Kinetics of trapped electrons in alkalihalide crystals under electron injection

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Abstract : An injection experiment is performed in single crystals of KCl and Kl under space charge limited condition. The kinetics of electron traps like nature of traps, shallow or deep and drift mobility of carriers are determined. Variation of the drift mobility of carriers with colouration is also studied to have a comparative idea of the density of states in conduction bend for these two types of crystals.

 Keywords
 : Electron injection, colour center, density of states

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1. Introduction

The electrical performances of the contact between an insulating solid like ionic crystal and metal is a difficult problem till date. The first stringent condition to be fulfilled is that the ionic processes in the crystal create conditions at the cathode crystal interface which are the pre-requisite for the onset of the injection of electrons from the cathode into the crystal [1]. The ionic transport paves the path for the formation of a new secondary cathode of alkali metal. Essentially, this process allows the electron injection during the second and third zone [2]. The secondary contact is termed as Ohmic and with such contact, the current voltage relationship is nonlinear and depends upon number of factors [3]. The term 'Ohmic' is inappropiate so far as the current voltage relationship is concerned and the linear conduction is achieved only at low fields. The conduction becomes nonlinear when the carrier injection from the electrode or the space-charge effect predominates. In other words, an Ohmic contact can also be realised as one which creates [4] an accumulation of charges extended from the interface of the metal-insulator to the interior of the solid. When a suitable contact is obtained, SCL current dominates the conduction in an ionic crystal containing large number of trapping sites [5].

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The present paper deals with the determination of some kinetics of trapped electrons like mobility and thereby obtain a comparative picture of the density of states of the conduction level of the crystals.

2. Experimental

Crystal flakes of KCl and KI cleaved along <100> directions of dimensions 0.86 cm x $0.73 \text{ cm} \times 0.61 \text{ cm}$ and $1.00 \text{ cm} \times 0.60 \text{ cm} \times 0.40 \text{ cm}$ respectively, were obtained from the single crystal blocks grown in the laboratory, adopting Kyropoulos method [5]. A crystal flake was mounted between a pointed brass cathode and a flat platinum anode. An electron injection experiment [6] was performed using these crystals at a constant temperature of 723 K under the application of different electrical fields between 925 and 1100 V cm⁻¹ for KCl <100>; 100 and 175 V cm⁻¹ for KI <100> separately. The injection current and colouration growth have been recorded simultaneously as a function of time by Bausch and Lomb series 5000 double pen recorder with pen speed 2.5 cm min⁻¹ for KCl and 5 cm min⁻¹ for KI at each injection field. The optical measurement of the colouration growth have been carried out by shinning maximum F absorption light for KCl and Kl on a small portion of the specimen very near to the pointed cathode with the help of an Oriel grating monochromator. The injection operation was stopped well before the advent of the third zone [7]. From the accumulated data, graphs of current and optical density against time were plotted for each electrical fields for KCl and KI crystal as shown in Figure 1.



Figure 1(a). Growth of injection current and optical density against time at 723 K under an injection field of 925 V cm⁻¹ for KCl single crystal.



Figure 1(b). Growth of injection current and optical density against time at 723 K under an injection field of 1050 V $\rm cm^{-1}$ for KCl single crystals



Figure 1(c). Growth of injection current and optical density against time at 723 K under an injection field of 1100 V cm^{-1} for KCl single crystals.

3. Results and discussions

Figures 1(a), 1(b) and 1(c) show the growth of current and optical density (colouration) for KCl crystal in which the ionic zone is shown to be in existence for a brief period of time when the necessary conditions for contact are satisfied to ensure the flow of the space charge limited (SCL) current through the crystal well within the second zone. The time scale in recording current and optical density (colouration) is arbitrarily truncated in each injection process. Similarly, the growth of current and colouration for KI crystal is exhibited in Figures 1(d), 1(e) and 1(f). Comparing the current of growth of KCl and KI, it



Figure 1(d). Growth of injection current and optical density against time at 723 K under an injection field of 100 V cm⁻¹ for K1 single crystals

is observed that KI needs a much lower electrical field than KCl, while the SCL current flow is many times more in KI. The flat nature of the current growth curve in KCl for all the fields, suggests that the growth rate is sluggish which may be due to the deep lying traps in KCl [8]. However, in KI crystal, the current grows very rapidly under quite low electrical fields, suggesting that the traps may be shallower in nature. Thus, the current and colouration growth of KCl and KI are quite distinguishable from each other.

