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Permittivity, vibration frequency, and Tan δ of Crystalline CDP

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Abstract: In the present paper, we shall modify the pseudo-spin lattice Hamiltonian with phonon anharmonic factors, electric field factors, as well as two additional lattice factors to study vibration frequency, permittivity, and Tan δ. Derivations for formulae for the above quantities for CH_2PO_4. Temperature variations of these quantities will be calculated for CDP and compared with the practical value data given by Robert B. et al (1979).

Keywords: Transition • Vibration frequency • Susceptibility • tangent delta.

Introduction

Ferroelectric crystals exhibit spontaneous electric polarization, which can be reversed by stress or an electric field. These crystals have found numerous applications, including high capacitor dielectrics, memory device materials, light modulators, and electro-optic and piezoelectric materials. Cesium dihydrogen phosphate (CDP) exhibits ferroelectric behavior below 109 K. It is orthorhombic below 109 K and tetragonal above 109 K. The crystal constants are $a = 7.6$ Å, $b = 7.6$ Å, $c = 7.2$ Å, and $\beta = 90°$. KDP, KDA, and CDA crystals are collectively referred to as CDP crystals. Gridnev and Kravchenko (2000) have studied experimentally the shear modulus and internal friction of CDP crystals.

Sriprakash et al. (2013) have conducted experimental crystal structure studies. Naili et al. (2001) have investigated the effect of replacing P by As in the CDP crystal. Bu and Xu (2018) worked out the emissivity of CH_2PO_4. Koval et al. (2002) worked out the isotope effects in the transition isotope effect in the CDP crystal.

We shall modify the PLCM model by adding phonon anharmonic, electric field, as well as the addition of the phonon-spin factors with the aid of Zubarev's (1960) function method. We shall obtain formulas for permittivity, vibration frequency, as well as *tan* δ for CH_2PO_4. We shall obtain the thermal variation of the above quantities for the CDP crystal. Results will be compared to the practical values of Robert et al. (1979) for CH_2PO_4.

Model Hamiltonian

We shall modify the earlier model Hamiltonian PLCM model given in the Ganguli et al paper.

$$H = -2\Omega\sum_i S_i^x - \frac{1}{2}\sum_{ij} J_{ij} S_i^z S_j^z + \frac{1}{4}\sum_k \omega_k \left(A_k^\dagger A_k + B_k^\dagger B_k\right) - \sum_{ik} (V_{ik} S_i^z A_k)$$
$$+ \sum_{k_1 k_2 k_3} V^{(3)}(k_1,k_2,k_3) A_{k_1} A_{k_2} A_{k_3} + \sum_{k_1 k_2 k_3 k_4} V^{(4)} A_{k_1} A_{k_2} A_{k_3} A_{k_4} - 2\mu E\sum_i (S_i^z) - \sum_{ik} (V_{ik} S_i^z A_k) + \sum_{ik} (V_i$$

In equation (1), the first four terms constitute the PLCM model of Ganguli et al. We have added the 5th to 9th terms to modify the (PLCM) model.

Theory

Green Function, Shift Weight, and Normal Mode Frequency.

Consider the double–time thermal Greens function,

$$G(t-t') = -i\Theta(t-t')\langle[S_i^z(t); S_j^z(t')]\rangle \quad \text{-(4)}$$

We shall differentiate equation (4) two times, then convert it into a Fourier transform, and we obtain

$$(\omega^2-4\Omega^2)\, G(\omega)=\delta(t-t')/2\pi<[f,S^x_j]> + <<F(t);S^x_j(t')>> \qquad -(5)$$

Differentiating last term on the other side of equation two times with t', taking the Fourier transform, we obtain

$$(\omega^2-4\Omega^2)\, T(\omega)=\delta(t-t')/2\pi<[F,S^x_j]> + <<F(t);F^x_j(t')>> \qquad -(6)$$

From eqn. (5), and (6), put it into what is called the equation of F.J. Dyson. This gives the value of the Green function.

$$G(\omega) = \Omega<S^x_i>\delta_{ij} / \pi[\omega^2 - \hat{\Omega}^2 - 2i\Omega\, \Gamma(\omega)] \qquad -(7)$$

In the above Equations

$$\hat{\Omega}^2 = 2\Omega\,\Delta(\omega) + \tilde{\tilde{\Omega}}^2 \qquad -(8)$$

And

$$\tilde{\tilde{\Omega}}^2 = \Delta_s(\omega) + \tilde{\Omega}^2 \qquad -(9)$$

With

$$\tilde{\Omega}^2 = a^2+b^2-bc \qquad -(10)$$

$$a= (J_{ij}<S^z> + 2\,\omega E)<S^z> \qquad -(11)$$

$$b= 2\,\Omega \qquad -(12)$$

$$c= J_y<S^x_i> \qquad -(13)$$

$\Delta(\omega)$ and $\tau(\omega)$ are the shift and width of the frequency response P(ω) is obtained as.

