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Crossover from Efros-Shklovskii to Mott Variable Range Hopping in Amorphous Thin Ni_xSi_{1-x} Films

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The temperature dependence of the electrical conductivity of insulating amorphous Ni_xSi_{1-x} alloys is studied in the temperature range 1–160 K. At low temperatures, Efros-Shklovskii (ES) variable range hopping (VRH) is observed. This is assumed to occur because of the creation of the Coulomb gap (CG) in the vicinity of the Fermi level. With increasing temperature, the CG vanishes and the measured conductivity can be described by the Mott VRH model, where the density of states is constant. The criterion of the crossover ES from to Mott VRH is assessed by extracting the related parameters.

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I. INTRODUCTION

At low temperatures when the thermal energy k_BT (k_B = Boltzmann's constant) is of the order of or smaller than the disorder or the Coulomb interaction energy between the carriers, transport in disordered semiconductors continues to attract a great deal of theoretical and experimental interest. Under these thermal conditions, the empty sites in the entourages of a given occupied state become few, and the phonon energies are not high enough to ensure the nearest-neighbor-hopping (NNH) conduction.

In three-dimensional systems, Mott [1, 2] has assumed that the density of states (DOS) is constant in the vicinity of the Fermi level. The related VRH regime can be described by

$$\rho = \rho_{\mathrm{Mott}} \left(\frac{T_{\mathrm{Mott}}}{T} \right)^{\frac{1}{4}}, \tag{1}$$

where ρ_{Mott} is a resistivity parameter, and T_{Mott} is a characteristic temperature.

On the other hand, Efros and Shklovskii (ES) [3, 4] have shown that long range electron–electron interactions create a soft Coulomb gap (CG). Therefore the DOS takes

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the form $N(E) \propto (E\text{-}E_F)^{1/2}$ in three-dimensional systems. Under this assumption the conductivity may behave as:

$$\rho = \rho_{ES} \left(\frac{T_{ES}}{T} \right)^{\frac{1}{2}}, \tag{2}$$

where ρ_{ES} and T_{ES} are constant.

The universal equation is given by

$$\rho = \rho_0 \left(\frac{T_0}{T} \right)^{p}, \tag{3}$$

where $p = (n+1)/(n+4)$. $n = 2$ and $p = 0.5$ for ES VRH and $n = 0$ and $p = 0.25$ for Mott VRH. The crossover from ES to Mott VRH with increasing temperature has been widely observed in several semiconductors [5–10].

It is worth pointing out that very recently a few theoretical studies (e.g., [11, 12]) and some experiments [13–15] have shown that the exponent p is different from the above predictions. Deutscher *et al.* [11] have considered the hopping between superlocalized states and predicted that $p > 1/4$. This has also been shown in carbon black-PVC [13]. In 2004, Fogler, Teber and Shklovskii (FTS) [12] studied the interaction between the electron and the positive charge that it left behind. This consideration leads to $p = (1 + n)/(1 + n + d)$, with $n = 0$, 1, 2 and d the dimensionality of the system. This expression permits not only the exponent in Eq. (3) to be $p = 1/2$ or $1/4$ but also other values, such as $2/5$ in 3D systems. Moreover, studies of VRH in insulating media have led to assessing some parameters such as the localization length [16, 17] and the relative permittivity [18]. On the other hand, tunneling conductivity in granular films has been included in several applications of spintronics [19, 20]. Its technological applications include use for information storage [21] and reading by magnetic sensors [22].

In this work, we have studied the electrical resistivity of amorphous silicon nickel alloys Ni_xSi_{1-x} in the temperature range 1–160 K [23]. The analysed data obtained in Ref. [23] are for seven insulating samples where $x = 19.5\%$, 20.3%, 21.2%, 22.3%, 22.5%, 23.5, and 24.8%, respectively. This study is similar to our previous report [5] focused on hydrogenated amorphous alloys a-$Si_{1-y}Ni_y$:H where hydrogen saturates and passivates bonds of the amorphous silicon.

