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# The Effect of Scattering of Phonons, Size and Grain Boundary on Electrical Properties for Ruthenium Nano Metals

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## Abstract

The study examines the impact of thickness on the electrical resistance of Ruthenium at room temperature. By applying the Fuchs-Sondheier and Mayadas Shatzkces models, the study establishes a linear relationship between thickness and grain boundary scattering. The M.S. model is crucial in calculating the size impact, accounting for all types of scattering affecting grain boundaries. On the other hand, the F.S. model focuses on explaining conduction electron scattering on material surfaces, particularly on tiny grains. The study's equation, derived from these two models, considers surface scattering and metal resistance to determine an experimental thickness that depends on metal resistivity. The Boltzmann Equation can be utilized to solve this equation. The study highlights the significance of Ruthenium as a common component of electrical and electronic circuits in producing electronic chips due to its excellent electrical conductivity.

**Keywords:** Phonons, electrical properties, size, grain.

## 1. Introduction

Ruthenium (Ru) is a versatile material that finds applications in various fields. In the electronic and electrical industry, Ru is used for the production of electronic chips due to its excellent electrical conductivity. This property of Ru can also be utilized in the production of solar cells to generate solar energy. It is worth noting that Russian chemist Karl Karlovich Klaus (1796-1864) discovered Ruthenium. He provided positive evidence for new elements derived from platinum and suggested naming the newly discovered element (Ruthenium) after the name of the ancient Russian country (Ruthenia) (1) . When materials are at the nanoscale level, resistance increases due to more scattering centers that conduct electrons, primarily at the boundaries between grains and surfaces. As the size approaches the average electron-free route, more resistance is observed. Electrons only collide with surfaces and grain boundaries at that point, becoming significant compared to their collision with other lattice errors such as impurities, point defects, and vacancies. Understanding the difference between surface and grain boundary contributions is essential when studying the resistive behavior of polycrystalline thin films (2) . Theoretical studies estimate the size effect by applying the F.S. model to surface electron dispersion, characterized by the surface effect coefficient (p), and the M.S. (3) . It is observed that electrical resistivity increases as thickness decreases because resistivity thickness depends on Fermi surface area values and metal-free paths (4,5). The uneven surface of the Grain boundary reflection in the F.S. and M.S. Models allows for the identification of different metals. To match the F.S. and M.S. theories to the experimental data, a simple equation was developed. This equation enables quick fitting of the two-theory model to the experimental data(6).

## 2. Materials and Methods

The grain boundary reflection coefficient (R) represents the limit of electron scattering(3). Moreover, the statistical study of the conduction electron distribution created by varying the collision mechanism's enforced rate of change forms the basis of the (F.S.) and (M.S.) theories. When two fields, an electric field (E) and a magnetic field (H), exist simultaneously, Boltzmann's equation takes the following form(7-9):

$$-\frac{e}{m^*}\left(\overline{V}+\overline{H}+\overline{E}\right).\mathrm{grad}\ \bar{v}\ f+\bar{v}.\mathrm{grad}\ \bar{r}\ f=\left(\frac{\partial f}{\partial t}\right)\mathrm{coll.}=-\frac{f-f_0}{\tau} \quad (1)$$

$$f_1(V,Z)=\frac{e\,E\,\tau_0}{m^*}\frac{\partial f_0}{\partial V_X}\left[1+F(V)\exp\left(\frac{-Z}{\tau_0\,V_Z}\right)\right] \quad (2)$$

