



Effects of Phonons, Surface and Grain Boundary Scattering in Electrical Resistivity of Nanometallics Nb

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Abstract

The electrical resistivity of nanometallic Niobium (Nb) as a function of thickness was studied, with thickness ranging from 5 to 100 nm at room temperature. The nanometallic Nb exhibited an increase in electrical resistivity with decreasing thickness, particularly when the thickness approached the mean free path of electrons. In this work, the (F-S) model and (M-S) model were applied to describe the increase in the electrical resistivity for nanometallic Nb. The results show the failure of the (F-S) model to describe the size effect in nanometallic Nb and the success of the (M-S) model, which shows good agreement between the fitted experimental and theoretical curves. This indicates that surface scattering is not the sole contributor to the increase in electrical resistivity and that grain boundary scattering is a major contributor to the size effect phenomenon. The values of surface and grain boundary scattering were determined ($p=0.32$ and $R=0.0122$) in this work.

Keywords: Grain boundary scattering, Size effect, Fuch-Sondheimer, Niobium

1. Introduction

Electrical properties of material are affected when their dimensions are reduced to the nanoscale¹, as the electrical resistivity of nanoscale metals shows a significant increase with decreasing thickness, particularly when thickness approaches the mean free path of electrons in these nanometals. This phenomenon is called the size effect^{2,3}. The increase in electrical resistivity in nanometallic is attributed to the appearance of additional types of scattering⁴, such as surface scattering, which is described by the Fuchs-Sondheimer (F-S) model⁵, and grain boundary scattering, which is described by the Mayadas-Shatzkes (M-S) model, in addition to background scattering⁶.

Niobium (Nb) metal is considered one of the important metals in this context, as it is characterized by good structure stability, which makes it a suitable element for studying the phenomenon of the size effect in nanometallics. Although the electrical resistivity of nanometallic (Nb) increases, it still preserves its basic electronic properties, which make it suitable for use in nanoelectronic applications such as interconnects in the integral circuit^{7,8}.

2. Material and methods

2.1. Background scattering

The bulk resistivity of metals is described by the Drude classical model, which assumed that the behavior of the transport electrons in metals undergoes uniform bulk background scattering from structures, effects, and phonons⁹. Electrical conductivity is given¹⁰:

$$\sigma = \frac{ne^2\tau}{m} \quad (1)$$

$$\rho_0 = \frac{1}{\sigma} = \frac{m}{ne^2\tau} \quad (2)$$

Where: n is the concentration of electrons per cubic meter, e is the electronic charge, τ is the relaxing time, m is the mass of one electron, and

$$\tau = \frac{l_\infty}{V_f} \quad (3)$$

l_∞ is mean free path, V_f is velocity of electrons at the Fermi surface¹¹.

2.2. Fuch-Sondheimer theory (F-S) model

The F-S model shows the increase that happens in electrical resistivity for nanometals, which is a result of surface scattering of these nanometallics, and through solving the transport equation of Boltzmann and Fuch, they got **Equation 2**, which describes the electrical resistivity in nanometallic¹².

$$\rho = \rho_0 \left[1 + \frac{3}{8} \frac{(1-p)}{\lambda} \right] \quad (4)$$

Where: ρ the electric resistivity in nanometallics, the Fuch surface scattering parameter (its values between 1, representing complete elastic scattering, and zero, representing complete diffuse scattering)¹³, and the ratio between nanometallics thickness (t) and l_∞ .

2.3. Mayadas-Shatzkes (M-S) model

The grain boundary scattering is a major contributor to the size effect phenomenon¹⁴. The (M-S) model describes this scattering where the electrical resistivity exhibits a significant increase when the size of the grain (D) approaches the mean free path (l_∞)¹⁵. And by solving the Boltzmann transport equation to the following equation, they arrived¹⁶:

$$\rho = \rho_0 \left[1 + \frac{3}{2} \alpha \right] \quad (5)$$

Where:

$$\alpha = \frac{l_\infty R}{D(1-R)} \quad (6)$$

R is grain boundary scattering parameter which its values between 1, representing complete elastic scattering, and zero, representing complete diffuse scattering¹⁷.