II. EXPERIMENTAL DETAILS

The experimental data quoted are for a-$Si_{1-x}Ni_x$ alloys reported by Rosenbaum *et al.* [23]. They prepared films by co-evaporating silicon and nickel using two electron guns. 7 to 8 narrow glass pieces of a width of 2.5 mm were used to avoid shadowing problems, which can be caused by using a single mask [23]. To vary the nickel content, Rosenbaum and co-workers placed three microscope glass slides 'end to end' above and between the nickel and silicon graphite boats. Small broken glass fragments which have been coated with

photoresist were placed between the glued glass pieces, so that EDAX (energy-dispersive analysis of X-rays) samples would also be available. Typical evaporation rates were 1.4 Å/s and 7 Å/s for the nickel and silicon sources. The evaporations were performed in high vacuum (10^{-6} mm Hg), and the glass slides were held at room temperature. The purity of nickel and silicon are 99.9% and 99.97%, respectively.

III. RESULTS AND DISCUSSION

At zero magnetic field, we used the method developed by Zabrodskii and Zinoveva [9] to see whether the Mott VRH regime or ES VRH regime is suitable for describing the experimental data. Using Eq. (3), Zabrodskii and Zinoveva [9] give the following function

$$w(T) = \ln\left[\frac{d\ln(\sigma)}{d\ln(T)}\right] = \ln(p) + p\ln(T_0) - p\ln(T)\,, \tag{4}$$

where σ is the electrical conductivity ($\sigma = 1/\rho$).

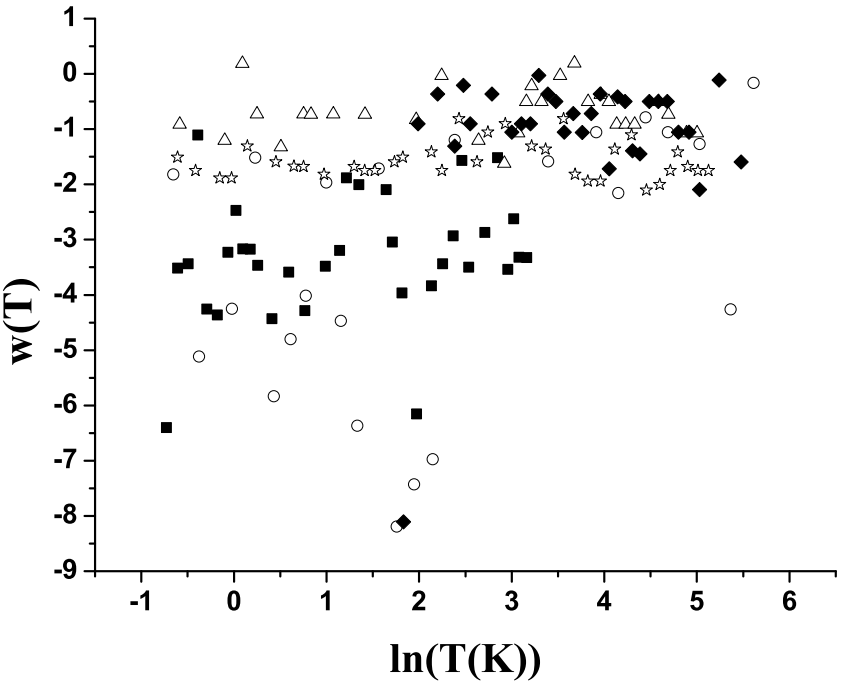

FIG. 1: The function $w(T)$ vs $\ln(T)$ for the samples referenced 28.2%, 24.8%, 23.5%, 22.3%, and 21.2%. The dispersion of the points means that these samples are close to the MIT.

In Fig. 1, we plot the function $w(T)$ versus $\ln(T)$ for the samples referenced 28.2%, 24.8%, 23.5%, 22.3%, and 21.2% [23]. The data points seem to scatter, and thus neither ES VRH nor Mott VRH can be used to describe the transport data. These films are therefore located very close to the MIT.