In this context, $f_0$ represents the Fermi Dirac function, while f represents the distribution function of the charge carriers. Meanwhile, τ represents the relaxation time, e represents the charge of the electron, m* represents the effective electron mass, t represents the integration variable, and v represents the electron velocity. It is worth noting that two electron distribution functions exist: one with $V_Z > 0$ and another with $f_1$- for electrons with $V_Z < 0$.(9,10)

$$f_1^{+}(V,Z)=\frac{e\,E\,\tau_0}{m^*}\frac{\partial f}{\partial V_X}\left\{1-\exp\left(\frac{-Z}{\tau_0 V_Z}\right)\right\} \qquad V_Z>0 \quad (3)$$

$$f_1^{-}(V,Z)=\frac{e\,E\,\tau_0}{m^*}\frac{\partial f_0}{\partial V_X}\left\{1-\exp\left(\frac{d-Z}{\tau_0 V_Z}\right)\right\} \qquad V_Z<0 \quad (4)$$

$$J(Z)=-2\,e\left(\frac{m^*}{h}\right)^3\int\int\int V_X\,f_1\ dV_X\,dV_y\,dV_Z \quad (5)$$

The Fermi surface (F.S.) integral is typically denoted as A(Z, P) and is a function of the atomic number (Z) and momentum (P). The integral is used to calculate various properties of metals, including their electrical conductivity, and Planck's constant (h). (11,12) :

$$A\,(Z,P)=\int_1^{\infty}\left(\frac{1}{t^3}-\frac{1}{t^5}\right)\frac{1-\exp\,(-Z\,t)}{1-p\exp\,(-Z\,t)}\ dt \quad (6)$$

Where is $B\,(Z,P,\propto)$ the integral of M.S. as given by [11][9][13] :

$$B\,(Z,p,\propto)=\int_0^{\pi/2}d\emptyset\int_1^{\infty}\frac{\cos^2\emptyset}{H\,(t\,,\emptyset)}\left[\frac{1}{t^3}-\frac{1}{t^5}\right]X\frac{1-\exp\,[-Z\,t\,H\,(t,\emptyset)]}{1-p\exp[-Z\,t\,H\,(t,\emptyset)]}dt \quad (7)$$

elucidation of the resistivity rate ( $\rho_f / \rho_0$ ) to the bulk metal (9,14) :

$$\frac{\rho_f}{\rho_0} = \frac{3}{8Z}(1 - \mathrm{p}) + 1 \tag{8}$$

In this context, $\rho_0$ represents the bulk resistivity, while $\rho_f$ represents the thin resistivity. Z denotes the rate, which is equal to (Z = d/$l_0$), where d represents thickness and $l_0$ represents the mean free path. p represents the surface scattering coefficient. To find the total resistivity of metals, the condensed solution based on the (F.S) and (M.S) models computes the surface scattering and grain boundary reflection coefficient (15,16). When calculating the electrical resistivity of conducting electrons as a function of thickness, the scattering at grain boundaries is crucial. (17-19).

$$\propto = \frac{\mathrm{l}}{\mathrm{Z}} \frac{\mathrm{R}}{1 - \mathrm{R}} \tag{9}$$

The parameters (R) are utilized to determine the coefficient of reflection at the Ru grain boundary, with (∝) equaling R = 0.043 for Ru (13), to make it easier to evaluate resistivity (16)and grain size at different grain sizes, while analyzed, goes on (20,21). The electron surface scattering-related Fuchs-Sondheier estimate in Eq (8) is used to determine the resistance of metals, while M.S. electron scattering for grain boundaries is determined from Eq 10 (22).

$$\frac{\rho_f}{\rho_0} = 1 + \frac{3}{8Z}(1 - p) + \frac{3}{2}\propto \quad \mathrm{Z} \gg 1 \ \propto \ll 1 \tag{10}$$

The two models show that Ru is one of the conductive metals (23) . Its dependent temperature in terms of electrical resistance increases with decreased thickness(4,24). Grain boundary scattering is dependent on the average linear distance between grain boundaries, whereas surface scattering is directly related to film thickness and scattering (25). Grain-boundary scattering is achieved by solving a (Boltzmann equation) with background and electrical resistance(7). The concentration of a material influences the electrical properties of metals (26,27). Lastly, it was discovered that the temperature of all conductor metals affects electrical resistivity (28,29). has an inverse relationship with thickness(30-32). which equal ($\rho_0$ = 7.8 × $10^{-8}\Omega$m), mean free path (MFP) equal ($l_0$ = 6.6 nm), ($\rho_0 l_0$ = 51.48 × $10^{-17}\Omega m^2$ ) (33).

