# Crossover from the Mott Variable Range Hopping Conduction Regime to Nearest Neighbor Site Hopping Regime in ZnS<sub>x</sub>Se<sub>1-x</sub> Thin Films

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Abstract. In this work, we study the behavior of resistivity as a function of temperature and for several samples of  $ZnS_xSe_{1-x}$  thin films with x = 0, 0.2, 0.4, 0.5, 0.6, 0.8 and 1.0 respectively. In fact, we re-analyze in our investigation experimental measurements obtained by M. Popa et al. [1] in the range of temperature from 300 K to 500 K. We showed that the resistivity follows a nearest neighbor site hopping conduction mechanism with  $\rho = \rho_0 \exp(\frac{E_a}{k_B T})$  for very high temperatures and Mott variable range hopping conduction with  $\rho = \rho_c \exp(\frac{T_0}{T})^{1/4}$  for relatively low temperatures. The crossover between the two regimes can be explained by the competition between the localization length scale  $\xi_{loc}$  and the hopping length scale  $R_{hop}$ .

Keywords: Variable Range Hopping, localization length, hopping length, thin films

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## 1. Introduction

In this work, we try to explain the crossover from the Mott Variable Range Hopping (VRH) conduction regime to nearest neighbor site hopping regime with activation energy  $E_a$  in ZnS<sub>x</sub>Se<sub>1-x</sub> thin films. We re-analyzed the experimental measurements obtained by M. Popa et al. [1], with x = 0, 0.2, 0.4, 0.5, 0.6, 0.8 and 1.0 respectively and in the range of temperatures between 300-500 K. In the last decade, we published more papers in 2D and 3D systems [2-12], which highlight the crossover from the Mott VRH regime [13] to Efros Shklovskii (ES) VRH regime [14] and vice versa depending on the material studied. We noted that in the VRH regime according to Mott the Density of State (DOS) is constant, on the other hand in the VRH regime according to ES the DOS has a parabolic shape due to the existence of a Coulomb Gap (CG).

### 2. Results and discussion

In Fig. 1 we plot  $\ln(\rho)$  against 1000/T for different values of the parameter x in the composition of samples of  $ZnS_xSe_{1-x}$  thin films  $(0 \le x \le 1)$  [1]. We notice for all the curves a change of slope when the temperature decreases. This change is obtained at a temperature value noted  $T_c$  and who is different for each sample. In Fig. 2 we present  $T_c$  versus x with  $0 \le x \le 1$ .  $T_c$  is in the range 360-381 K. For  $T > T_c$  and according to Mott [15], when the energy states are strongly localized and the temperature enough high, the expression of the resistivity  $\rho$  is given by

$$\rho = \rho_0 \exp\left(\frac{E_a}{k_B T}\right),\tag{1}$$

where  $E_a$  is the energy distance between two neighboring sites. Expression (1) is known as nearest neighbor energy site hopping conduction.



**Fig. 1.**  $\ln(\rho)$  against *1000/T* for different values of the parameter *x* in the composition of samples of  $\operatorname{ZnS}_{x}\operatorname{Se}_{1-x}$  thin films ( $0 \le x \le 1$ ). Experimental measurements obtained by M. Popa et al. [1].



**Fig. 2.**  $T_c$  versus x with  $0 \le x \le 1$ .

In Fig. 3, for  $T>T_c$ , we plot  $\ln(\rho)$  against 1/T for different values of the parameter x in the composition of samples of  $\operatorname{ZnS}_x\operatorname{Se}_{1-x}$  thin films  $(0 \le x \le 1)$ . We obtain straight lines. The parameters  $\rho_0$  and  $E_a$  in expression (1) are determined by linear regression.

In Fig. 4 we present the energy distance between two neighboring sites  $E_a$  against the parameter x in the composition of samples of  $ZnS_xSe_{1-x}$  thin films ( $0 \le x \le 1$ ). We find that  $E_a$  increases as the parameter x increases. In this temperature zone ( $T>T_c$ ), the electrons are highly localized and the thermal energy received by these electrons only allows them jump to the nearest neighboring energy site.

For  $T < T_c$ , when the states are weakly localized and the temperature relatively high, Mott [15-18] suggests a VRH conduction. Indeed, the electron jumps towards the energetically most favorable site. The expression of the resistivity  $\rho$  is given by

$$\rho = \rho_c \exp\left(\frac{T_0}{T}\right)^{\frac{1}{4}}.$$
(2)



Fig. 3.  $\ln(\rho)$  against 1/T for different values of the parameter x in the composition of samples of  $\operatorname{ZnS}_{x}\operatorname{Se}_{1-x}$  thin films  $(0 \le x \le 1)$  [1].



**Fig. 4.**  $E_a$  against the parameter x in the composition of samples of  $ZnS_xSe_{1-x}$  thin films ( $0 \le x \le 1$ ).

In Fig. 5 we present ln ( $\rho$ ) versus  $\frac{1}{T^{1/4}}$  for  $T < T_c$ . We obtain straight lines. The parameters  $\rho_c$  and  $T_0$  ( $T_0$  has the dimension of a temperature) in expression (2) are determined by linear regression.

