MOTT-VARIABLE RANGE HOPPING MECHANISM IN *N*-TYPE $CuIn_3Se_5$

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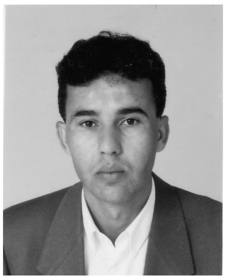
Variable range hopping conduction of Mott type, where the magnetoresistance follows the relation $\rho(B) = \rho_0 \exp[T_0(B)/T]^{1/4}$, is observed in *n*-type $CuIn_3Se_5$ in two different temperature ranges at different magnetic field values up to 27 tesla. The positive magnetoresistance data are analyzed using the theoretical models of Shklovskii and Efros. We obtained a good but only in the lower temperature range. The observed discrepancy in range I needs to be investigated.

Keywords: ordered defect compounds, variable range hopping, magnetoresistance



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Introduction

Electrical conduction due to Mott type variable range hopping mechanism of (M-VRH) has been reported in many materials [1, 2] and explained as a result of the presence of strong localization of the charge carriers in the impurity band. Under this mechanism, electrical resistivity (ρ) follows the relation $\rho = \rho_0 \exp [T_0/T]^{1/4}$, where T_0 is the characteristic temperature and ρ_0 is taken as a constant. This is for a 3-D system when the electron density of states around the Fermi energy level is constant or varies very slowly.

In the present work, we report on the effect of the presence of ordered arrays of donor-acceptor defect pair (DADP) on the localized states in *n*-type $CuIn_3Se_5$ samples. The ordered defect compound (ODC) $CuIn_3Se_5$ can be derived from a repeat of one unit of the interacting donor-acceptor ($InCu^{+2}$, $2VCu^{-1}$) defect pair in each 5 units of $CuInSe_2$ (CIS) [3, 4]. The temperature dependence of the electrical resistivity (ρ) below 70 K and the positive magnetoresistance (PMR) up to 27 T are measured. The experimental results are analysed with the existing theoretical models. The details about the crystal growth and the techniques used to measure ρ and PMR are reported earlier [5].

Experimental results

In Fig. 1, we plot the logarithmic variation of ρ with $T^{-1/4}$. This variation can be separated into three well-defined temperature regions that are between 67 and 24.5 K, 24.5 and 9 K, and below 9 K. These are referred to as I, II, and III, respectively. The linear dependenceon this plot establishes that the electrical conduction by VRH mechanism of Mott type (M-VRH), where $\rho = \rho_0 \exp [T_0/T]^{1/4}$, is dominant in the first two ranges. From the theoretical fits, we find $\rho_{0I} = 2.37 \cdot 10^{-7} \Omega^{\text{-cm}}$, $T_{0I} = 8.01 \cdot 10^6$ K and $\rho_{0II} = 3.01 \cdot 10^{-2}\ \Omega^{\text{-cm}}$, $T_{0II} = 2.44 \cdot 10^5$ K in I and II, respectively. This suggests that the localized states, caused by the ordered arrays of DADPs or defects, start to form just below 70 K. Tne variations of the relative magnetoresistance $\Delta\rho/\rho = (\rho(B) - \rho(0))/\rho(0)$ as a function of the magnetic field *B* up to 27 *T* for different fixed temperatures from 10 to 77 K is shown in the insert. The magnetoresistance is positive and decreases when the temperature increases.

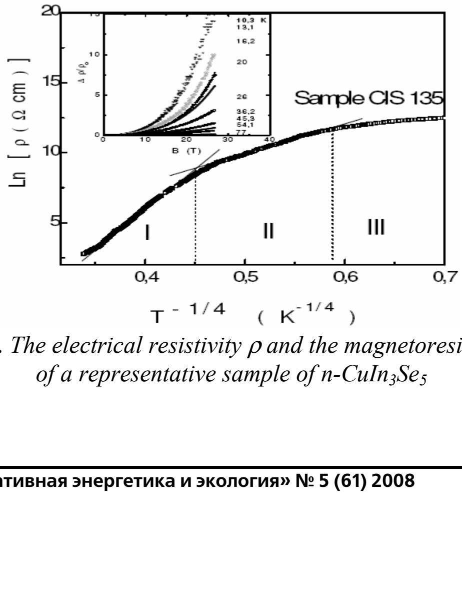


Fig. 1. *The electrical resistivity ρ and the magnetoresistance of a representative sample of n-$CuIn_3Se_5$*