Figure 2 and Figure 3 show $w(T)$ versus $\ln(T)$ for the samples referenced 19.5% and 20.3%, respectively [23]. The same behavior is observed for both samples; for $T < T_C$, where T_C is the critical temperature, the slope is found to be close to 1/2, indicating the ES VRH with creation of CG. For $T > T_C$, the slope becomes close to 1/4, suggesting the vanishing of CG and consequently the crossover from ES to Mott VRH. The values of the critical temperatures and the slopes for $T < T_C$ and $T > T_C$, respectively, are shown in Table I.

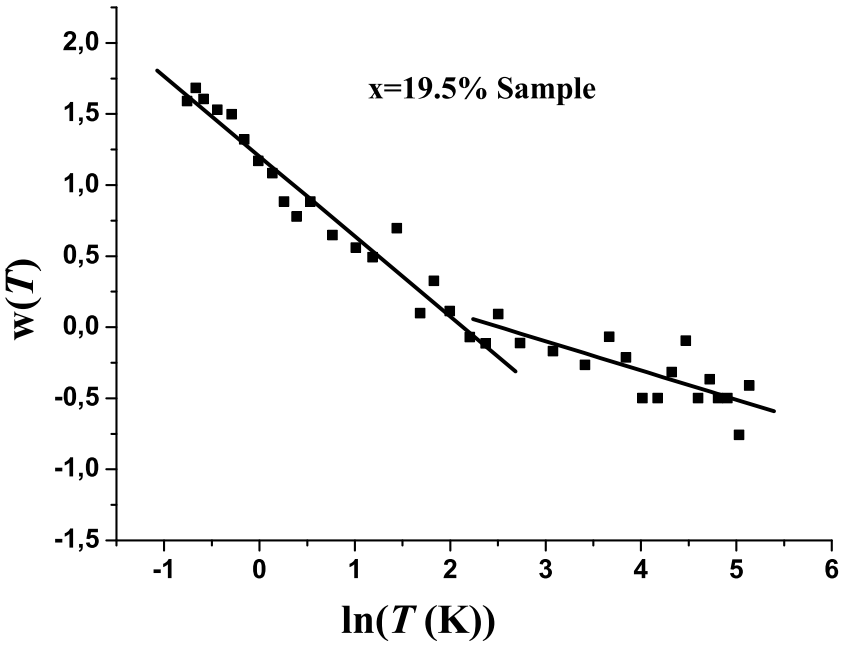

FIG. 2: Observation of the crossover from ES to Mott VRH for the sample referenced 19.5% by plotting the function $w(T)$ vs $\ln(T)$.

Figure 4 (a) and Figure 4 (b) show the variation in the logarithm of resistivity with $T^{-1/2}$ and $T^{-1/4}$ for the samples where we have observed the VRH regimes [23]. For both samples, these figures show that $\ln(\rho)$ varies linearly with $T^{-1/2}$ (ES VRH) for $T < T_C$ and with $T^{-1/4}$ for $T > T_C$ (Mott VRH) (fits analogous to the procedure adopt in Ref. [10]). It is worth noting that temperatures below the coulomb gap effect have been determined in Figs. 2 and 3.