Finally, the total electric resistivity in nanometallic is given by¹⁸:

$$\rho = \rho_0 \left[1 + \frac{3}{8} \frac{(1-p)}{\lambda} + \frac{3}{2} \alpha \right] \quad (7)$$

The three term on the right hand side of **Equation 7** represent the contributors in the total resistivity in nanometallics⁶.

2.4. Method

Niobium (Nb) thin films were deposited using direct current (DC) magnetron sputtering in an ultrahigh vacuum system with a base pressure of 10^{-19} Torr. The films were grown on Al₂O₃ (aluminum oxide) (sapphire) substrates that were ultrasonically cleaned in successive solvent baths and degassed at 500C for 1 hour prior to deposition^{19, 20}.

The deposition process was carried out at a working pressure of 3 mTorr with an applied power in the range of 60–180 W, while maintaining a fixed target-to-substrate distance of 30 cm, enabling control over the deposition rate and film thickness within the range of 4–400 nm¹⁹⁻²¹.

Electrical resistivity was measured using an in situ linear four-point probe technique at room temperature, with an applied current ranging from 1 to 100 mA¹⁹⁻²².

3.Results

The experimental resistivity of nanometallic Nb on the y-axis and corresponding thickness on the x-axis at room temperature were showed in **Figure 1**. The figure shows the inverse relationship between electrical resistivity and thickness from nanometallics Nb, where the electrical resistivity exponentially decreases with increased thickness.

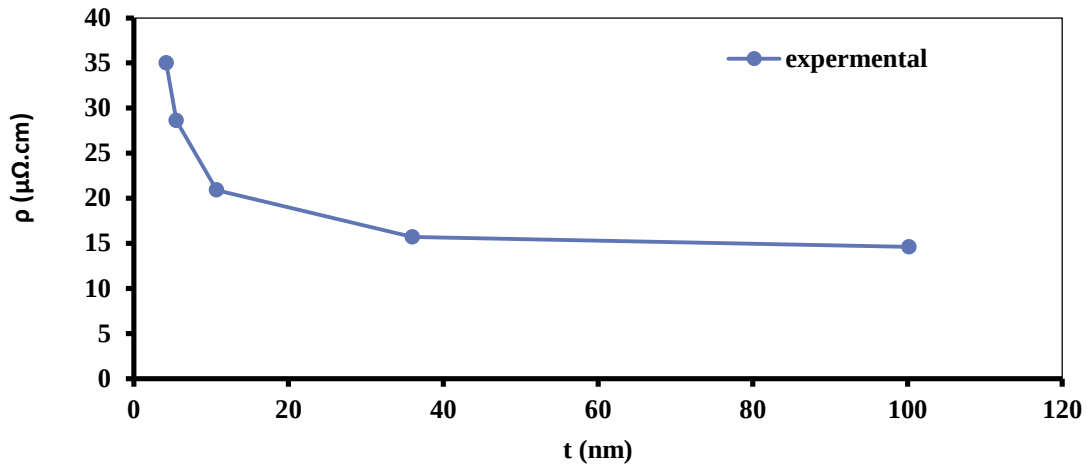


Figure 1. Room-temperature experimental electrical resistivity(ρ) as a function of film thickness (t) for Niobium (Nb).

Figure 2 shows the linear relationship between (ρt) on y-axis and t on x-axis, according to **Equation 8**. The slope represents bulk resistivity of nonmetallic Nb, which ($15.2\mu\Omega cm$). The obtained slope value is ($13.974 \mu\Omega cm$), which shows good agreement with the reported bulk resistivity

$$\rho t = \rho_0 t + \frac{3}{8} \rho_0 l_\infty (1 - p) \quad (8)$$

The value of parameter p was calculated from intercept of **Figure 2**, which is equal to 77.655. Using a value of l_∞ equal 20nm the calculated value of p is (0.32)

