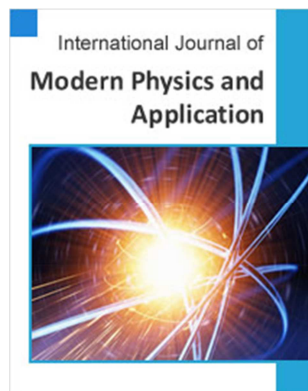




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Characterization of the Metal Insulator Transition in Thin Ni_xSi_{1-x} Films

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Abstract

In R. Rosenbaum, A. Heines, A. Palevski, M. Karpovski, A. Gladkikh, M. Pilosof, A. J. Daneshvar, M. R. Graham, T. Wright, J. T. Nicholls, C. J. Adkins, M. Witcomb, V. Proseky, W. Przybylowicz, R. Preterious, J. Phys.: Condens. Matter. 9, 5395–5411 (1997), the authors have observed a metal-insulator transition in films Si_{1-x}Ni_x at x_c=0.24 and observed WL and EEI phenomena at low temperatures. Using results obtained on these films we have performed calculations using Boltzmann' theory and weak localization theory near the MIT. Our new results show that Ioffe-Regel criterion is obeyed and the conduction is governed by weak localization and electron - electron interactions phenomena, in agreement with the results obtained by Rosenbaum *et al.*

1. Introduction

Depending on their electrical properties, films can be classified as metallic or insulating. Insulating three-dimensional (3D) films display infinite resistivity or zero conductivity, σ , at $T = 0$ K. On the other hand, metallic 3D films have non-zero positive conductivity at $T = 0$ K provided that they do not become superconducting. Transport properties of 3D films are fascinating as they allow one to probe interesting physics such as variable range hopping (VRH), weak localization and electron-electron interactions.

The electrical transport in strongly insulating films could be governed by VRH phenomenon. This mechanism can be found with a constant density of states (DOS) (Mott VRH [1, 2]) or with the creation of the Coulomb Gap (CG) in the vicinity of the Fermi level (Efros and Shklovskii' - (ES) VRH [3-5]). In both cases (Mott VRH or ES VRH), the conductivity is given by the following formula:

$$\sigma = \sigma_0 \exp \left[- \left(\frac{T_0}{T} \right)^p \right], \quad (1)$$

where σ_0 is the prefactor, T_0 the characteristic temperature, and $p = (n+1)/(n+4)$. When $n=0$, no CG is created and $p=0.25$, corresponding to the Mott VRH [1, 2]. When $n=2$, the DOS varies in the vicinity of the Fermi level and $p=0.5$, corresponding to ES VRH [3-5] with creation of CG.

The electrical conductivity of the 3D metal films at sufficiently low temperatures can be written as:

$$\sigma = \sigma(T=0) + mT^s, \quad (2)$$

where $\sigma(T=0)$ is the zero temperature conductivity, m is the magnitude of the correction term and the adjustable parameter s is equal to 1/3 or 1/2. We note that formula (2) is used for doped crystalline and amorphous semiconductors [6-8].

2. Results and Discussion

We have re-analyzed the experimental data obtained on the alloys $a\text{-Si}_{1-x}\text{Ni}_x$ prepared and published by Rosenbaum *et al.* in reference [9]. Films No.16 ($x = 28.2\%$) and No.18 ($x = 24.8\%$) are two pure metallic films; their electrical conductivity is calculated using theory the Boltzmann's by the following formula:

$$\sigma_B = \sigma(T=0) = \frac{Ne^2\tau_0}{m^*}, \quad (3)$$

where N is the carrier density, $m^*=0.26m_0$ is the electron effective mass in silicon alloys, m_0 is the free electron mass,

$\tau_0 = \frac{l_0}{v_F}$ is the relaxation time, l_0 is the free mean path of the

electron, $v_F = \frac{\hbar k_F}{m^*}$ the speed of the Fermi and

$k_F = (3\pi^2 N)^{1/3}$ the Fermi vector. We note that the carrier density N is calculated using the formula $N = (3/4\pi a^3)$, with a denotes the average distance between impurities ($a \approx 4 \text{ \AA}$).

By using the theory of Boltzmann, we found $l_0 = 0.71 \text{ \AA}$ and $k_F l_0 = 0.12$ for film No.16. On the other hand, we obtained $l_0 = 0.25 \text{ \AA}$ and $k_F l_0 = 0.34$ for film No.18. These two films are close to the MIT (see later). We note that the free mean path l_0 of two metal films No.16 and No.18 are shorter than the average distance between impurities ($a \approx 4 \text{ \AA}$) and also the parameter $k_F l_0$ is much less than π . The results are summarized in table1.

We note that, if the two alloys are metallic, then l_0 should be larger than a . To further study this possible contradiction, we use the theory of weak localization where the conductivity [10-12] at $T = 0 \text{ K}$ is given by the following expression:

$$\sigma_0 = \sigma_B g^2 \left(1 - C / g^2 (k_F l_0)^2 \right), \quad (4)$$

where C is the coefficient ranging between 1 and 3, $g = 1/3$ is

the factor calculated by Mott representing the decrease in the density of states by the disorder.

