



A Review on Paraelectric Behavior of KI: OH⁻ System

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Abstract: Within the framework of two parameter octahedral potential for a dipolar impurity in ionic crystals, it is possible for impurity to possess minimum energy orientational configurations in two crystallographic directions simultaneously. Two combinations are $\langle 111 \rangle + \langle 110 \rangle$ and $\langle 111 \rangle + \langle 100 \rangle$. Taking first model, I have tried to explain theoretically the paraelectric behavior of KI: OH⁻ system with applied electric field in $\langle 110 \rangle$ and $\langle 100 \rangle$ directions. The data gives good agreement for backward lines with the experimental data.

Key Words: Paraelectric, Tunneling models, Paraelectricity, backward lines

I. Introduction

Oriental tunneling motion of the defects in solids have received considerable attention in the past few years, numbers of experiments have been performed on such system as Li^+ , OH^- CN⁻ and NO_2^- in alkali halide crystals [1]. Many qualitative features were interpreted in terms of pocket state model proposed by Gomez et al [2]. Potassium iodide doped with hydroxyl ion, KI:OH⁻ is a paraelectric system whose behavior has been investigated by a variety of techniques [3,4,5]. Since paraelectric resonance is extremely useful in investigating paraelectricity, because three important parameters, namely the dipole moment, dipole orientation and the tunneling parameters. So the initial paraelectric resonance data [3] taken on KI:OH⁻ between 12 and 75 GHz have some interesting features, which provided compelling motivations which was later done by Kelly et al [5]. The observation of lines that moves to lower electric field as the frequency is increased plus strong temperature dependence of some resonance can apparently be most easily explained by presence of a second multiplet of energy level within 200 GHz of the usual ground state tunneling multiplet. This is entirely unexpected result which has not been observed in any other paraelectric system. In addition the KI:OH⁻ paraelectric resonance system contains an unusually large number of lines, many of which are relatively narrow, which should facilitate more accurate measurement of the system parameters. The more detailed experimental examination of this system was done and has been published [5] which are in good agreement with a tunneling model [2]. Later Pandey et al [6, 7] says that there is possibility of simultaneous occurrence of potential minima along two crystallographic directions in an octahedral potential. The two possible combinations are $\langle 111 \rangle + \langle 110 \rangle$ and $\langle 111 \rangle + \langle 100 \rangle$, and later on using $\langle 111 \rangle + \langle 100 \rangle$ tunneling model Raj Kumar et al [8] explains the paraelectric behavior of KI: OH⁻ with applied electric field in $\langle 110 \rangle$ and $\langle 100 \rangle$ direction. So in present paper, I try to explain paraelectric behavior of KI doped with OH⁻ ion with the help of $\langle 110 \rangle + \langle 111 \rangle$ tunneling model with applied electric field in $\langle 110 \rangle$ and $\langle 100 \rangle$ direction only.

II. Theory

Different approaches have been made to explain the experimental data of paraelectric resonance of KI: OH⁻ system by different workers. For this purpose they have been taken two type of models, one is Hinder Rotor model and another is Two multiplet tunneling model. Taking second approach we will explain the experimental result of paraelectric resonance of KI:OH⁻ system in present model i.e. $\langle 111 \rangle + \langle 110 \rangle$ tunneling model.

When the wave functions are expressed according to the irreducible representation of O_h group then the transformed Hamiltonian H' for the model impurity under the influence of electric field will be

$$H' = H_0 + H_E$$

Where $H_0 = T + V$ and $H_E = eE_{loc}(\alpha x + \beta y + \gamma z)$

Hence

$$H' = T + V + eE_{loc}(\alpha x + \beta y + \gamma z)$$

Where V is the multiwell potential, E_{loc} is the field seen by impurity, e is the charge of impurity and α, β, γ are the direction cosines of the field with respect to x, y and z axis. Hamiltonian H' is obtained using the above equation and the wave function for twelve $\langle 110 \rangle$ well and eight $\langle 111 \rangle$ wells [2].

III. Conclusions

On diagonalizing the Hamiltonian H' we have studied the variation of electric field with frequency. The result of present model with $\eta = 20$ GHz, $\eta' = 105$ GHz, $\chi = 10$ GHz and dipole moments along $\langle 110 \rangle$ and $\langle 111 \rangle$ directions are 4 Deby each is shown in fig.1 and 2 respectively, by solid lines and experimental points are also plotted for ready comparison by solid circles which was performed by Kelly et al [5]. When electric field is applied parallel to $\langle 110 \rangle$ and $\langle 100 \rangle$ directions respectively.

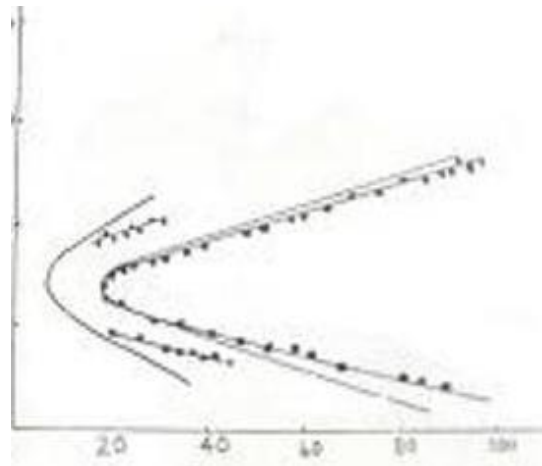


Fig 1 Variation of electric field (KV/ cm, on Y- axis) with frequency (GHz, on X- axis) for KI: OH⁻ system

a). ●●●●●●●●●● Represents experimental data for $E_{dc} || E_{ref} || \langle 110 \rangle$

b). Solid lines represents the result of present theoretical investigation for $\langle 110 \rangle + \langle 111 \rangle$ tunneling model.

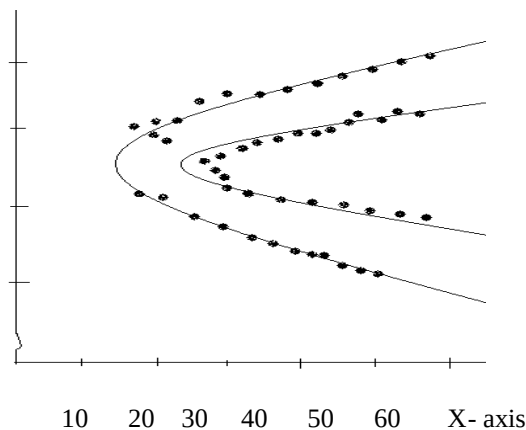


Fig 2 Variation of electric field (KV/ cm, on Y- axis) with frequency (GHz, on X- axis) for KI: OH⁻ system

a). ●●●●●●●●●● Represents experimental data for $E_{dc} || E_{ref} || \langle 100 \rangle$

b). Solid lines represents the result of present theoretical investigation for $\langle 110 \rangle + \langle 111 \rangle$ tunneling model.

From fig. 1 & 2 we can say that the theoretical result of the investigation have good agreements with experimental data because it can explain the backward lines of KI:OH⁻ systems the turned around frequency 17 GHz and 22 GHz respectively [9] comes out approximately same as experimental value performed by Kelly et al [5]. The variation of electric field with frequency is also satisfactory except slope of line is greater in case of present model. This can be removed by taking the higher order interaction term in the Hamiltonian. One important thing in the analysis is that in the experimental curve there are two lines which have opposite slope but they could not meet at a point near 7 GHz and 14 GHz. So this provide occurrence of another backward lines with turn around frequency 7 GHz and 14 GHz. Hence for this purpose experimental facts should be verified further.

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