According to Mott analysis by using transition probability theory [19-21] and to the work of Biskupski et al. [22] equation (2) can be written as

$$\rho = A'T^{-\frac{1}{4}} exp(B'T^{-\frac{1}{4}})$$
(3)

and

$$Ln\left(\rho T^{\frac{1}{4}}\right) = Ln(A') + B'^{T^{-\frac{1}{4}}},$$
(4)

where

$$A' = \frac{1}{A}; A = \frac{e^{6}E_{d}^{2}}{12\pi\mu_{0}S^{5}\hbar^{4}} \left(\frac{8\pi N(E_{F})k_{B}\alpha}{9}\right)^{\frac{1}{4}} \left(\frac{\alpha}{2k}\right)^{2}.$$
 (5)



**Fig. 5.**  $\ln(\rho)$  against  $\frac{1}{T^{1/4}}$  for different values of the parameter *x* in the composition of samples of ZnS<sub>x</sub>Se<sub>1-x</sub> thin films ( $0 \le x \le 1$ ) [1].

By using the expression

$$Q = \frac{e^{6}E_{d}^{2}}{12\pi\mu_{0}S^{5}\hbar^{4}} \left(\frac{8\pi k_{B}}{9}\right)^{\frac{1}{4}} \left(\frac{1}{2k}\right)^{2} \quad , \tag{6}$$

where k is the dielectric constant and  $N(E_F)$  the DOS at the Fermi level. S is a speed of sound in air. Equation (5) becomes

$$A = Q(N(E_F))^{\frac{1}{4}} \alpha^{\frac{9}{4}} (7)$$

B' is given by

$$B' = 2.063 \left(\frac{\alpha^3}{N(E_F)k_B}\right)^{\frac{1}{4}}$$
(8)

and

$$\alpha = \frac{1}{\xi_{loc}},\tag{9}$$

where  $\xi_{loc}$  is the localization lenght. Using equations (7) and (8), we obtain

$$\xi_{loc} = \left(\frac{2.063Q}{AB' k_B^{1/4}}\right)^{1/3}.$$
(10)

Mott [13] gives the following expressions of  $T_0$  and the hopping lenght  $R_{hop}$ 

$$T_0 = \frac{18}{k_B N(E_F) \xi_{loc}^3},\tag{11}$$

$$R_{hop} = 0.4 \xi_{loc} \left(\frac{T_0}{T}\right)^{1/4}$$
 (12)

In Fig. 6 we present  $\ln (\rho T^{1/4})$  versus  $\frac{1}{T^{1/4}}$  for  $T < T_c$ . We obtain straight lines and the parameters *A'*, *B'* and *A* in expression (3) are determined by linear regression.  $\xi_{loc}$  and  $R_{hop}$  can be calculated using equations (11) and (12).



In Fig. 7 we present  $\xi_{loc}$  and  $R_{hop}$  versus the parameters *x* in the composition of samples of  $ZnS_xSe_{1-x}$  thin films ( $0 \le x \le 1$ ) for  $T < T_c$ . We observe that  $R_{hop}$  is greater than  $\xi_{loc}$  for  $T < T_c$ .



Fig. 7.  $\xi_{loc}$  and  $R_{hop}$  versus the parameters x in the composition of samples of  $\text{ZnS}_x\text{Se}_{1-x}$  thin films ( $0 \le x \le 1$ ) for  $T < T_c$ .

We can therefore consider that we begin to obtain a crossover from the Mott VRH conduction regime to nearest neighbor site hopping regime when the hopping length  $R_{hop}$  becomes greater than the localization length  $\xi_{loc}$ .

#### 3. Conclusions

In this work, we showed that when the temperature is relatively low the hopping length  $R_{hop}$  becomes larger than the localization length  $\xi_{loc}$ , which produces Mott VRH mechanism conduction indicating that the DOS in constant at the Fermi level  $E_F$ . The electron jumps to the

most energetically favorable site. However, when the temperature increases the electrons are more localized and the jump of the electrons is done at the nearest neighboring site. Indeed, the electrons use the thermal energy to free themselves and jump towards the nearest site because they do not have enough energy to jump towards distant energy sites.

In a previous work [2] we also used the competition between scale lengths to explain the behavior of the electrical conductivity of the metallic side of the Metal-Insulator Transition (MIT) which varied from a temperature dependence in  $T^{1/2}$  far from the TMI to a dependence in  $T^{1/3}$  very close to the MIT. In this case we had to compare the correlation length  $\xi_{cor}$  to the interaction length  $L_{int}$  to explain the crossover of the dependence of the metallic electrical conductivity at  $T^{1/2}$  far from the MIT to  $T^{1/3}$  near the MIT. In fact, we showed that when  $L_{int} > \xi_{cor}$ ,  $\sigma \propto T^{1/2}$ , but when  $L_{int} < \xi_{cor}$ ,  $\sigma \propto T^{1/3}$ .

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