The Influence of the Density of States to the Resistivity in the Dimensional Crossover Regime

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ABSTRACT

It has already been established from experimental and theoretical results that the properties of nanostructures are different from their bulk counter part if that property is some expression of an internal length scale. This work focuses on a thin film model that was used to observe how metals change their electrical resistivity as their size change. Using the thin film model, the behavior as to when it will exhibit a bulk or thin film behavior was determined by observing the density of states transition from 3D to 2D.

INTRODUCTION

Experimental and theoretical studies show that electrical resistivity increases as size reduces [1]. However, there is a limit as to how small a conductor or semiconductor gets before it shows scattering and quantum mechanical effects in which different results can arise [2]. The electronic resistivity of a material is related to the density of states (DOS). The latter determines the number of different states that the electrons can occupy. Many intensive properties such as the specific heat capacity, magnetic susceptibility, electrical conductivity, and thermal conductivity which by definition, do not depend on the amount of matter present but it is experimentally shown that DOS can be expressed in terms of the of dimensions of a material [3]. Since the aforementioned intensive properties of a material depend on DOS, these intensive properties can now be expressed as functions of the size of the system. Hence, known intensive properties in bulk can be seen as extensive properties in nanostructures. The DOS is usually expressed in three different equations, for 1D, 2D, and 3D. The equation for DOS is given as [8]:

$$D^{0-D}(E) = \lim_{\sigma\to 0}\sqrt{\frac{2}{\pi\sigma^2}}\left(\frac{1}{L_xL_yL_z}\right)\times \sum_{n_x,n_y,n_z}^{\infty}\exp\left(\frac{-\left[E-\left\{\frac{\hbar^2\pi^2}{2m^*}\left(\frac{n_x^2}{L_x^2}+\frac{n_y^2}{L_y^2}+\frac{n_z^2}{L_z^2}\right)\right\}\right]^2}{2\sigma^2}\right) \qquad (1.1)$$

where L_x, L_y, L_z are the lengths of for each dimension of the material and n_x, n_y, n_z are quantum numbers and σ is the standard deviation of the Gaussian function.

Experiments show that changing the size of material will result to changes on its properties [4, 5]. To understand the effects of changing the dimension of the material, a theoretical model for thin film was used to understand the relationship between size of the material, temperature, and resistivity in the presence of scattering.

$$\rho = c\rho_0\left[\frac{1}{\frac{\left(2\sqrt[8]{\gamma/kT}-b\right)(\tau_1/\tau_2+1)}{2a+b}}\right] \quad \text{if thickness} \geq 2\lambda \qquad (1.13)$$

$$\rho = \frac{c\rho_0}{k'[1-\ln(k')]}\left[\frac{1}{\frac{\left(2\sqrt[8]{\gamma/kT}-b\right)(\tau_1/\tau_2+1)}{2a+b}}\right] \quad \text{if thickness} \leq 2\lambda \qquad (1.14)$$

where *k'* is related to thickness of the material, *c* describes how rough the surface of the material, ρ_0 is the bulk resistivity of the material, γ is a parameter that depends on the material that is related to the energy equation of the restoring force of the moving atoms in the system, τ_1/τ_2 is the average time of travel of the electrons before they are scattered by phonons, *a* is the atomic radius, and *b* is the distance between atoms inside the unit cell.

RESULTS

Data are generated from this model to examine the effects of scattering in the resistivity of the material.