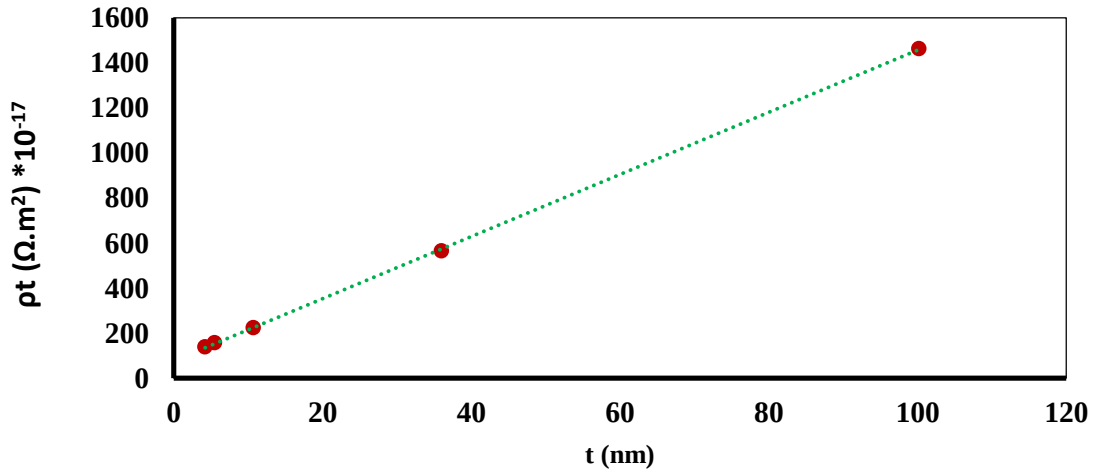


Figure 2. Resistivity multiplied by thickness ρt vs thickness t .

The electrical resistivity values corresponding to different nanometallic Nb thicknesses were calculated using **Equation 4** based on the (F-S) model and are represented by the yellow curve in **Figure 3**. **Figure 3** shows disagreement between the experimental and theoretical curves at small Nb thicknesses, indicating that the (F-S) model fails to accurately describe the size effect in this regime.

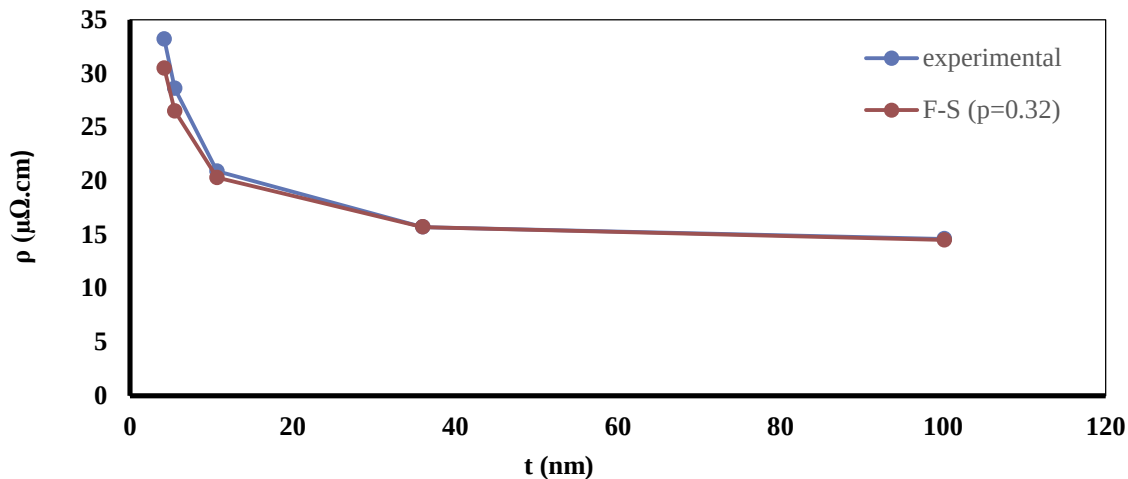


Figure 3. Fit of Niobium Experimental Results with Fuch-Sondheimer Model at Room Temperature.

Based on the M-S model and using **Equation 7**, the grain boundary parameter R was calculated, to be (0.0122). Using the approximation $D = t$, where the grain size in nanostructured metals is considered equivalent to the thickness of the nanometallic film, which is a commonly adopted approximation in this field.

Figure 4 shows good agreement between the experimental and theoretical curves of electrical resistivity as a function of thickness for nanometallic Nb, calculating using the (M-S) model according to **Equation (7)**. This agreement indicates that the (M-S) model successfully describes the size effect well.

