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Thermal variations of crystal vibrational frequency, capacitivity, and dissipation loss in crystalline Rubidium Dihydrogen Arsenate (RDA)

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Abstract: The crystal vibrational frequency, capacitivity and dissipation loss in crystalline RDA are studied using an extended lattice coupled pseudospin Hamiltonian. Statistical two-time Zubarev's Green function approach has been employed for derivations. In the model, four spin coupled term, anharmonic vibrational terms, additional lattice coupled-spins terms as well as static electric field term have been added. Theoretical formulae for capacitivity, dissipation loss and crystal vibrational frequency are developed. Thermal variations of above quantities are found for RDA crystal by fitting model values. Theoretical findings satisfactorily agree with Blinc and Burgar et al. (1973).

Keywords: Crystal vibrational frequency • Curie temperature • Ferroelectric • Capacitivity • Dissipation loss

Introduction

The ferroelectric materials have got important applications in different fields. Transducers, demodulators, deflectors, high permittivity capacitors, electro-optic materials, pyroelectric detectors and gas sensing devices are just a few examples for these materials. Rubidium dihydrogen arsenate (RDA) crystal shows ferroelectric transition at 110.2K. T_c shifts to 176.5K on deuteration, exhibiting a significant isotope effect. Crystal constants of RDA at normal temperature are a=7.7033 Å , b=7.7933 Å ,c=7.466 Å and β=90°.Chouchene et al (2017) have worked out structural and thermal properties of RDA crystal as well as temperature dependent behaviour of RDA. Seliger et al (2011) have done NQR study of RDA crystal. Truesdale et al (1980) worked out X-ray experiments on RDA crystal. K. Kato (1995) has studied generation of X-ray using RDA. Leung et al (1973) studied RDA crystal's soft mode behavior. Adhav (1969) has researched the RDA crystal's physical characteristics. V Rama and T. Tomoyashu (1977) as well as Nath et al (1980) have employed pseudospin model Hamiltonian for their study of RDA crystal (KDP-type crystals). R. Deepali and Trilok (2016), Pawan and Trilok (2020) and Kuldeep and Trilok (2022) have earlier studied KDP-type crystals by using pseudospin model with some extension of model. Riya Upadhyay and SC Bhatt (2022) have studied temperature variations of crystal vibrational frequency, capacitivity and dissipation loss in potassium dihydrogen phosphate KH_2PO_4(KDP)crystal. By including the phonon anharmonic (Riya Upadhyay and SC Bhatt.,2022), four spin couplings, electrostatic energy as well as and additional lattice coupled pseudospins, we have extended the original model Hamiltonian. For derivations we used Riya Upadhyay and SC Bhatt (2022) for crystal vibrational frequency, capacitivity, as well as dissipation loss for crystalline RDA crystal. We used Zubarev two-time method of statistical Green functions (Zubarev., 1960). To find temperature variations of aforementioned quantities for RDA crystal, model values are employed. For RDA crystal, computed data have been compared with practical data from (Blinc and Burgar et al., 1973). Unlike Nath et al., (1980) we have considered more terms in Hamiltonian and done decoupling at proper stage. Unlike Deepali and Trilok (2016) we considered more terms in Hamiltonian. Unlike

Pawan and Trilok (2020) we have neglected direct spin-spin factor and complicated decoupling as well. We considered four spin term. Similarly, unlike Kumar and Upadhyay (2022) we have neglected direct spin-spin term in our work.

Theory

Shift and Width

The extended Hamiltonian (Riya Upadhyay and SC Bhatt.,2022) is expressed as:

$$H = -2\Omega\sum_i S_i^x - \frac{1}{2}\Sigma_{ij}J_{ij}S_i^zS_j^z + \frac{1}{4}\Sigma_k\omega_k(A_k^+A_k + B_k^+B_k) - \Sigma_{ik}V_{ik}S_i^zA_k + \sum_{k_1k_2k_3}V^3A_{k_1}A_{k_2}A_{k_3} + \sum_{k_1k_2k_3k_4}V^4A_{k_1}A_{k_2}A_{k_3}A_{k_4} - \Sigma_{ik}S_i^zV_{ik}A_k - \Sigma_{ik}S_i^xV_{ik}A_k^2 - \frac{1}{4}\sum_{ijkl}J_{ijkl}^{'}S_i^zS_j^zS_k^zS_l^z - 2\mu E\sum_i S_i^z$$

In Equation (1), the proton tunnelling frequency (Riya Upadhyay and SC Bhatt.,2022) and exchange interaction between O-H-O bonds are provided. Components of spin 1/2 operator are S_i^x , S_i^z . Spin-lattice interaction is V_{ik}. Displacement and momentum operators are A_k and B_k. Phonon frequency is ω_k. $J_{ijkl}^{'}$ is four spin interaction constant while V^3 (Riya Upadhyay and SC Bhatt.,2022) and V^4(Riya Upadhyay and SC Bhatt.,2022) represent anharmonic phonons factors. Extra spin lattice terms make up the seventh and eighth terms while the electric field term makes up the tenth term.

