Tungsten as an Interconnect Material for Next-Generation IC Design

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***Abstract*—Over the last few decades, technology have seamlessly transfer from Aluminium to Copper, as aluminium has deemed as an unsuitable metal when it is in the nanoscale due to associated drawbacks. Although with the challenge of having to replace copper, it has been one of the most consistent materials in the wire dimension area. However, getting a material as ideal as copper is proving to be more inefficient as scale down the wire deeper. There has been a spurt in the research of Tungsten (W) and its Oxides (WOx) as a potential replacement to the issues posed by copper. In general, tungsten has been proven to be superior to most existing interconnect materials and has been only put behind Silver and Copper. However, as technology reach the nanoscale, there has been increasing studies on how to fabricate tungsten and its subsidiaries as an alternate to other materials. The purpose of this research is to study Tungsten and other existing interconnect materials and compare them on theoretical and observational basis. The number of simulations has been carried out using the COMSOL software in various environments in order to see how tungsten behaves in all environments and propose whether it is suitable in the upcoming generation of ICs and beyond.**

Keywords—Nanoelectronics, Interconnects, Tungsten, Conductivity, Resistivity, Integrated Circuits, Conducting materials.

I. INTRODUCTION

There has been a considerable growth over the years in the research of nanowires and other related structures. The reach of this field has touched the disciplines of solid-state chemistry, quantum mechanics, biomedical engineering, condensed matter physics, photonics, opto-electronics etc. However, one of the fields that have benefitted the most is the Nano-electronics/Nanomachines and Integrated Circuit (IC) design. As the IC scale down, the real challenge lies in reducing the dimension of the wire itself. Since the onset of the industrial revolution and even in instances before, wires have been a part of our daily lives for centuries together. Powerlines are utilized efficiently to transmit electricity to households everywhere, the optical fibres have been introduced to transmit information over long and short distance. It has been more than a decade that the researchers all over the world have investigated different processes and techniques and have come up with methods which can be used to synthesize nanowires which are thousands of times thinner than the hair. These nanowires have allowed the onset of the next generation of application in fields like advanced computing, photonics and photosensitive applications, efficient energy utilization and especially it has enhanced applications in the biomedical field as well [1-5].

The material which have been scaled down to the nanoscale in the form of nanotubes, nanorods and nanowires have been under the spotlight due to their plethora of applications in semiconductors, interconnects and other nanoscale devices. These materials give the insight on the study of properties like electrical, mechanical and thermal which have changed due to scaling down to the nanoscale. These properties can be studied and altered for development and advancement of novel applications in different fields and focusing on the nanoelectronics.

Choi and Barmak [6], in their research have discussed the potential of Tungsten as future interconnects and have reviewed the current availability of different technology, processing methods and the required nanostructure. Moreover, they have studied the resistivity Copper and Tungsten nanowires using the Mayadas-Shatzkes grain boundary and Fuchs-Sondheimer surface scattering model model. It is observed that Tungsten nanowires exhibit lower resistivity than Copper. Bien *et al.* [7] have extensively studied a synthesis method for fabricating Tungsten nanowires which are self-aligned, by the use of a Poly-Si core. They formed nanowires in the neighbourhood of 10nm using the Poly-Si transfer technology followed by CVD of tungsten using WF6 as the precursor solution. They also characterized the conductivity of the nanowires to see how this method influenced physical properties and found it to be 40% higher than doped Poly-Si nanowires of the same scale. Further, Wu *et al.* [8] has proposed tungsten oxide materials as a photothermal nanomaterial. They found that WO_x structures have an unusual oxygen defect and allow excellent photo-absorption of various wavelengths in the NIR region. Moreover, Min and Ahn [9,10] have reported the synthesis of W nanostructures by a simple process of thermally treating tungsten films, which are characterized by self-catalysing layer formation and have astounding field emission (FE) properties. This easy fabrication could be the gateway for building nano-level interconnection materials and nano-machine components. Chen *et al.* [11] have come up with a novel method which involves the usage of solution-based printing of thermoelectric generators (TEG) and metal contacts and Ni *et al.* have also discussed the improvement in thermoelectric properties using a PEDOT nanowire film to coat Te, which can also be investigated in the use case of tungsten [12].

From above literature, it is observed that the Tungsten has been extensively investigated and utilized for various applications as an interconnect. Moreover, it can be used in energy applications, biomedical, chemical, photothermal etc. The versatility of tungsten, along with its inter-miscibility

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with other metals to form alloys can help to investigate oxides of W, Carbides and even Sulphides as an alternative. Therefore, in this paper an extensive experimentation is carried out the possibilities of Tungsten as an interconnect for IC design has been investigated.