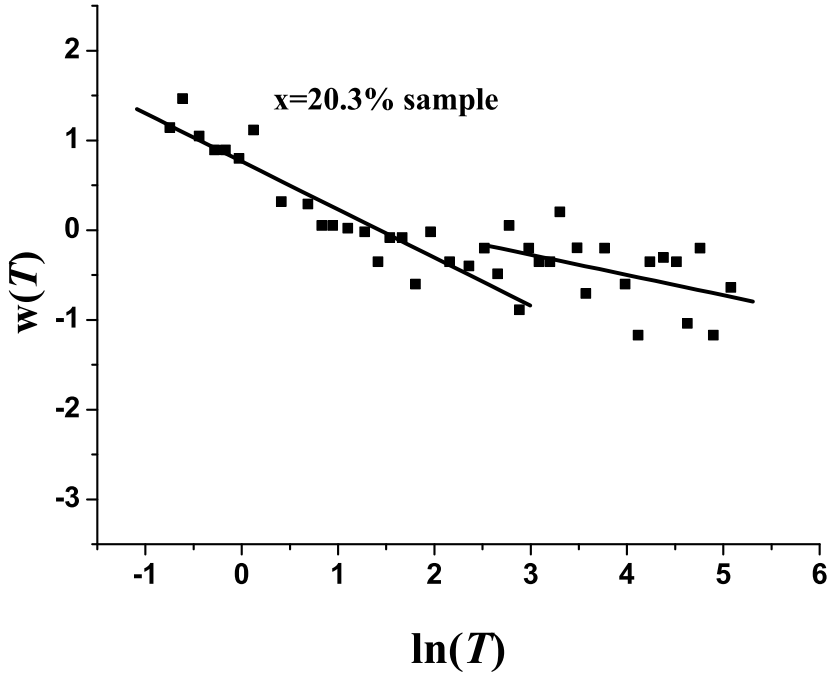

FIG. 3: Observation of the crossover from ES to Mott VRH for the sample referenced 20.3% by plotting the function $w(T)$ vs $\ln(T)$.

TABLE I: Values of $T_{\rm Mott}$, $T_{\rm ES}$, the experimental and theoretical critical temperatures T_C, and the ratio $T_{\rm Mott}/T_{\rm ES}$ for the samples referenced 20.3% and 19.5%.

Samples	Exponent p for $T < T_C$	Exponent p for $T > T_C$	$T_{\rm Mott}$ (K)	$T_{\rm ES}$ (K)	T_C (exp) (K)	T_C (The) (K)	$T_{\rm Mott}/T_{\rm ES}$
20.3%	0.61	0.18	1833.4	20.84	10	4.118	87. 97
19.5%	0.52	0.19	8458.13	43.87	16	8.67	192.8

Let us now discuss the ES to Mott VRH crossover criterion. By using fits in Figures 4 (a) and 4 b), we have extracted the values of $T_{\rm Mott}$ (in Eq. (1)) and $T_{\rm ES}$ (in Eq. (2)) for $T > T_C$ and $T < T_C$, respectively. These values have been confronted to those proposed by Rosenbaum [24],

$$T_C = \frac{T_{\rm ES}}{5.06} \text{ and } \frac{T_{\rm Mott}}{T_{\rm ES}} = 81 \tag{5}$$

The values of $T_{\rm Mott}$, $T_{\rm ES}$, and the ratio $T_{\rm Mott}/T_{\rm ES}$ are shown in Table I. We notice