The effective drift mobility (μ) of the electrons undergoing trapping-detrapping under thermal equilibrium, is determined using the equation of the form

$$\mu = \frac{J}{neE},\tag{1}$$

where E is the applied field, e is the electronic charge and n is the number of electrons per unit volume of the specimen n is given by

$$n = \frac{1}{eL\alpha} \int_0^{L/\nu} i dt, \qquad (2)$$

where α is the cross section of the specimen, v is the drift velocity of the carrier in this trapping-detrapping zone and i the current through the specimen.



Figure 1(e). Growth of injection current and optical density against time at 723 K under an injection field of 150 V cm⁻¹ for KI single crystals.

From the nature of the experimental data, the best fit equation for current appears to be a nonlinear function of time

$$i = a t^b. ag{3}$$

After some algebraic manipulations and using eqs. (1) and (2), the mobility is obtained as,

$$\mu = \frac{L}{E} \left[\frac{a}{i(b+1)} \right]^{1/b}.$$
(4)

The value of a and b have been deduced by the method of averages from the available data using eq. (4). Mobility of the electrons at the experimental temperature of 723 K have been evaluated and variations of mobility values with trapped centre (in terms of optical density) have been plotted for different fields as shown in Figure 2.



Figure 1(f). Growth of injection current and optical density against time at 723 K under an injection field of 175 V cm^{-1} for K1 single crystals

It is clear from Figures 2(a) and 2(b) that the mobility value decreases in a manner more or less like a rectangular hyperbola, as the optical density (colour centers) increases. Let us try to understand the situation from the physical point of view. At the very beginning of the growth of colouration (also the current growth), there is an ample scope for trapping and detrapping of the carriers injected from the secondary contact. Practically at first, the trapping occurs along the least path which is from the pointed cathode to the anode in a straight line and then in all possible directions randomly. Consequently, the velocity of the electrons is more sensitive on how many and in what fashion the electrons are being trapped. With time, the electrons on their way through the bulk solid are trapped with increasing number when they become less mobile, thereby decreasing in mobility value. As most of the vacant traps are persistently filled up, randomness in trapping appears to be restricted, which attributes the mobility to attain a constant value, while during the trapping process, the number of electrons to reach the anode from the pointed source of infinite resorvoir of carriers are increased causing the increase in current. This situation may also be realised from a theoretical standpoint. If the free electron concentration is disturbed from its thermal equilibrium value (N_0) by injecting to a new value (N), then on a time-scale long compared to the microscopic trapping and detrapping times, the population (N_t) of the electron traps will be in quasithermal equilibrium with N [9]. Then the entire body of the injected electrons will predominantly be the trapped electrons, and the presence of



Figure 2(a). Mobility of injected carriers against optical density under different injection fields at 723 K for KCl single crystals

thermally generated free electrons will be insignificant in number in contrast to N_{I} . The drift mobility (μ) will follow an equation of the type [10]

$$\mu = \mu_0 \Big[1 + (N_{,}/N_{c}) \exp(W_{,}/KT) \Big]^{-1},$$
(5)

where N_c is the density of states in conduction band, W_r is the activation energy for the formation of F center, and is of the order of 1 eV for KI and KCl, K and T are respectively Boltzmann's constant and temperature of the experiment. For the crystalline materials in question, at the working temperature of 723 K, $(N_r/N_c) \exp(W_r/KT)$ \rangle 1, as $(N_r/N_c) 10^{-1} - 10^{-3}$ and the eq. (5) takes the simple form

$$\mu = \mu_0 (N_c / N_r) \exp(-W_r / KT).$$
(6)

From eq. (6), it is clear that at a particular temperature and for a specific specimen as N_t being the intrinsic property of the material, all the terms other than N_t in the right hand side of the equation are constant and μ bears an inverse relationship with N_p , which is justified



experimentally by Figure 2. From the plot of μ vs 1/N, in the curved portion of Figure 2, an approximate straight line is obtained as shown in Figure 3. The slope of the straight line



Figure 3(a). Mobility of injected carriers against inverse of colour center per c.c. for KCl single crystals.

will provide the value of $\mu_0 N_c \exp(-W_t / KT)$ for the specimens. If we assume that the carrier mobility (μ_0) of the ideal crystal be of the same order for both KCl and Kl, then N_c for Kl turns out to be approximately ten times higher which is an indication of higher

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conduction power of KI in constrast to KCl. We have seen experimentally that KCl requires much higher field approximately ten times compared to the field required for KI to produce



Figure 3(b). Mobility of injected carriers against inverse of colour center per c.c. for KI single crystals.

colour center. This result may be the consequence of higher density of states in conduction band of KI as compared to KCl. Thus, this can be a very interesting field of study and can provide us with significant information about the Space Charge Limited conduction in alkalihalide crystals.

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