## 3. Results and Discussion

The experimental portion of Ru is shown in **Figure 1**, from which the data for the surface reflection coefficient was obtained by using equation (8) for (F.S) It seems that the theory developed by Fuchs-Sondheimer provides a way to obtain numerical values for the surface scattering coefficient in the range of (0-0.9), as well as the lowered resistivity based on equations with varying thicknesses. This measurement is dependent on the Fuchs-Sondheimer theory, which also takes into account conduction electron scattering on metal surfaces, particularly background scattering and grain boundaries (33,34).

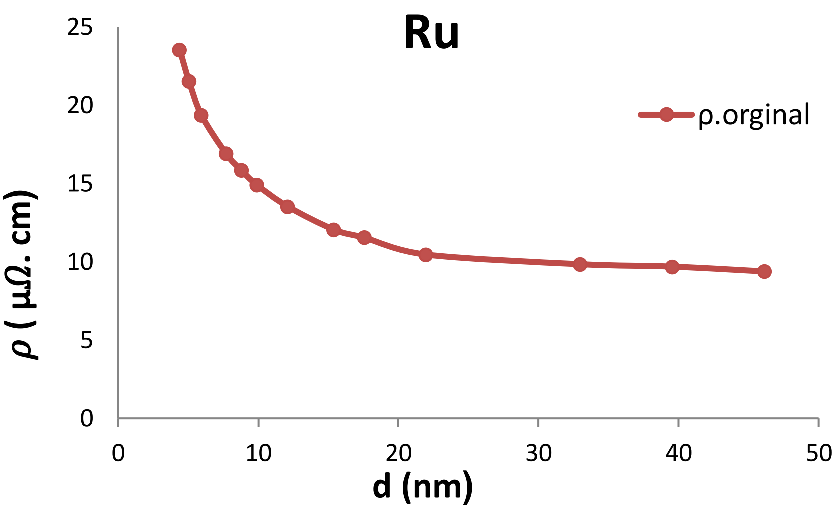


**Figure 1.** Resistance versus thickness for Ruthenium.

The intersection point of Ruthenium, originally ($\rho d$), and the slopes of Ruthenium, determined using values between (ρ and d), where d is the (x-axis) and ρ is the (y-axis), are obtained from the preceding **Figure 1**, Then Intersection point for (Ru= 68.03 * $10^{-17} \Omega m^2$), while slope of $\rho_0$ Ru (7.878 μ$\Omega$. cm ) as a following **Figure 2**. It seems that in the theoretical study shown in the **Figure 1**, the intersection point represents the resistance of the metal. However, due to defects, the difference in resistance at that point is very small.

