



Behaviour of Electrical Pressure with Temperature and Electric Field for <100> Tunnelling Model

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Abstract: In the present paper we have investigated theoretically the variation of electrical pressure with temperature and electric field for <100> tunnelling model along different direction. Which may be used to explain various experimentally available data and may be also used for further theoretical investigations.

Keywords: Dielectric constant, Tunneling model & Electrical Pressure

I. Introduction

Diatomic and off-centered monoatomic impurities alter the properties of host crystal drastically. There has been considerable recent interest in the impurity modes of ions substituted at lattice sites in alkali halide crystals. A small concentration of impurity doped in certain alkali halides cause a large rise in dielectric constant at low temperature.[1].The octahedral potential for the angular motion of the diatomic impurity in solid state matrices was first presented by Devonshire[2].Many experimental results for system such as OH⁻ and CN⁻ ions in alkali halide matrices[3,4] and HCl, HBr etc impurities in rare gas matrices[5] have successfully explained. The effects of externally applied electric field on induced dipole moment of the impurity were studied by Gomez et al[6] using tunnelling models.

Theory - The electric field polarisation for the <110> off centered model and for the model of simultaneous minima along the direction <110> + <111> has been explained by Pandey et al [7,8].Theoretical study of polarisation and dielectric constant for the various tunnelling models have been obtained by Raj Kumar et al [9,10,11,12] using the relation

$$\epsilon = \frac{dP}{dE} \quad 1.1$$

The expression of polarisation and dielectric constant for electric field along different crystallographic direction for system<100>is listed in Table-1 with $x = \frac{\mu E}{kT}$

Table 1

Direction of applied electric field	Polarisation as expected from the simple<100> model	Dielectric constant
<100>	$P = N\mu \frac{e^x - e^{-x}}{4 + e^x + e^{-x}}$	$\epsilon = \frac{4N\mu^2(1 + e^x + e^{-x})}{kT(4 + e^x + e^{-x})^2}$
<110>	$P = \frac{N\mu}{\sqrt{2}} \left[\frac{e^{x/\sqrt{2}} - e^{-x/\sqrt{2}}}{1 + e^{x/\sqrt{2}} + e^{-x/\sqrt{2}}} \right]$	$\epsilon = \frac{N\mu^2 \left(4 + e^{x/\sqrt{2}} + e^{-x/\sqrt{2}} \right)}{2kT \left(1 + e^{x/\sqrt{2}} + e^{-x/\sqrt{2}} \right)^2}$
<111>	$P = \frac{N\mu}{\sqrt{3}} \left[\frac{e^{x/\sqrt{3}} - e^{-x/\sqrt{3}}}{e^{x/\sqrt{3}} + e^{-x/\sqrt{3}}} \right]$	$\epsilon = \frac{4N\mu^2}{3kT \left(e^{x/\sqrt{3}} + e^{-x/\sqrt{3}} \right)^2}$

The expression for electric pressure is given by

$$S = \frac{\sigma^2}{2\epsilon} \quad 1.2$$

Where σ = surface density of charge.

Using the expression of dielectric constant as listed in Table 1, we have obtained the expression for electrical pressure and given below.

Case-I: Electric field along <100> direction-

The expression for electrical pressure for system<100> and the electric field along the direction<100> is worked out and given as

$$S = \frac{\sigma^2 kT (4 + e^x + e^{-x})^2}{8N\mu^2 (1 + e^x + e^{-x})} \quad 1.3$$

Case-II: Electric field along<110>direction-

The expression for electrical pressure for system<100> and the electric field along the direction<110> is worked out and given as

$$S = \frac{\sigma^2 kT \left(1 + e^{x/\sqrt{2}} + e^{-x/\sqrt{2}} \right)^2}{8N\mu^2 \left(4 + e^{x/\sqrt{2}} + e^{-x/\sqrt{2}} \right)} \quad 1.4$$

Case-III: Electric field along<111>direction-

The expression for electrical pressure for system<100> and the electric field along the direction<111> is worked out and given as

$$S = \frac{3\sigma^2 kT \left(e^{x/\sqrt{3}} + e^{-x/\sqrt{3}} \right)^2}{8N\mu^2} \quad 1.5$$

The variation of electric pressure with temperature is shown in the figure1.1 and1.2 as given by equation1.3,1.4 and1.5.