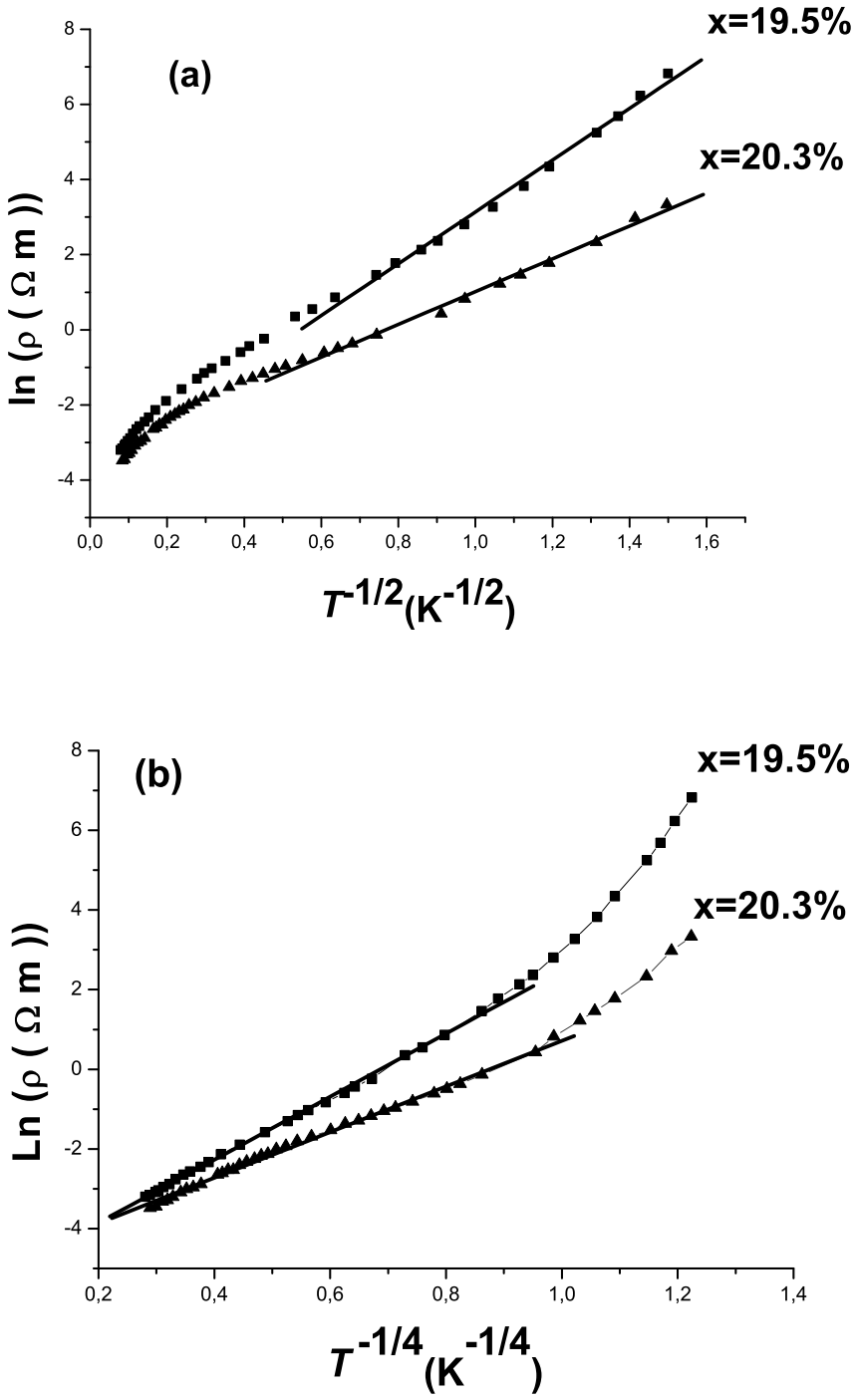

FIG. 4: Variation of resistivity of the $x = 19.5\%$ and $x = 20.3\%$ samples. (a) $\ln(\rho)$ versus $T^{-1/2}$ and linear fits in the ES VRH for $T < T_C$, (b) $\ln(\rho)$ versus$T^{-1/4}$ and linear fits in the Mott VRH for $T > T_C$.

that the ratio $T_{\mathrm{Mott}}/T_{\mathrm{ES}}$ is consistent with Eq. (5) for the $x = 20.3\%$ film and roughly two times greater for the $x = 19.5\%$ sample. For both the $x = 20.3\%$ and $x = 19.5\%$ samples, the theoretical value of T_C is almost two times smaller than the experimental value.

We have confirmed our results by adopting the percentage deviation while fitting the experimental resistivity $\rho_i(T_i)$ to Eq. (3). ρ_0 and T_0 are taken as adjustable parameters. In this procedure, we have varied the exponent p from 0.01 to 1 with a step of 0.05 (and of 0.01 near the minimum deviation). For each value of p, we have extracted the values of ρ_0 and T_0 and calculated the percentage deviation:

$$\mathrm{Dev}(\%) = \left[\frac{1}{n}\sum_{i=1}^{n}\left(\frac{100}{\sigma_i}\left(\sigma_0 \exp\left[-\left(T_0/T\right)^p\right] - \sigma_i\right)\right)^2\right]^{1/2}, \tag{6}$$

where $\sigma_0 = 1/\rho_0$ and n is the number of experimental points.

By using the above fitting procedure, we have confirmed the results obtained using the variation of $w(T)$ against $\ln(T)$ given by Eq. (4), as shown in Figs. 2 and 3. This approach was employed below and above T_C to check the possible conductivity by the VRH mechanism with different adjustable parameters.