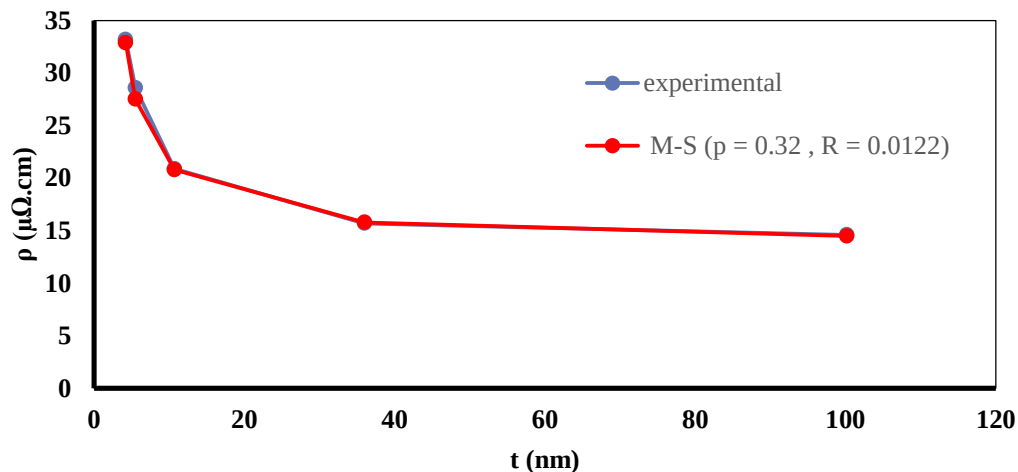


Figure 4. Fit of Niobium Experimental Results with the Mayadas-Shatzkes Model at Room Temperature

4. Discussion

The increase that happened in the value of electric resistivity for nanometallics Nb is attributed to surface and grain boundary scattering, as described by (F-S) and (M-S) models^{23,24}. The discrepancy between the experimental and theoretical curves obtained using the (F-S) model at small thickness indicates that this model alone cannot adequately describe the size effect. This suggests that surface scattering not the only mechanism contributing to increase in electrical resistivity in nanometallics Nb²⁵.

The good agreement between the experimental and theoretical curves of the (M-S) model, indicating its success in describing the phenomenon of size effect well. This suggests that grain boundary scattering is the main contributor to the increase in electrical of nanometallic Nb as the metal thickness decreases²⁶.

The theoretical curve of electrical resistivity values calculated according to (F-S) model, which agrees with the experimental curve at thicknesses (greater than the mean free path). At these thicknesses, the electrical resistivity of nanometallic Nb approaches the bulk value, ($\rho_0 = 15.2 \mu\Omega cm$), which can be attributed to the reduced influence of surface and grain boundary scattering. In this regime, the resistivity is primarily governed by background scattering²⁹. Furthermore, the fitting between the experimental and theoretical curves indicates that both surface and grain boundary scattering increase as the thickness decrease becomes smaller than the electron mean free path of electron. Therefore, both mechanisms act as major contributors to the electrical resistivity for nanometallic Nb²⁷.

When comparing the surface scattering parameter ($p=0.32$) and grain boundary scattering parameter ($R=0.0122$) values obtained for the nanometallic Nb with those previously obtained by Fairouz for the element copper ($p=0$) and ($R=0.0017$). These results show that the nanometallic Nb is less affected by the size phenomenon than the copper, as its value, despite the similarity in the value of grain boundary scattering, indicates a complete diffuse scattering of the incident electrons on the surfaces of the copper nanometallic. From this, it can be concluded that the Nb element can be used in the manufacture of interconnects used in integrated electronic circuits as an alternative to copper²⁸⁻³⁰.

5. Conclusion

The electrical resistivity of nanometallic Nb increases significantly as its thickness approaches the electron mean free path. The F-S model fails to accurately describe this increase when applied alone, whereas the M-S model provides a better description of the size effect phenomenon in nanometallic Nb. This indicated that both surface scattering and grain boundary scattering contribute to increasing the electrical resistivity of this material. The surface scattering parameter (p) was calculated to be (0.32), while the grain boundary scattering parameter (R) was found to be (0.0122).

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Conflict of Interest

The authors declare that they have no conflicts of interest.

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Ethical Clearance

No animals were used in this study.

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