The Green's function (Riya Upadhyay and SC Bhatt.,2022) $G(\omega)$ is finally obtained (simplified one) derived as follows using double-time Green's function and Hamiltonian Equation (1)

$$G(\omega) = \pi^{-1}\Omega\langle S_i^x\rangle\delta_{ij}\left[\left(\omega^2 - \widehat{\Omega}^2\right) + 2\Omega\Gamma(\omega)\right]^{-1} \quad (2)$$

With (Riya Upadhyay and SC Bhatt.,2022)

$$\widehat{\Omega}^2 = \widetilde{\Omega}^2 + \Delta(\omega) \quad (3)$$

And (Riya Upadhyay and SC Bhatt.,2022)

$$\widetilde{\Omega}^2 = a^2 + b^2 - bc. \quad (4)$$

where

$$a = \left(2\mu E + J + 3J^{'}\langle S_i^z\rangle^2\langle S_{ii}^z\rangle\right) \quad (5)$$

$$b = 2\Omega \quad (6)$$

As well as

$$c = \left(J + 3J^{'}\langle S_i^z\rangle^2\langle S_{ii}^z\rangle\right) \quad (7)$$

In the above Eq. (2) and (3), Δ(ω) and Γ(ω) (Riya Upadhyay and SC Bhatt., 2022) stand for frequency shift and frequency width. These naturally appear when we solve Green function following:-

$$G(\omega) = \pi^{-1}\Omega\langle S_i^x\rangle\delta_{ij}\left[\left(\omega^2 - 4\Omega^2 - \widetilde{P}(\omega)\right)\right]^{-1} \quad (8)$$

Crystal vibrational frequency

When we solve Eq. (3) we obtain crystal vibrational frequency as

$$\widehat{\Omega}^2 = \frac{1}{2}\left\{\left(\widetilde{\Omega}^2 + \widetilde{\omega}_k^{\,2}\right) \pm \left[\left(\widetilde{\Omega}^2 - \widetilde{\omega}_k^{\,2}\right) + \ldots + 16V_{ik}\langle S_i^x\rangle\Omega + \ldots\right]^{\frac{1}{2}}\right\}$$

Capacitivity

Both capacitivity and electric susceptibility are connected to Green function $G(\omega)$ is related to susceptibility $\chi(\omega)$ and hence to $\epsilon(\omega)$ as

$$\chi(\omega) = \lim_{x\to 0} 2\pi N\mu^2 G(\omega); \epsilon(\omega) = 1 + 4\pi\chi$$

. In ferroelectric crystals $\epsilon(\omega) \gg 1$ so $\epsilon(\omega) = 4\pi\chi$ that .(Riya Upadhyay and SC Bhatt.,2022).So we obtain

$$\varepsilon(\omega) = \frac{-8\pi N\Omega\mu^2 \ll S_i^x \gg}{[(\omega^2 - \widehat{\Omega}^2) + 4\Omega^2\Gamma^2]} \quad (10)$$

Dissipation Loss

Dissipation loss (Riya Upadhyay and SC Bhatt.,2022) $(tan\delta)$ is given as

$$tan\delta = \frac{\epsilon^{''}}{\epsilon^{'}} = \frac{-2\Omega\Gamma(\omega)}{(\omega^2 - \widehat{\Omega}^2)} \quad (11)$$

Results

With the help of Eq. (9-11), when we put values from following table, we obtain crystal vibrational frequency, capacitivity, dissipation loss versus temperature curves (Fig.1-3)

J $(cm)^{-1}$	$\dot{J}$ $(cm)^{-1}$	V_{ik} $(cm)^{-1}$	Ω $(cm)^{-1}$	ω_k $(cm)^{-1}$	T_c (K)	$N_k \times 10^{-22}$ (esu-cm)	$\mu \times 10^{18}$ $(cm)^{-3}$
238.8	321.5	14.66	.9	26	110.25	.76	1.5

We have therefore obtained our theoretical data for RDA which are compared with practical data. (Blinc and Burgar.,1973)