$$P(\omega) = <<F(t);F^x_j(t')>> / \Omega< S^z_i > \qquad -(14)$$

In eqn. (14). $<<F_i(t);F^x_j(t')>>$ are higher-order Green functions which are decoupled using the symmetric truncation formula. Thus, decoupled simple Green functions are solved and substituted into Equation (14), i.e., Equation (7). Thus, we obtained. $\Delta_s(\omega)$, $\Delta(\omega)$ *and* $\tau(\omega)$ Shift and width are the real and imaginary parts of P(ω). Equations (8), (9), and (10) represent the normal mode frequency, normalized pseudo-spin frequency, and bare pseudo-spin frequency of the CDP Crystal, respectively. From Equation (8), we obtain the normal mode frequency $\hat{\Omega}$ as.

$$\hat{\Omega} = 1/2\,(\tilde{\tilde{\Omega}}^2-\tilde{\Omega}^2) \pm 1/2\,\sqrt{[(\omega^{\aleph 2}{}_k-\tilde{\tilde{\Omega}}^2) + 16\Omega V^2_{ik}<S^x_i><\omega_k> + 2aV^2_{ik}<S^z_i><\omega_k>/2\Omega + 4\omega^2 E^2 V^2_{ik}<S^y_i>\omega_k]} \qquad -(15)$$

Dielectric Constant

The electric constant ϵ is related to susceptibility χ as $\epsilon = 1 + 4\pi\chi$. In ferroelectric $\epsilon >>1$, so $\epsilon=4\pi\chi$. Susceptibility χ is related to Zubarev's function as $x=-2\pi N\mu^2 G\ (\omega)$. From equation (15), we obtain with its real part as

$$\epsilon' =8\pi N\mu^2\ \Omega<S^x_i>(\omega^2 - \hat{\Omega}^2\ )/[(\omega^2 - \hat{\Omega}^2)^2 + 4\Omega^2\, T(\omega^2)\,] \qquad -(16)$$

In eqn. 16 in the denominator, the second term is minimal as compared to 1st term, and $\omega\ <<\hat{\Omega}$ equation (16) gets simplified.

Dissipation Loss

Energy loss in dielectrics is obtained by dividing ϵ'' by ϵ' i.e.

$$Tan\,\delta = \frac{\epsilon''}{\epsilon'} \qquad -(17)$$

From the Equation.(16), we obtain

$$Tan\,\delta = \frac{-2\Omega\ \ \Omega(\omega)}{(\omega^2 - \hat{\Omega}^2)} \qquad -(18)$$

In Equation (18) at radio frequency $\omega\ <<\hat{\Omega}$, so that equation. (18) gets simplified.

$$Tan\,\delta = 2\Omega\Gamma / \hat{\Omega}^2 \qquad -(19)$$

Numerical calculation and comparison with experiments.

Putting the various parameter values for CDP in the expression, 15, 16, 18, thermal variations of $\hat{\Omega}$, ϵ and $tan\,\delta$ are calculated. These values are plotted in Figures 1, 2, and 3. Experimental Data of Blinc et al. [8] are also plotted in these figures for comparison. It is observed that our theoretical values meet to match with practical values reported by Robert, B. et al. 1979 for CDP.

Ω (cm^{-1})	J (cm^{-1})	J' (cm^{-1})	Tc (K)	V_{ik} (cm^{-1})	ω_k (cm^{-1})	μ * 10^18 esu-cm	N*10^22 (cm^{-3})
82	350	450	154	25	130	1.8	0.8

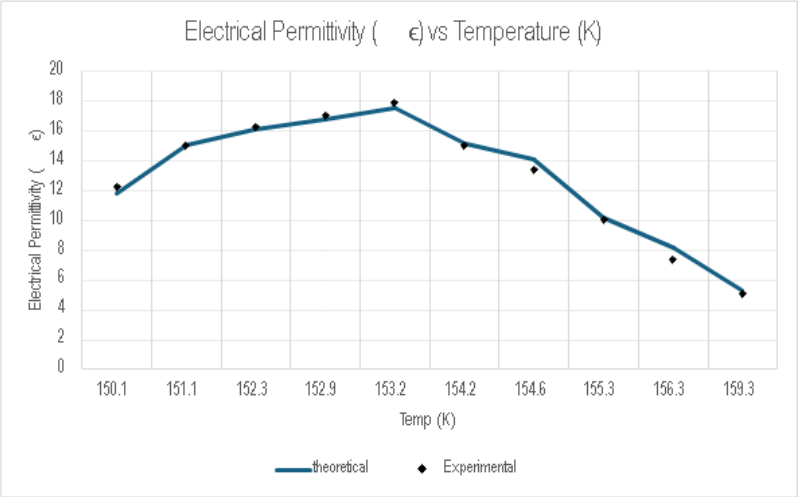

Fig. 1 Present computed values of permittivity against T(K) for CDP data (solid line); Practical values of Robert, B. et al., 1979.[8] (Dashed)