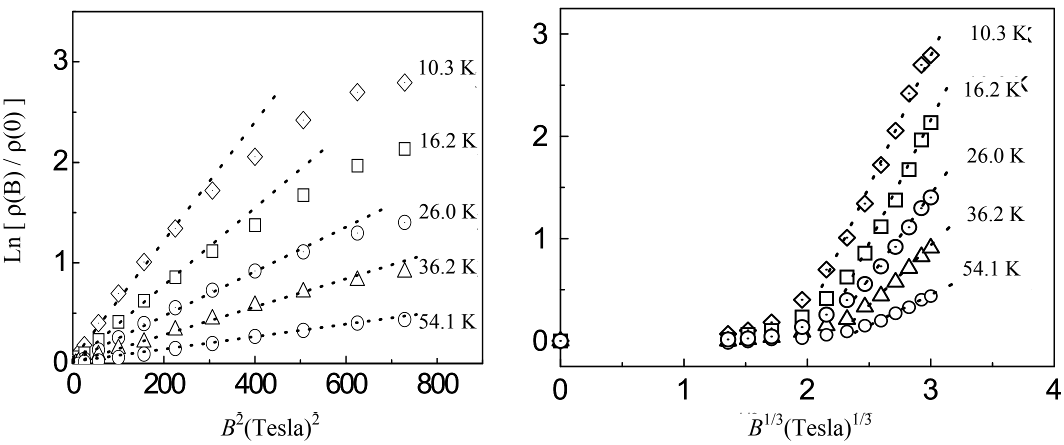
A similar behaviour around 20 K in n-$CuInSe_2$ with conduction by a M-VRH mechanism both above and below this temperature with different T_0 has been reported [6]. PMR in the hopping regime is caused by the shrinkage of the electronic wave function in a direction perpendicular to the applied magnetic field. To analyze the data, the model proposed by Efros and Shklovskii [7] for the field and temperature dependence of the PMR in the variable range hopping conduction regime is used. The main mathematical expressions, although reported by us earlier [5], are as follows:

$$\ln\left[\frac{\rho(B)}{\rho(0)}\right] = K_S B^2;\ B < B_c \tag{1}$$

and

$$\ln\left[\frac{\rho(B)}{\rho(0)}\right] = \left[\frac{T_0(B)}{T}\right]^{1/3} = PB^{1/3};\ B > B_c. \tag{2}$$

In these expressions K_s is proportional to $T^{-3/4}$ and depends on the effective Bohr radius a_H^* and the zero field characteristic temperature T_0, whereas $T_0(B)$, in the high field region, is proportional to B and depends on the constant density of states $N(E_F)$ at the Fermi level and a_H^*. The critical field B_c that separates the low from high field regime is expected to vary with the temperature as $T^{-1/4}$ [5]. From Eq. (1) and (2) one should expect that at fixed temperatures $\ln[\rho(B)/\rho(0)]$ should vary as B^2 and $B^{1/3}$ below and above B_c in the case of Mott type VRH conduction and at fixed magnetic fields it should be proportional to $T^{-3/4}$ and $T^{-1/3}$, respectively. Also, the variation of $\ln K_s$ and $\ln P$ with $\ln T$ should give a respective slope of -3/4 and -1/3. As in Fig. 1 of Ref. 5, we plot in Fig. 2 $\mathrm{Ln}[\rho(B)/\rho(0)]$ as a function B^2 and $B^{1/3}$ at several fixed temperatures from 10 to 54 K.



a *b*

Fig. 2. *Ln [ρ(B)/ρ(0)] as a function of B^2 (a) and $B^{1/3}$ (b) at various fixed temperatures*

We can see the linear dependence, represented by the straight dotted lines, of Ln $[\rho(B)/\rho(0)]$ with B^2 for lower fields and $B^{1/3}$ for higher values of B. The cross-over from B^2 to $B^{1/3}$ dependence occurs at a critical field B_c that separates the low from the high field regime. As in the case of n-$CuInSe_2$ [5], these linear behaviours thus observed in low fields (Fig. 2, *a*) and in high field region (Fig. 2, *b*) show that our data are in agreement with the variable range hopping theoretical model of Shklovskii and Efros [7].

In Fig. 3, we plot $\mathrm{Ln}K_S$ (left scale) and $\mathrm{Ln}P$ (right scale), where K_S and P are the slopes of $\mathrm{Ln}[\rho(B)/\rho(0)]$ vs B^2 and $\mathrm{Ln}[\rho(B)/\rho(0)]$ vs $B^{1/3}$ dependence, against $\mathrm{Ln}T$.

The expected theoretical dependence [7] is shown by straight lines. An excellent agreement is found, but only, in range II. Although M-VRH conduction is also valid in range I, the origin of nearly three times higher slope of K_S and P is noted and yet not clear.

In conclusion, it is established that the electrical resistivity in n-type $CuIn_3Se_5$ follows M-VRH conduction in two different temperature ranges. The observed variation of $\mathrm{Ln}[\rho_{(B)}/\rho_{(0)}]$ with the magnetic field is in complete agreement with the theoretical model. However, the corresponding temperature variation of the slopes agrees only with the data of range II. The observed discrepancy in range I needs to be investigated.

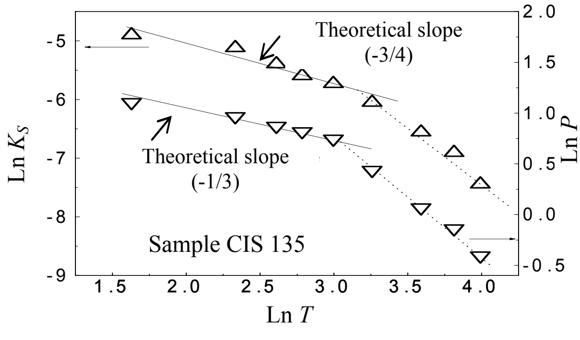


Fig. 3. *$\mathrm{Ln}K_S$ (left scale) and LnP (right scale) as a function of LnT*

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