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# The Effect of Scattering of Phonons, Surface and Grain Boundary on electrical Properties for Tungsten Nanometallic

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**Abstract**
In the context of increasing the use of nanometals in electrical and electronic applications and improving their unique electrical properties, this research explains the effect of the mechanisms of scattering of phonons at room-temperature (293K) in addition to the scattering and reflection of electrons at the surface and at grain boundary on the electrical resistivity of Tungsten metal at different thicknesses. The electrical resistivity of Tungsten was obtained by solving the Boltzmann transport equation which the electron scattering coefficient at the surface (p) is calculated by the Fuch-Sondheimer model, and the grain boundary reflection coefficient (R) by the Mayadas-Shatzkes model were calculated as (p=0.89) and (R=0.18) for Tungsten metal based on the mean of the free path of the electrons. The results showed that there is a linear relationship between the mechanisms of scattering and resistivity, and an inverse relation between electrical resistivity (ρ) and the thickness of the nanometal (d) and extending to a large range of thicknesses. Moreover, the defects of the crystal lattice and the roughness of the surface have an evident impact on the electrical properties of Tungsten metal. In addition, we obtained an excellent consistency between experimental data and theoretical results of electrical resistivity. These results provide important predictions for the use of nano-Tungsten as an interconnection between micro integrated electronic circuits and in various electrical devices.
**Keywords:** Tungsten, Mayadas, Nanometals, Scattering, Resistivity.

## 1. Introduction

The effects of limited size on the resistivity of nanometals have been the subject of research for several years from an applied and basic point of view. Understanding the resistivity of nanometals is of great importance because nanometals form the interconnection structures used in micro-integrated electronic circuits. At present, the thickness of nanometals used for interconnection is in the range of (25-30 nm), and expected that their dimensions to reach about (10 nm) in the coming years. At these dimensions, the grain boundary and surface scattering in tungsten dominate the phonon scattering, leading to a much bigger resistivity than that in the bulk (1-5). While the scattering of the phonon and possibly impurities dominate the bulk resistivity of the metals at room temperature, surface scattering of electrons can become dominant when the thickness of nanostructured metals is reduced (6-8).

Furthermore, it has been found that the grain sizes of polycrystalline nanostructured metals typically decrease with decreasing metal thickness, which leads to an increased contribution of grain boundary scattering in nanostructured metals (9-11). Eventually, when the metal thickness becomes within a few nanometers, the effects of electron trapping will also change the resistivity of nanostructured metals (8,12-19). Recently, Tungsten has become a good candidate to replace copper for semiconductor metallurgy for two reasons (20-24). The first reason is that tungsten has a very high melting point (3695K), much higher than that of copper (1358K), which is expected to improve interconnection problems such as voltage discharge and electromigration due to the large activation energy of tungsten diffusion (25-28). The second reason is the expected decrease in the size effect of resistivity due to the much shorter mean free path of electrons of Tungsten than that of copper (19.1nm) at 293K (9).

## 2. Materials and Methods

Mayadas and Shatzkes developed an extension of Boltzmann’s transport equation to include the transport and reflection of electrons at the surface and grain boundary of a polycrystalline metal (30). In addition to presenting their model for grain boundaries and phonon scattering, Shatzkes and Mayadas derived a more complex model that combines the scattering effect of phonons, surfaces, and grain boundaries in nanometals and includes the interactions between these effects (11). The electrical resistivity of nanometals is calculated based on the Fuchs-Sondheimer model by (6,31):

$$\rho_f = \rho_0 \left[ 1 + \frac{3}{8K}(1 - \mathrm{p}) \right] \quad , K > 0.1 \tag{1}$$

Where $\rho_0$ = resistivity of nanometal, ρf = the final resistivity, K = ratio of thickness (d), to the electron mean free path (ℓ), p = the surface scattering coefficient. The probability of scattering of the electron scattered on the surface (1-p) and thus the value of the surface scattering coefficient (p) can also be calculated from equation (1) and within the range ($0 \le p < 1$) (32,33).

In 1970, Mayadas-Shatzkes developed the above equation, introducing an additional term that includes the grain boundary scattering coefficient (R) that has values in the range ($0 \le R < 1$), as follows (11):

$$\rho_f = \rho_0 \left[ 1 + \frac{3}{8K}(1 - p) + \frac{3}{2}\delta \right] \quad , \delta \ll 1 \tag{2}$$

Where $\boldsymbol{\delta} = \ell_{\circ}$ R / d (1- R ) is the grain boundary scattering power dependent on thickness(d) , electron mean free path and grain boundaries reflection coefficient (R).