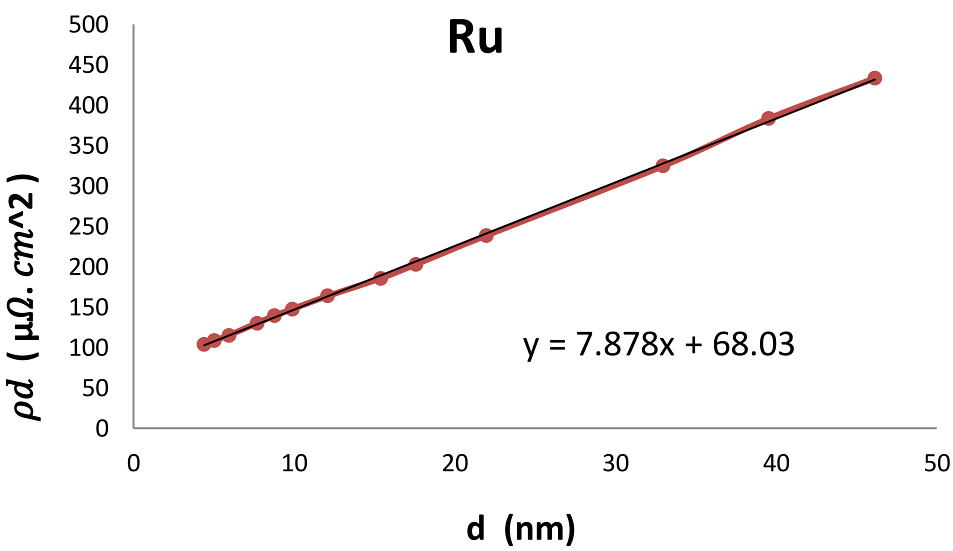


**Figure 2.** Point of intersection Ruthenium with thickness.

Then as indicated in Equation (8) application. Determine the surface scattering coefficient ($p$) for Ru, where ($p_{Ru}$= 0.6) (33,34). based on total scattering, as shown in the figures below **Figure 3**.

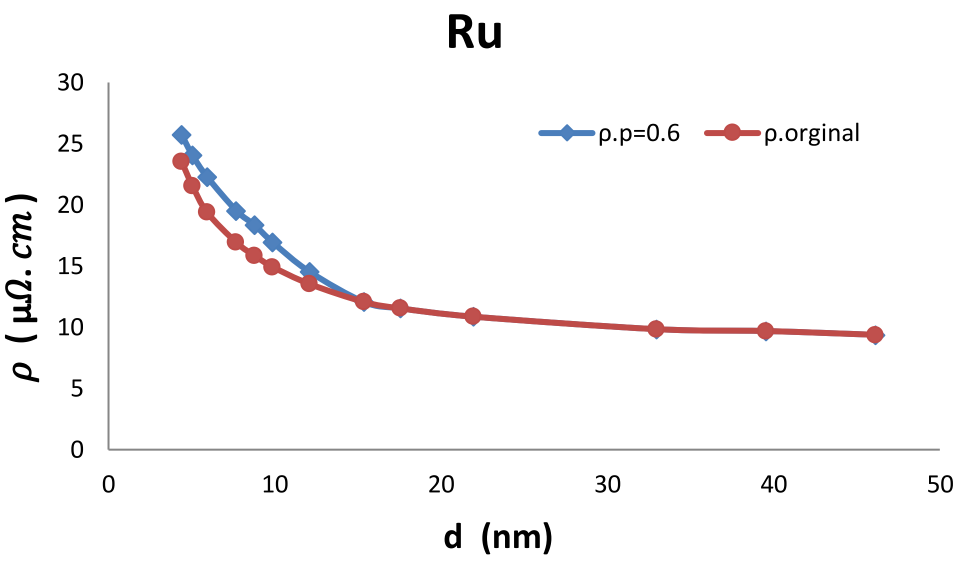


**Figure3**. Theoretical changing of the resistivity and thickness of Ruthenium.

Using the M.S. model, equation (10) calculated the reflection coefficient for Ruthenium at grain boundaries. Additionally, the value of bulk resistivity for Ru ($\rho_0$ = 6.8 × $10^{-8}$ Ωm), ($l_0$ = 6.6 nm), ln ($\rho_0 l_0$ = 51.48 × $10^{-17}\Omega m^2$) (33-37). As the result shown in the staying **Figure 4**, we computed the new resistivity by applying the surface scattering coefficient (p) and reflection coefficient (R) in Equation 10 for Ru. The Mayadas-Shatzkes model takes into consideration three scattering mechanisms, namely background scattering, grain-boundary scattering, and external surface scattering. Background scattering refers to the scattering of particles in the same direction in which they radiate after passing through a thick material. Grain-boundary scattering, on the other hand, is caused by binary defects in the crystalline structure of a solid that reduce electrical conductivity. Finally, external surface scattering results in a reduction of electrical conductivity as the scattered electron loses its velocity along the direction parallel to the surface of the conduction direction (5).