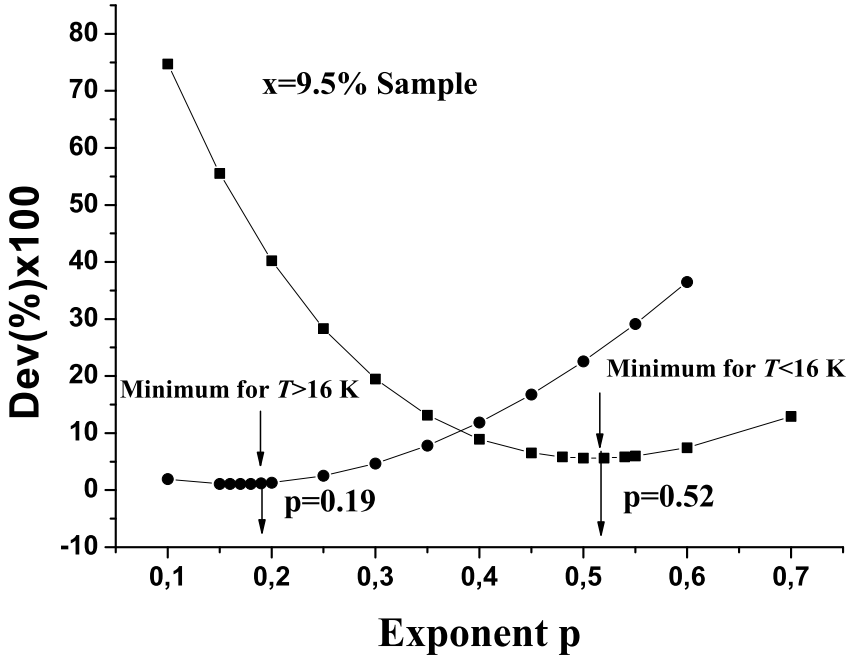

FIG. 5: Percentage deviation Dev(%) versus exponent p in the whole temperature range 1–160 K for the $x = 19.5\%$ sample. The minimums for $T < T_C$ and $T > T_C$ are consistent with ES and Mott VRH, respectively.

The percentage deviation for the different ranges of temperature are displayed in Figs. 4 and 5 for the $x = 19.5\%$ and $x = 20.3\%$ samples, respectively [23].

For the $x = 19.5\%$ sample, when $T < T_C$ ($T_C = 16$ K) the minimum for Dev(%) is obtained for $p = 0.52$. This value is very close to 0.5. In this temperature range, the DOS is characterized by CG near the Fermi level with ES VRH conduction. For $T > T_C$, the minimum for Dev(%) corresponds to $p = 0.19$ (close to 0.25). This means that the DOS is almost constant near the Fermi level with Mott VRH conduction.

The same behavior is shown for the $x = 20.3\%$ sample. When $T < T_C$ the minimum deviation is obtained for $p = 0.61$ (close to 0.5), suggesting the existence of ES VRH. When $T > T_C$ the minimum corresponds to $p = 0.18$ (close to 0.25), which is in agreement with Mott VRH.

The VRH conduction depends on the magnitude of the hopping energies Δ_{ES} for $T > T_C$, Δ_{Mott} for $T < T_C$, and on the CG width. Very close to the MIT, only Mott VRH conduction occurs, because the CG becomes so narrow. This has been confirmed in Si:(P,B) [25].