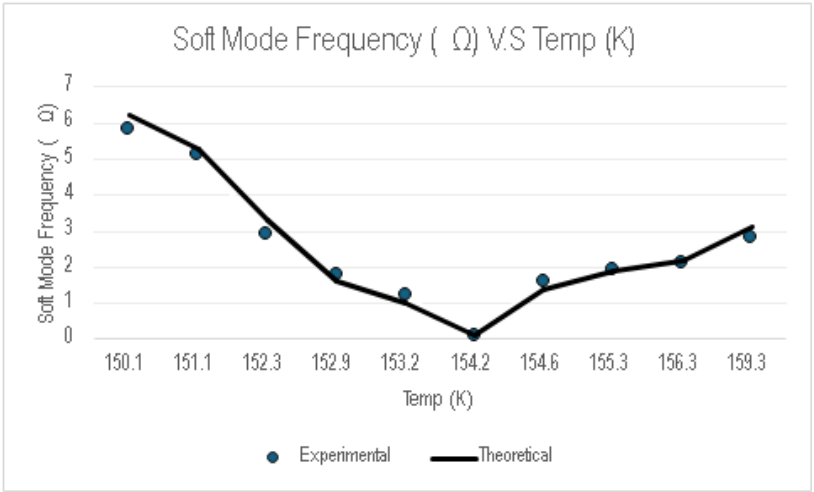

Fig. 2 Our Computed values for vibration frequency against T(K) in CDP. Our data (solid) Practical values extracted from dielectric data of Robert B. et al, 1979.[8] (Dashed)

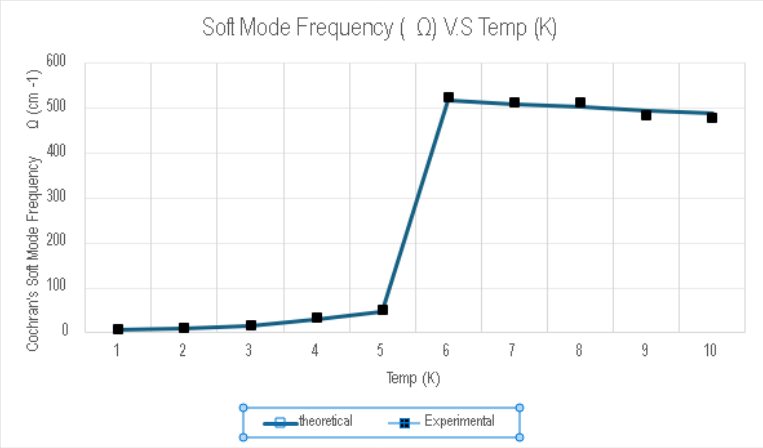

Fig. 3 Theoretical (Tan δ) against T for CDP; our computed data(solid line); practical data of Robert B. et.al 1979.[8] (Square)

Discussion & Conclusion

Our expressions 15, 16, and 18 clearly demonstrate that the terms we have added to the model contribute to explaining permittivity, vibration frequency, and Tan δ for CDP Crystal. Expression (15) predicts experimental data for the vibrational frequency in the CDP Crystal. The normal mode frequency first decreases from below Tc, then becomes anomalously small, and then increases around Tc. Our expression 16 predicts the behavior of the dielectric constant in accordance with experimental results. It first increases from below Tc, then becomes large, and then decreases above Tc. Similar behavior is observed for the loss tangent of the CDP crystal. Therefore, it is concluded that the modified model is suitable for explaining the behavior of CDP-type crystals. We have set E = 0 in all numerical calculations.

References

Bu H and Xu C (2018). Optical properties of materials. *Optical Materials*, 84, 109–114.

Ganguli S, Nath D and Chaudhuri B K (1980). Ferroelectric behavior in solid-state systems. *Physical Review B*, 21, 2937.

Gridnev S A and Kravchenko S A (2000). Solid-state properties of crystalline structures. *Physics of the Solid State*, 42(11), 2137–2141.

Koval SJ, Kahanoff RL et al. (2002). Structural analysis of ferroelectric compounds. *Physical Review Letters*, 89, 187602.

Kumar K and Upadhyay TC (2022). Structural and dielectric properties of materials. *Materials Today: Proceedings*, 49, 2360–2364.

Naili H, Vedier L, Jaud J and Mhiri T (2001). Crystal structure and solid-state characterization. *Solid State Sciences*, 3(6), 647–677.

Robert B and Zeks B et al (1979). Ferroelectric phase transitions and polarization behavior. *Physical Review Letters*, 43, 231.

Singh P and Upadhyay TC (2020). Studies on functional materials. *Materials Today: Proceedings*, 28, 146.

Sriprakash G, Ramesh KP and Rukmania K (2013). Spectroscopic and dynamic studies of solid-state materials. *Journal of Spectroscopy and Dynamics*, 3(2).

Upadhyay R and Bhatt SC (2023). Ferroelectric behavior of ceramic compounds. *Ferroelectrics*, 616, 33.

Zubarev DN (1960). Double-time Green functions in statistical physics. *Soviet Physics Uspekhi*, 3, 320.