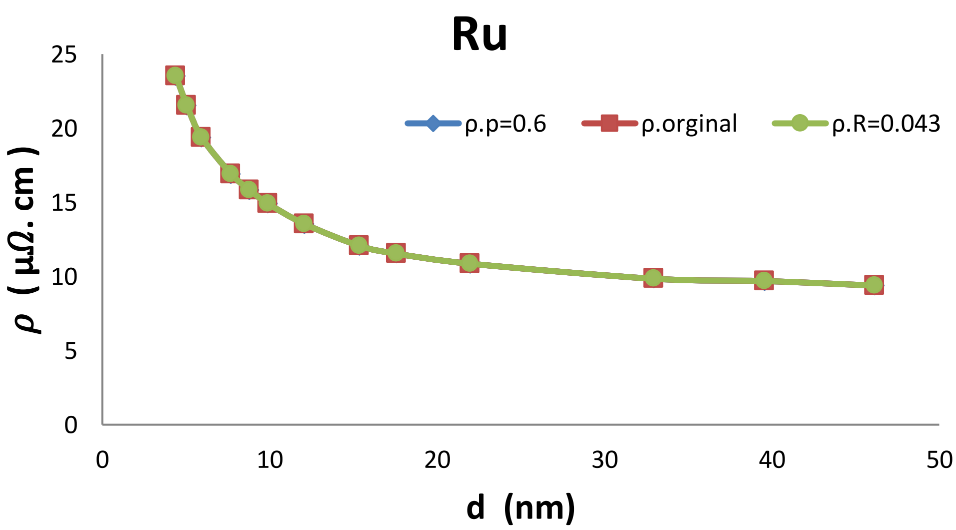


**Figure 4**. Resistivity and thickness of Ruthenium.

## 4. Conclusion

The electrical resistivity of Ru metal was calculated in this study using the Boltzmann equation's solution due to its strong electrical conductivity and numerous other advantages, the most important being its use in electrical and electronic circuits to produce electronic chips. Utilizing a Fermi surface, Fuchs-Sondheimer observed a phenomenon known as the size effect hypothesis for the free electron model. The statistical analysis used in their theory is based on the Boltzmann equation, which describes the distribution of conduction. As a result, F.S. theory is also used to describe conduction electron scattering on metal surfaces, focusing on background scattering and grain boundaries. The Fuchs-Sondheier model-based Equation 8 was used to calculate the surface scattering coefficient. In contrast, Equation 10 was used to obtain the grain-boundary reflection coefficient, which is based on the F.S and M.S models. In conclusion, using bulk resistivity reveals an inverse relationship between thickness and electrical resistivity, increasing resistivity as thickness decreases.

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## Conflict of Interest

No conflicts of interest exist for me.

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## Ethical Clearance

No animals were used in this study.

## References

1. Cheng YL, Lee CY, Huang YL. Properties and Applications of Ruthenium. Intech Open. 2016;11(13):377-390. https://DOI:10.5772/intechopen.76393
2. Sahu AK, Dash DK, Mishra K, Mishra SP, Yadav R, Kashyap P. Properties and applications of ruthenium. In Noble and precious metals-properties, nanoscale effects and applications. Intech Open. 2018;23(12):23-34. https://DOI:10.5772/intechopen.76393
3. Marom H, Eizenber M. The effect of surface roughness on the resistivity increase in nanometric dimensions. J Appl Phys. 2006;99(12):1-8. https://doi:10.1063/1.2204349
4. Lim JW, Mimura K, Isshiki M. Thickness dependence of resistivity for Cu films deposited by ion beam deposition. Appl Surf Sci.. 2003;217(23):95-99. https://doi:10.1016/S0169-4332(03)00522
5. Dutta SK, Moors K. Thickness dependence of the resistivity of platinum-group metal thin films. J Appl Phys. 2017;122(2):1-30. https://doi:10.1016/S0169-4332(03)00522-1
7. Gall D. Electron mean free path in elemental metals. J Appl Phys. 2016;119(8):1-5. https://doi:10.1063/1.4942216
8. Moraga L, Arenas C, Henriquez R, Bravo S, Solis B. The electrical conductivity of polycrystalline metallic films. Phys. B. Condens Matter. 2016;499:17–23. https://doi:10.1016/j.physb.2016.07.001
9. Moraga L, Arenas C, Henriquez R, Bravo S, Solis B. The effect of surface roughness and grain-boundary