## 3. Results and Discussion

Experimental results of electrical resistivity as a function of the thickness of Tungsten metal, which were measured at a temperature of 293 K, show that nano-tungsten shows a decrease in electrical resistivity with increasing thickness, as the thickness of the nano-metal, the more evident this effect is. That is, the relationship between resistivity and thickness is inverse (34), as in the following in **Figure 1.**

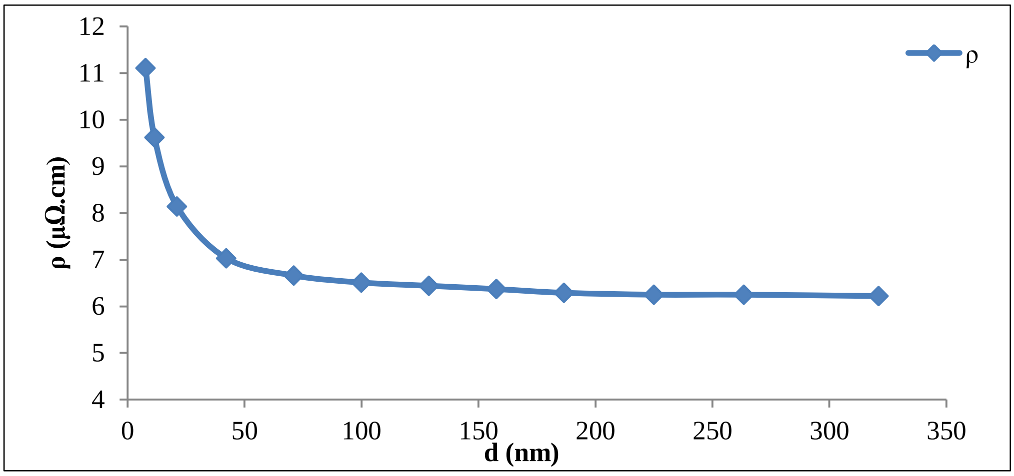


**Figure 1.** Experimental resistivity at room temperature as a function of thickness for Tungsten metal.

This effect is due to the surface scattering of the electron according to the Fuchs-Sondheimer theory and the effect of electrons' reflection at grain boundaries according to Mayadas-Shatzkes theory and the scattering of phonons, as well as the effect of size (35).
To calculate the values of slope and point of intersection, which represent the value of the bulk tungsten resistance and the point of intersection of the two axes, respectively, the values of (d) were plotted on the x-axis, and the values of (ρd) on the y-axis, so the relationship was represented by a straight line that does not cross the origin, and from the relation of the straight line (y=ax+b), the slope and the point of intersection were calculated as they are equal to ($\rho_{\circ}$) and (ρd) respectively. As in the following in **Figure 2.**

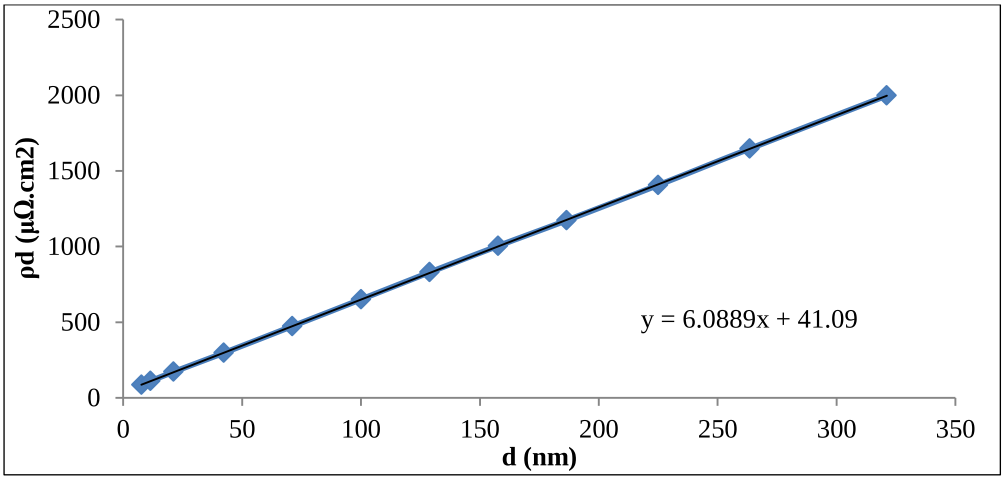


**Figure 2.** Resistivity multiplied by thickness ρd vs thickness d.

Through the Fuch-Sondheimer theorem, **Equation 1**, the value of surface scattering coefficient of an electron (p) of the Tungsten nanometal was calculated, where it was equal to (p=0.89), which represents the sum of the values of the scatterings (36). Then, based on it, we calculate new values of resistivity ($\rho_f$), and draw them as a function of thickness, also comparing them with the experimental results, where the green curve indicates the theoretical results and the blue is the experimental data. As in the following in **Figure 3.**