Using the latter theory and the expression of σ_B , the mean free path is given by the following formula:

$$l_0 = \frac{\sigma(0) + \sqrt{\sigma^2(0) + C \left(\frac{2g n e^2}{\hbar k_F^2} \right)^2}}{\frac{2g^2 n e^2}{\hbar k_F}}, \quad (5)$$

Now using the weak localization theory and choosing $C = 1$, we found $l_0 = 9.48 \text{ \AA}$ and $k_F l_0 = 4.54$ of film No.16, we obtained also $l_0 = 7.44 \text{ \AA}$ and $k_F l_0 = 3.56$ of film No.18, such as the two films are close to MIT (detailed later), the values of $k_F l_0$ are in accordance with the Ioffe-Regel criterion $k_F l_0 = \pi$. We present in table2 the parameters of the two films No.16 and No.18.

Table 1. Atomic percentages, free mean path of the electron and parameter $k_F l_0$ as calculated by using the Boltzmann' theory.

Film No.	x (at.% Ni)	l_0 (Å)	$K_F l_0$	σ_0 ($\Omega \text{ cm}$) ⁻¹
16	28.2	0.71	0.12	136
18	24.8	0.25	0.34	49,6

Table 2. Atomic percentages, free mean path of the electron and parameter $k_F l_0$ obtained by applying the weak localization theory.

Film No.	x (at.% Ni)	Carrier density $N (*10^{27} \text{ m}^{-3})$	Free mean path $l_0(\text{\AA})$	$K_F l_0$
16	28.2	3.73	9.48	4.54
18	24.8	3.73	7.44	3.56

Figure 1 shows the conductivity in the five $\text{Ni}_x\text{Si}_{1-x}$ films (films No.16 ($x=28.2\%$), No.18 ($x=24.8\%$), No.19 ($x=23.5\%$), No.20 ($x=22.3\%$), and No.21 ($x=21.2\%$)) [9] plotted against $T^{1/2}$. We have found the good regression with exponent, s , close to 0.5 in the alloys which are located in the vicinity of MIT ($s=0.52$ for film No. 16, $s=0.55$ for film No.18, $s=0.47$ for film No.19, $s=0.5$ for film No.20 and $s=0.47$ for film No.21).

These results are obtained with a good approximation by adopting the percentage deviation method [13-14]. We have adjusted the parameters σ_0 and m in equation (2) for each value of the exponent s ranging from 0 to 1 with a step 0.01. The percentage deviation is calculated using the following formula:

$$Dev(\%) = \left[\frac{1}{n} \sum_{i=1}^n \left(\frac{100}{\sigma_i} \left([\sigma(T=0) + mT^s] - \sigma_i \right) \right)^2 \right]^{1/2}, \quad (6)$$

where n is the number of experimental points and σ_i the experimental values of the electrical conductivity at different

temperatures. The minimum deviation corresponds to the best value of the exponent s .

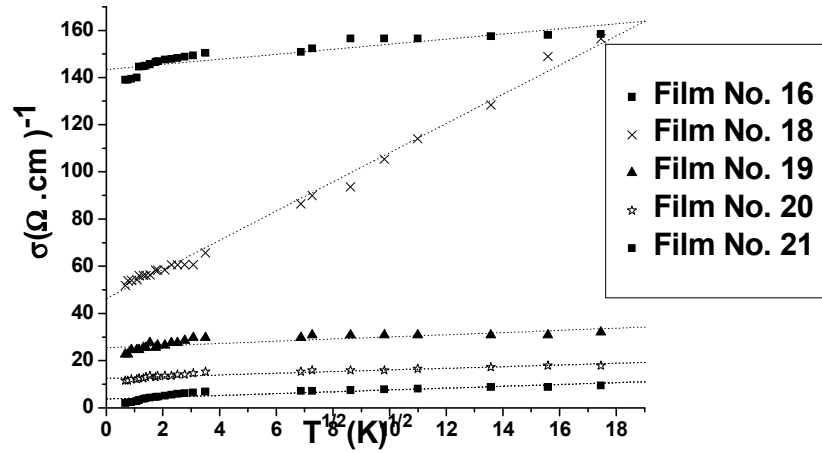


Figure 1. In the absence of the magnetic field, the electrical Conductivity plotted as a function of $T^{1/2}$ for the five $\text{Ni}_x\text{Si}_{1-x}$ films. As mentioned above, we have reanalyzed experimental data obtained in Ref. [9].

Figure 2 shows the percentage deviation as function of exponent s for films No.16, No. 18 and No. 19 [9]. The analysis of this figure shows us that the minimums of Dev (%) is obtained for the values of s very close 0.5 ($s = 0.51$ for film

No. 16 and $s = 0.54$ for film No.18 and $s = 0.47$ for film No. 19). This is well declared in ref [9] as it is in agreement with the 3D weak localization (WL) and electron-electron (EEI) theories [10-12].