scattering on the electrical conductivity of thin metallic wires, Phys. Status Solidi Basic Res. 2015;252:219–229. https://doi:10.1002/pssb.201451202
10. Tellier CR, Tosser AJ. A theoretical description of grain boundary electron scattering by an effective mean free path. Thin Solid Films. 1982;51(3):311-317. https://doi:10.1016/0040-6090(78)90293-6
11. Pazukha IM, Protsenko IY. Theoretical methods Investigation of the properties of thin film materials, 2017;11(2):101-120. http://essuir.sumdu.edu.ua/handle/123456789/59581
12. Van MJ. Size effects in double-layer metallic films. Concrete Fracture. 2012;7:184-219. https://doi:10.1201/b12968-13
13. Lucas MP. Size effects in double-layer metallic films. Thin Solid Films. 1971;7(6):435-444. https://doi.org/10.1016/0040-6090(71)90040-X
14. Mirigliano M, Milani P. Electrical conduction in nanogranular cluster-assembled metallic films. Adv Phys. 2021;6(1):1-40. https://doi:10.1103/PhysRevB.1.1382
15. Zhang QG, Zhang X, Cao BY, Fujii M, Takahashi K, Ikuta T. Influence of grain boundary scattering on the electrical properties of platinum nanofilms. Appl Phys. 2006;89(11):1-3. https://doi:10.1063/1.2338885
16. Jin JS, Lee JS, Kwon O. Electron effective mean free path and thermal conductivity predictions of metallic thin films. Appl Phys. Let. 2008;92(17):1–4. https://doi:10.1063/1.2917454
17. Meteab FA, Mohammed MA, Kanbur U. The effect of phonons-surface and grain-boundary scattering on electrical properties of metallic Ag. Ibn al-Haitham j pure appl sci. 2023;36(4):182-187. https://doi.org/10.30526/36.4.3234
18. Udachan L, Shiva L, Ayachit N, Banagar A, Kolkundi S, Bhairamadagi S. Impact of substrate temperature on surface and grain boundary reflection in thin chromium nanofilms. J Phys Conf Ser. 2019;1186(1):1-8. https://doi:10.1007/BF00552414
19. Zhang X, Huang H, Patlolla R, Wang W, Mont FW, Li J, Edelstein D. Ruthenium interconnect resistivity and reliability at 48 nm pitch. In 2016 IEEE International interconnect technology conference/advanced metallization conference (IITC/AMC). 2016;23(3):31–33. https://doi:10.1109/IITC-AMC.2016.7507650
20. Gall D. The search for the most conductive metal for narrow interconnect lines. J Appl Phys. 2020;127(5):112-134. https://doi.org/10.1063/1.5133671
21. Alderbas FAM, Najeeb MA. The effect of phonons-surface and grain-boundary scattering on electrical properties of metallic Al, Cu. In AIP Conference Proceedings. 2023;3018(1). https://doi.org/10.1063/5.0172558
22. Smith RS, Ryan ET, Hu CK, Motoyama K, Lanzillo N, Metzler D, Wright S. An evaluation of Fuchs-Sondheimer and Mayadas-Shatzkes models below 14nm node wide lines. AIP Adv. 2019;9(2):24-45. https://doi.org/10.1063/1.5063896
23. Henriquez R. Electron grain boundary scattering and the resistivity of nanometric metallic structures. The American Physical Society. 2010;82(11):2–5. https://doi:10.1103/PhysRevB.82.113409
24. Kim MS. Scaling Properties of Ru, Rh, and Ir for Future Generation Metallization. IEEE J Electron Devices Soc.. 2023;11:399–405. https://doi:10.1109/JEDS.2023.3292298
25. Shiva L, Ayachit N, Udachan L, Banagar A, Kolkundi S, Bhairamadagi S. A study on nucleation, growth and grain boundary reflection in thin tin nanofilms. J Phys Conf Ser. 2019;1186(1):1-11. https://doi:10.1088/1742-6596/1186/1/012006
26. Dutta SK, Vandemaele MC. Finite Size Effects in Highly Scaled Ruthenium Interconnects. IEEE Electron Device Lett. 2018;39(2):268-271. https://doi:10.1109/LED.2017.2788889
27. Milosevic E, Kerdsongpanya S, Gall D. The Resistivity Size Effect in Epitaxial Ru(0001) and Co(0001) Layers. IEEE Nanotechnol. 2019;1:1–5. https://doi:10.1109/NANOTECH.2018.8653560
28. Josell D, Brongersma SH, Tokei Z. Size-dependent resistivity in nanoscale interconnects. Annu Rev Mater Res. 2009;39:231-254. https://doi:10.1146/annurev-matsci-082908-145415
29. Bakonyi I. Accounting for the resistivity contribution of grain boundaries in metals: critical analysis of