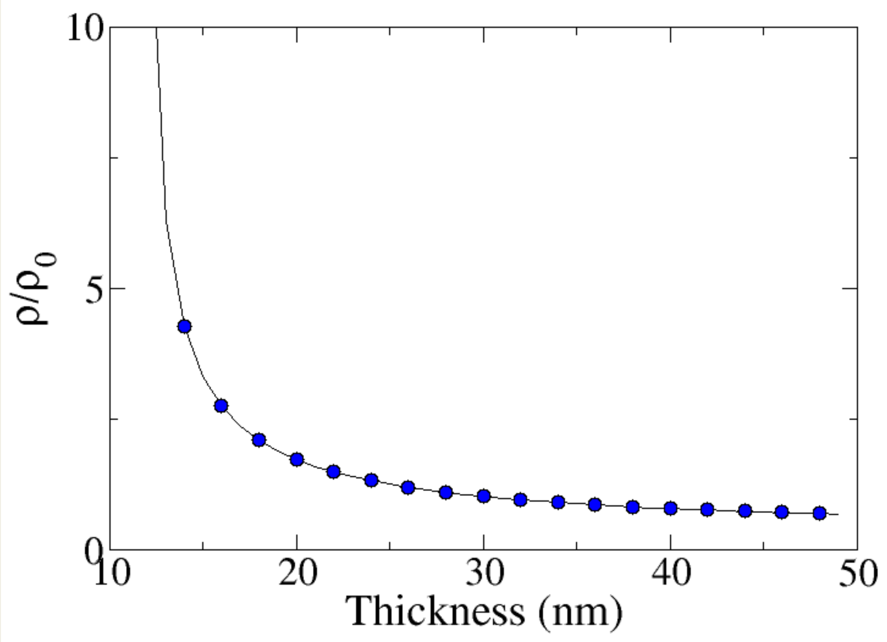

Figure 1. Resistivity of silver metal as a function of thickness

Equation 1.1 was used to observe the evolution of density of states while changing the thickness of the film. Results from Figures 1 and 2 fit together for observation of the crossover since the sudden increase in resistivity from 30nm to 10nm matches the change in shape of DOS from 3D to 2D. Even when the thickness of the thin film is the same as its λ (52 nm), it still exhibits its 3D signature of DOS since the transport of electrons can still transmit with no interaction to the surface of the material because the mean free path of the silver (52 nm) is still larger than the system.
By further decreasing the thickness of the film 20 nm lower than the mean free path of silver, the DOS starts to show a shape that is in between of 2D and 3D, this is where the crossover regime lies, it is where the resistivity starts to suddenly increase.

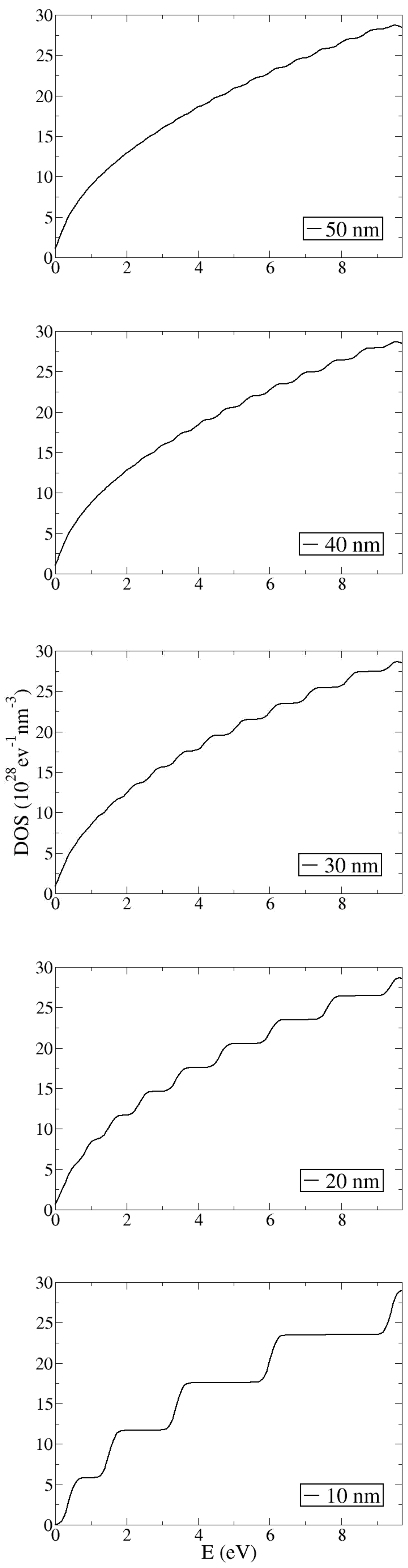

Figure 2. Density of states evolution from bulk to film

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CONCLUSIONS

Reducing the size of a conductor will randomize the momentum of electrons due to electron-surface scattering, which will result in increased resistivity. It is also observed that if the thickness of the film is the same or higher than the mean free path, λ, the value of the resistivity will stay constant. The sudden increase in resistivity is observed when the thickness of the film is half the length of λ. This is due to the crossover of density of states from 3D to 2D. However, there is a limit on how small the thickness of the thin film can reach before it shows quantum mechanical effects such as localization effects.

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