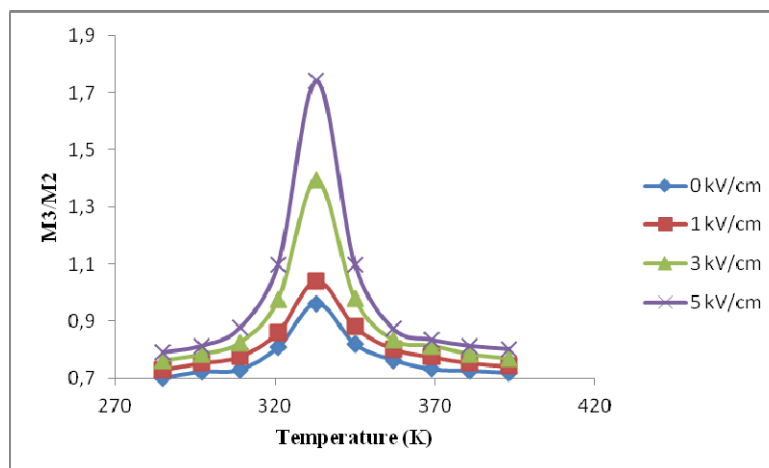


Figure 14. Temperature and electric field dependence of ratio of figure of merits ($M3/M2$) of deuterated triglycine sulphate crystal. (matched with experimental result of Banan et al [23] and Kushnir et al [9])

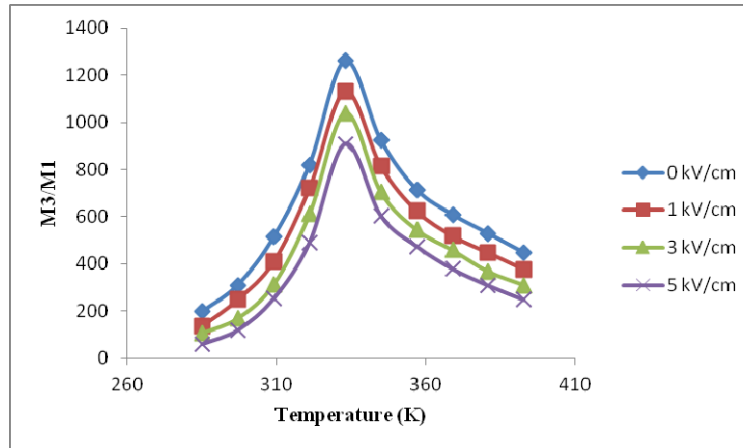


Figure 15. Temperature and electric field dependence of figure of merits ($M3/M1$) of deuterated triglycine sulphate crystal. (matched with experimental result of Banan et al [23] and Kushnir et al [9])

4. DISCUSSION

In this paper we have modified pseudo vibration theory by adding third and fourth order phonon anharmonic interaction terms in two sublattice modes for deuterated triglycine sulphate (DTGS) crystal. Using model values given by Chaudhuri et al [14,15], temperature dependence of shift, width of soft mode frequency, dielectric constant, loss tangent, quality factor, electric conductivity, smooth function, relaxation time and ratio of figure of merits have been obtained for deuterated triglycine sulphate crystal. Previous researchers [14,15,17] have not considered phonon anharmonic interactions, or two sublattice model and even not in a convincing way as they have decoupled the correlations at an early stage. As a result, some important interactions disappeared from their calculations. The width and shift of the present calculation reduce to the results of Chuoudhari et al. Previous researchers have not calculated the effect of electric field on soft mode frequency, dielectric constant, tangent loss, attenuation, quality factor, electric conductivity, smooth function, relaxation time and ratio of figure of merits of the crystal. All our calculated results are in good agreement with the experimental data. Thus, the study of deuterated triglycine sulphate crystal and their isomorphous forms can also be done in a similar way. The loss can be explained as the following, “A transverse radiation field derives the low lying transverse mode of the material in a forced vibration. Energy is transferred from the electromagnetic field to this lattice mode and is then degraded into other vibrational modes of the material. Due to anharmonic phonon interactions, decay processes take place, for

example, third order interaction leads to the decay of a virtual phonon in the real phonons or the virtual phonon may be destroyed by scattering a thermal excited phonon”. A ferroelectric field effect transistor in which a ferroelectric is used in place of metal gate on a field effect transistor would both decrease the main size of memory cell and provide nano structure read out; however, no commercial product has yet been developed as well as the application of random ferroelectrics memory (FRAMs). Ferroelectrics materials have a potential use in dynamics random access memory (DPAMs) because of their high dielectric constant in the vicinity of ferroelectrics phase transition (Kington, Maria, and Streiffer 2000). The leading computing technology in the long term for non-volatile computer includes FRAMs and magnetic access memory (MRAM). The main disadvantage of the above mentioned devices are accompanied by a write operation leading to faster degradation of the device. As a result much of the ferroelectric FET research has employed buffer layers, for example the first BaMnF4 FET made at symetrix (Scott 1998) used buffer layers for 40 nm of SiO₂, subsequently studies often used PZT (Scott 1998). Although the large remanent polarization in the case ($\sim 40 \mu\text{C}/\text{cm}^2$) is actually undesirable for a ferroelectrics FET gate. The direct contact of the ferroelectric on to Si produces a semiconductor junction that is quite different from the metal-dielectric interface the Schottky barrier height and for this case have been calculated by Peacock and Robertson (2002). It is also observed that stress widens the domain with compressive stress while a-stress widen domains with the c-stress the opposite tendency meanwhile the b-stress effect caused by AFM tip derive the domain switching towards the polar axis.

5. CONCLUSION

As conclusion we can say that deuterated triglycine sulphate crystal is conditionally a satisfactory crystal for memory devices, display devices and other pyroelectric devices.

6. ACKNOWLEDGEMENT

We are very thankful to professor P.K. Bajpai (Physics Dept., Guru Ghasidas Univ., Chhattisgarh, India), Prof. S. Mollah (Physics Dept., A. M. Univ., Aligarh, U.P., India) and Prof. S. K. Srivastava (Physics Dept., Bundelkhand Univ., Jhansi, U.P., India) for their kind support and advices.

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УЛОГА АКУСТИЧНИХ И ОПТИЧКИХ ВИБРАЦИОНИХ МОДА
У ТЕХНОЛОГИЈАМА ФЕРОЕЛЕКТРИЧНОГ КРИСТАЛА
(КРИСТАЛ ДЕУТЕРИСАНОГ ТРИГЛИЦИН-СУЛФАТА)

Сажетак: Модификована теорија Грине функције са теоријом псевдовибрација фероелектрике примијењена је на кристал деутерисаног триглицин-сулфата како би се предвидјеле примјене фероелектричног кристала у компјутерској технологији.

Кључне ријечи: фазни пријелаз, квантна стања, пребацивање.

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