reported experimental and theoretical data for Ni and Cu. Springer Berlin Heidelberg. 2021;136(4): 13360-01303. Https://doi:10.1016/j.mee.2004.07.041

30. Alsoltani KA, Harbbi KA. The Effect of Annealing Temperatures on Cu2O Nanoparticle Structural Properties. Ibn Al-Haitham J Pure Appl Sci. 2023;36(3):148-153. Https://doi.org/10.30526/36.3.3116
31. Palenskis V, Žitkevičius E. Phonon Mediated Electron-Electron Scattering in Metals. World J. Condens. Matter Phys. 2018;8(3):115–129. https://doi:10.1007/s10948-012-1507-3
32. Jasim KA, Fadhil RN. The Effects of Micro Aluminum Fillers in Epoxy Resin on the Thermal conductivity. J Phys Conf Ser. 2018;1003(1):012082. https://doi:10.1007/s10948-012-1507-3
33. Alsoltani KA, Harbbi KA. Effect of the Synthesis Time on Structural Properties of Copper Oxide. Ibn Al-Haitham J Pure Appl Sci.. 2023;36(2):181-198. https://doi.org/ 10.30526/36.1.2891
34. Ahmed ZW, Khadim AI, ALsarraf AHR. The effect of doping with some rare earth oxides on electrical features of ZnO varistor. Energy Procedia. 2019;157(20):909-917. https://doi:10.1016/j.egypro.2018.11.257
35. Jasim KA, Mohammed LA. The partial substitution of copper with nickel oxide on the Structural and electrical properties of HgBa2 Ca2 Cu3xNix O8+δ superconducting compound. J Phys Conf Ser. 2018;1003(1):012071. https://doi:10.1007/s10948-012-1507-3
36. Choi D. Potential of ruthenium and cobalt as next-generation semiconductor interconnects. J Korean Inst Met Mater. 2018;56(8):605-610. https://doi:10.3365/KJMM.2018.56.8.605
37. Zhao K, Hu Y, Du G, Dong J. Mechanisms of Scaling Effect for Emerging Nanoscale Interconnect Materials, Nanomaterials. 2022;12(10). https://doi:10.3390/nano12101760