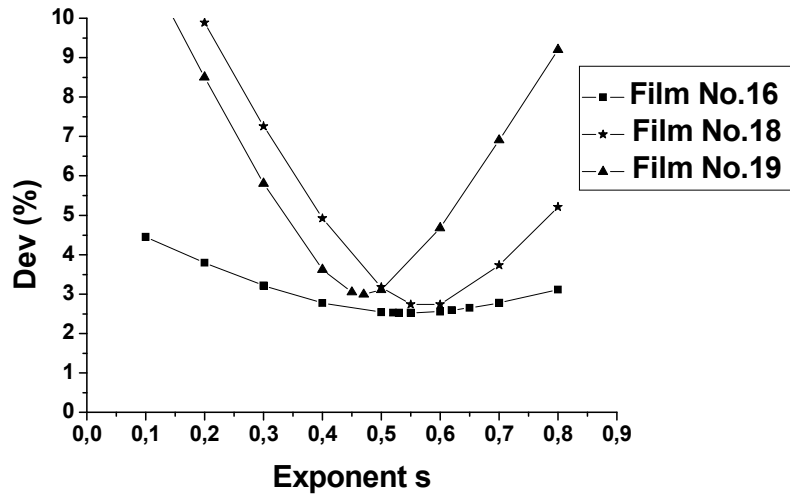


Figure 2. Percentage deviation Dev (%) versus exponent s in films No.16, No.18 and No.19.

In a previous study [15], we observed the competition between the interaction length L_T and the correlation length ξ leads to the transition of the law ($s = 1/2$) to the law ($s = 1/3$) at close the MIT. This competition was also observed in compensated n-type InP [16]. But generally this passage is not obvious for all the systems as examples Rosenbaum *et al* [9] and Narjis *et al* [17], they have not observed this behaviour in their works at close the MIT.

An interesting method has been introduced to distinguish between the metallic and insulating films is the calculation of

the mathematical function $w(T)$ [9, 18-20] defined by the formula:

$$w(T) = \left[\frac{d \ln(\sigma)}{d \ln(T)} \right], \quad (7)$$

Using the conductivity $\sigma(T_1)$ and $\sigma(T_2)$ of two neighboring points corresponding to the temperatures T_1 and T_2 , the function $w(T)$ is calculated by the following formula:

$$w(T) = \frac{\ln(\sigma_1) - \ln(\sigma_2)}{\ln(T_1) - \ln(T_2)}, \quad (8)$$

In Figure 3, we plot the function $w(T)$ for films No.16, No.18, No.19 and No.21 [9], where T is the average temperature of T_1 and T_2 . The analysis of this figure allows us to note that $w(T)$ approaches zero when the temperature decreases identifying these two films No.16 ($x=28.2\%$) and

No.18 ($x=24.8\%$) such as metallic films. On the other hand, the film No.21 ($x=21.2\%$) identifies an insulating film when $w(T)$ is finite and not equal to zero for temperatures approaching to zero. Furthermore, for the film No.19 ($x=23.5\%$), the function w is zero for some points and positive for others, which allows us to conclude that this film close to the MIT. The film No.19 is insulating and located slightly below the MIT. Thus, we can estimate the critical metallic content to be $X_C=0.24$.

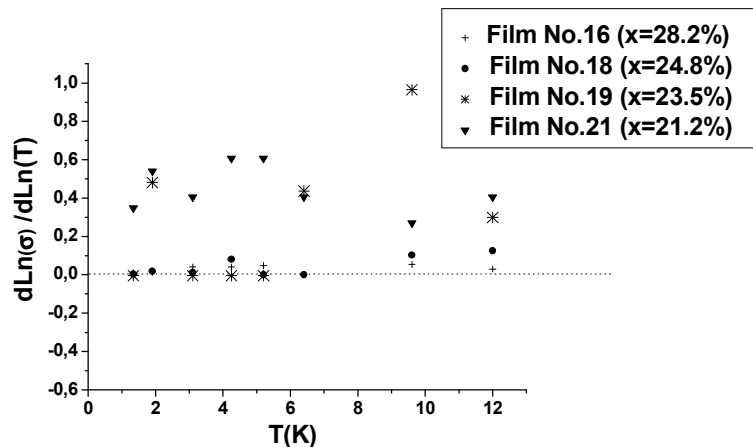


Figure 3. Function $W = (d\ln(\sigma) / d\ln(T))$ according to the temperature T of films No.16, No.18, No.19 and No.21.

3. Conclusion

Based on the Boltzmann theory and WL and EEI model, we re-analyzed the data obtained in $\text{Ni}_x\text{Si}_{1-x}$ films [9]. By using the function w and the deviation percentage, we have identified the critical nickel content for the MIT. Near this percentage conduction is governed by WL and EET phenomena. Our results show that Ioffe-Regel criterion is obeyed. These results are in agreement with those obtained by Resenbaum *et al.* [9].

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