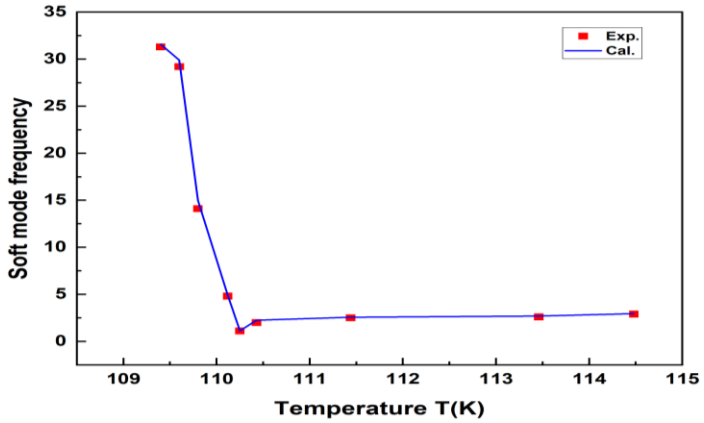

Fig.1 Variations of crystal vibrational frequency $(\hat{\Omega})$(cm^{-1}) with temperature in RDA crystal. Our computed values are denoted by (—) and practical values by (♦)

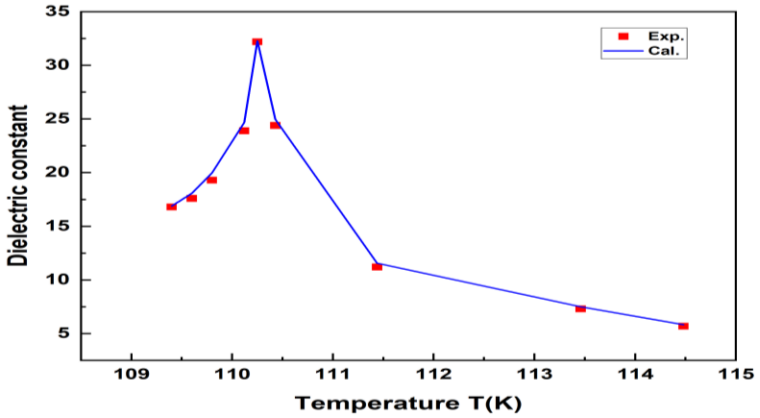

Fig.2 Variations of capacitivity(ε) with temperature in RDA crystal Our computed values are denoted by (—) and practical values by (♦)

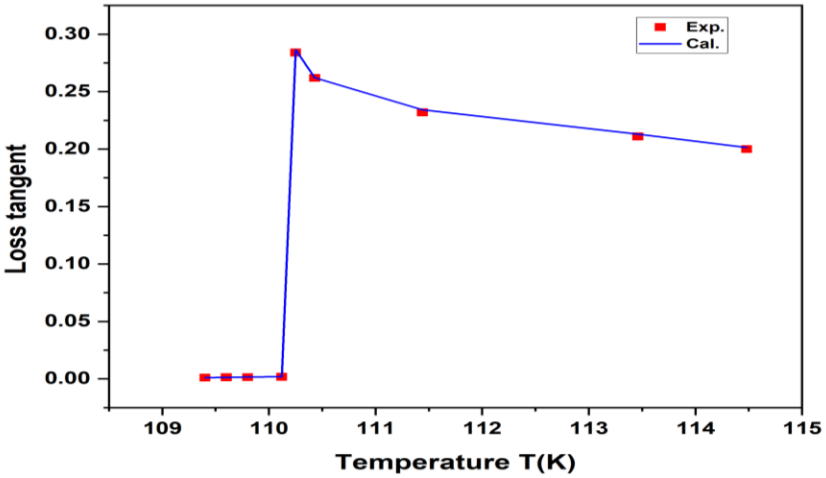

Fig.3 Variations of dissipation factor (tan δ) with temperature in RDA crystal Our computed values are denoted by (—) and practical values by (♦)

Discussion

It is observed that the correlated frequency values deduced from the dielectric data of (Blinc and Burgar.,1973) agree with temperature variations of the RDA crystal of crystal vibrational frequency. Agreements exist between our calculations of the capacitivity and dissipation loss with practical RDA data of (Blinc and Burgar.,1973). Our calculations show that our ability to describe the behaviours of $\epsilon(\omega)$, $tan\delta$ and $\widehat{\Omega}$ in RDA crystals are significantly impacted by the additional factors we took into account in our work.

Findings

It is the conclusion that present modified model Hamiltonian is adequate in explaining the experimentally observed thermal variations of dielectric properties of RDA crystal.

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