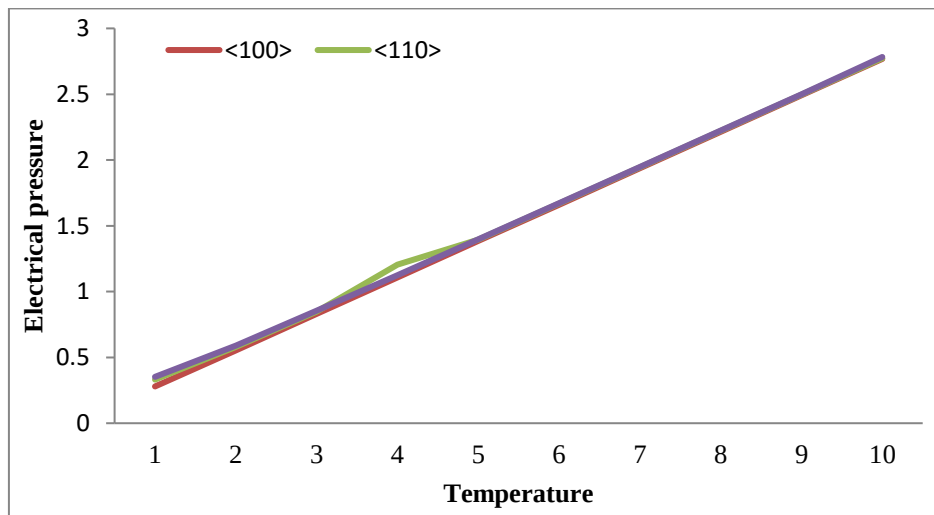


Fig1.1 variation of electrical pressure with temperature at constant electric field

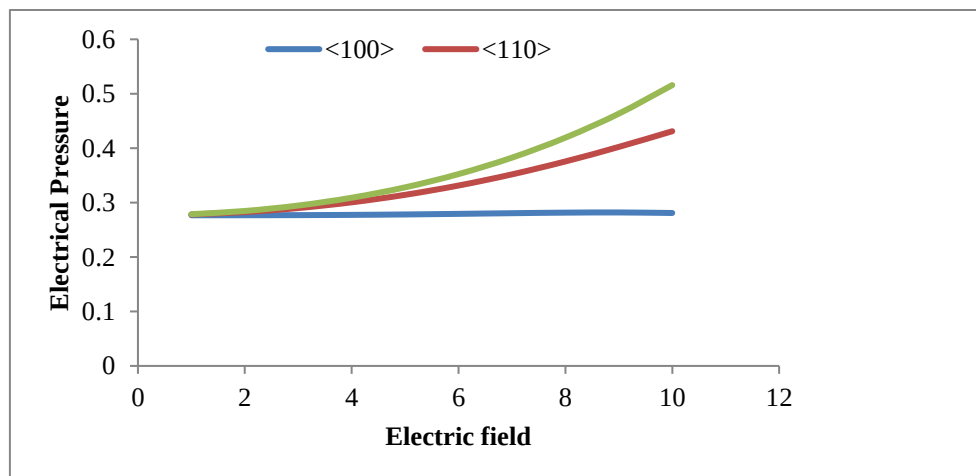


Fig 1.2 Variation of electrical pressure with electric field at constant temperature.

II. Result and discussion

With the study of dielectric constant for the different tunnelling models, we have studied the electrical pressure incorporated by electric field applied along $\langle 100 \rangle$, $\langle 110 \rangle$ & $\langle 111 \rangle$ direction for $\langle 100 \rangle$ tunnelling model. Also we have obtained the variation of electrical pressure with temperature at steady electric field. The expression for electrical pressure as a function of electric field and temperature is represented by equation 1.3, 1.4 & 1.5 for $\langle 100 \rangle$ tunnelling model. The variation of electrical pressure with electric field applied along the directions $\langle 100 \rangle$, $\langle 110 \rangle$ and $\langle 111 \rangle$ is plotted in the figure 1.1 at steady electric field 10^6V/m and fig 1.2 represent the variation of electrical pressure with electric field at constant temperature 10K. It is included that the electrical pressure increases with increase in electric field.

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