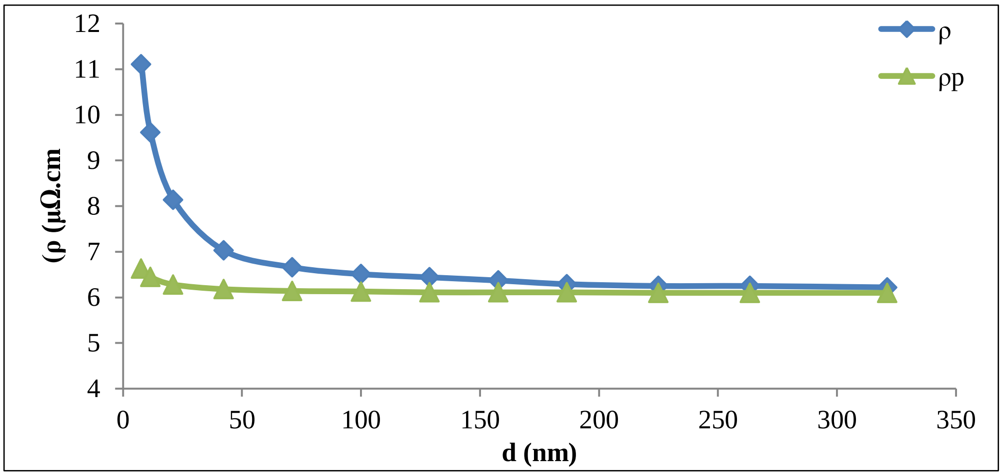


**Figure 3.** Fit of Tungsten Experimental Results with Fuch-Sondheimer Model at 293K.

The scattering of electrons at this Tungsten surface is due to crystalline metal defects, such as point defects (Schottky and Frenkel), vacancies and impurities, as well as surface roughness [37,38]. An increase in this type of scattering means an increase in the electrical resistivity of the metal according to the Fuch-Sondheimer theory (39).

From the Mayadas–Shatzkes theorem, equation 2, the value of the grain boundary (R) of Tungsten was calculated (40) so that it was equal to (R=0.18). The bulk resistivity of Tungsten is ($\rho_{\circ}$=5.28 μΩ.cm ), and the mean free path of the electron is ($\ell_{\circ}$=19.1 nm ), so that ($\rho_{\circ}\ell_{\circ}=101\times10^{-17}$ $\Omega.m^2$). After that, through equation 2 and using the values of (p, R), new values of resistivity were found, which were drawn and compared with the experimental results, as shown in the following in **Figure 4**, where the red curve represents the theoretical values obtained.

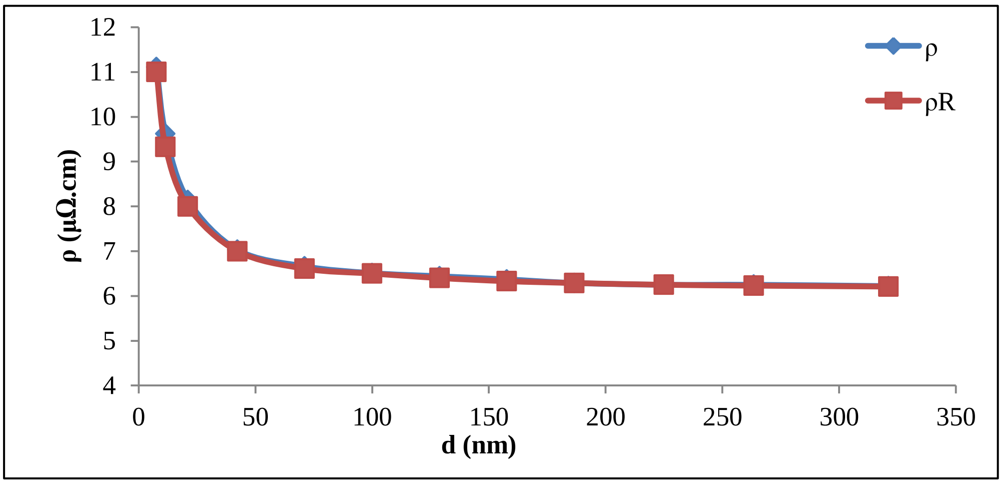


**Figure 4.** Fit of Tungsten Experimental Results with Mayadas-Shatzkes Model at 293K.

The above figure shows a good fit and consistency between the experimental values and the theoretical results of the Mayadas-Shatzkes model of grain boundaries scattering, that this model is based on the mean free path of electron-phonon scattering, as well as point defects in crystal structure and surface defects (e.g., roughness)(41).

Finally, in general, the scattering and reflection mechanisms of the surface electrons lead to a decrease in resistivity, because they slow down the speed of electron transition along the direction of conduction (33, 40).

## 4. Conclusion

In this research contribution, the mechanisms of scattering and reflection of grain boundaries and surface boundaries of conduction electrons and scattering of phonons at room temperature and their effect on the electrical properties of Tungsten nanometal were studied. The findings indicate that reducing the severity of these scatterings contributes to improved electrical conductivity and reduced resistivity by reducing the concentration of Tungsten metal crystal lattice defects as well as surface defects. Furthermore, it was found that the thickness of the nanometal has a noticeable impact on the electrical properties of Tungsten, as increasing the thickness decreases electrical resistance and vice versa. Finally, experimental data of resistivity (p) as a function of thickness (d) of Tungsten nanometal showed a good and appropriate match with the theoretical results calculated for electrical resistivity by the Mayadas-Shatzkes and Fuchs-Sondheimer models. The properties of this metal can be used in integrated electronic circuits as an interconnection structure.

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## Conflict of Interest

The authors declare that they have no conflicts of interest.

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The article is not supported financially.

## Ethical Clearance

No animals were used in this study.

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