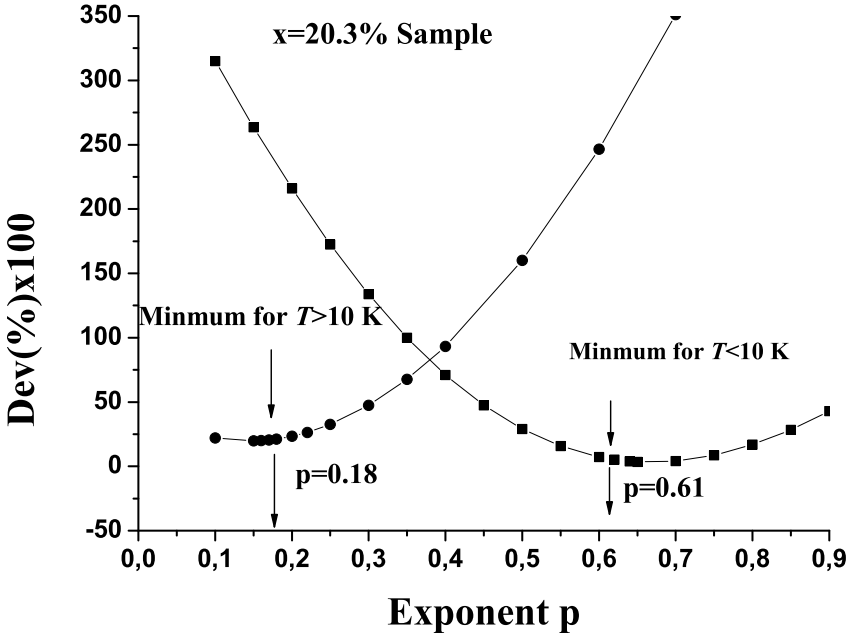

FIG. 6: Percentage deviation Dev(%) versus the exponent p in the whole temperature range 1–160 K for the sample referenced 20.3%. The minimums for $T < T_C$ and $T > T_C$ are also consistent with ES and Mott VRH, respectively.

Once we extract the related parameters by adopting the above procedure, we can clearly show the crossover from ES to Mott VRH conduction by increasing the measurement

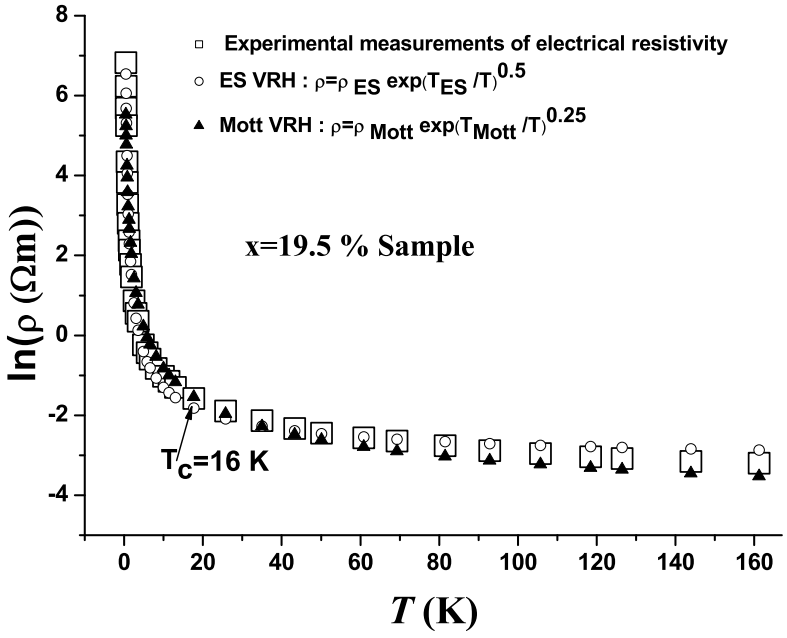

FIG. 7: Observation of the crossover from Mott to ES VRH by plotting $\ln(\rho)$ versus T for the $x = 19.5\%$ sample. We have used the related parameters extracted by using Eq. (1) for $T > T_C$ and Eq. (2) for $T < T_C$.

temperature. This is evidenced for the $x = 19.5\%$ and $x = 20.3\%$ samples, as shown in Figs. 6 and 7, respectively.

IV. CONCLUSION

We have studied the temperature dependence of the resistivity of amorphous Si_{1-x} Ni_x alloys on the insulating side of the MIT [23]. At low temperatures, the charge transport in the $x = 19.5\%$ and $x = 20.3\%$ films are found to be governed by VRH conduction with two distinct temperature behaviors of resistivity. The Mott VRH hoping law, $\ln(\rho) \propto T^{-1/4}$, and the ES VRH hopping law, $\ln(\rho) \propto T^{-1/2}$, are sequentially observed as the temperature is decreased. The agreement with the Rosenbaum prediction for the $x = 20.3\%$ sample indicates that the crossover ES to Mott VRH occurs when the relative magnitude of the hopping energies $\Delta_{\rm Mott}$ (in the Mott VRH) and $\Delta_{\rm ES}$ (in the ES VRH) become comparable. We note that this behavior is not observed in the $x = 19.5\%$ sample and thus requires further studies.

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