The rest of the paper is structured as follows: Section II describes the detailed explanation of the existing material and characteristics. Experimental evaluation and results are presented in Section III and conclusions are drawn in Section VI.

II. MATERIALS AND THEIR CHARACTERISTICS

This sub-heading explores the current available information on the current generation methods and the viable synthesis methods for such nanowires. There are a variety of metals available, which can be used for IC and Semiconductor design. Some metals which are commonly used are Silicon, Copper, Aluminium, Silver and Gold.

Silicon (Si) is the most commonly used material for IC design. Si is a semiconductor having the electrical behaviour is between that of a conductor and an insulator at room temperature. Polycrystalline silicon (Poly-Si) is used for making resistors or conductors in an integrated circuit. Si is also widely used in semiconductor packaging, being the main ingredient of plastic encapsulants for ICs and are used in die overcoats as well [13,14].

Another material Aluminium (Al) is a highly lightweight metal with silvery appearance. It is the most abundant metallic element on earth and used in many aspects of semiconductor manufacturing. On an IC, Al metal lines are commonly used as the main conductor between components due to low resistivity. As a thin film, it has good adherence to SiO_2. Al is used for the bonding and probing pads on the die. When used for IC metallization, it slightly doped with elements such as Si and/or Cu to improve its characteristics and reliability. In semiconductor assembly, ceramic packages are composed mainly of alumina. Al is also used for wire-bonding IC in ceramic packages. Aluminium is one of the most widely used metal for metallizing IC chips since it has a high conductivity, very low contact resistance and good compatibility to Si and SiO_2. However, Aluminium has many shortfalls when it is brought up in the interconnect argument like poor step coverage, spiking and migration of electrons [13-16].

Gold (Au), is a soft element which is a good conductor of heat and electricity. It is also the most malleable and ductile of all metals. Au is used in many aspects of semiconductor manufacturing, particularly in the assembly or packaging processes. Its most widespread use is in wire-bonding because of excellent conductivity and ductility. It is mainly used as wires for interconnect in ICs [17].

Silver (Ag), is another element which is next only to gold in terms of malleability and ductility and is also a good conductor of heat and electricity. Ag is the best conductor of electricity, better even than copper and gold. Ag is used in many facets of semiconductor manufacturing, more particularly in packaging processes. Most epoxy die attach materials contain Ag fillers for increased electrical and thermal conductivity. Ag is also used to cover the surfaces of the die pad and bonding fingers of the plastic packages to prevent chemical degradation of these areas, which may lead to die attach and bonding problems [18].

Copper (Cu), is one of the most widely used metals in the world, mainly because of its many desirable properties. It is the 2nd best conductor of electricity next to Ag. It is very malleable and ductile and good conductor of heat. Cu is also widely used in semiconductor assembly being an excellent conductor. Recent technological advancements though have already allowed the use of copper as metal lines in semiconductor devices [19]. The continued scaling down of semiconductor devices is proportional to the miniaturization of Cu interconnect lines as well. Although this scaling leads to improved working, it tends to exhibit a higher resistivity and hence in turn give rise to issues like increased power consumption, delayed signal transfer and increased resistivity.

With the onset of advance techniques of VLSI on circuit chips, the introduction of new processes and materials which are capable of matching or improving the density of packing and high-performance are remains the challenge for researchers. There is a need of a material which can help in shunting out Poly-Si gate and thereby reduce the sheet resistance, electro-migration, junction spiking and a high contact resistance.

From literature, it has been observed that the Tungsten can be considered as a potential candidate to replace Cu for metallization for two main reasons. The first is the very high melting point (3695) compared with Cu, which is expected to improve interconnect reliability such as electromigration and stress. The second reason is the anticipated reduction of resistivity effect due to significantly shorter EMFP of 19.1 nm at 293˚K as compared to Cu. However, given the fact that the room-temperature bulk resistivity of W at 5.3 μΩ-cm is higher than that for Cu at 1.7 μΩ-cm, it is important to quantify the contributions of size-dependent scattering mechanisms in order to determine whether W can favourably compare with Cu as a nanoscale interconnect. The theoretical nanowires properties of existing interconnect material is summarised in Table 1.

The metallic Tungsten has well-known chemical, physical, electrical, and mechanical properties that makes it very useful for various applications [20-22]. Especially for nanodevices below 100 nm, a gate material such as W with a mid-gap work function is desirable as a metal gate of CMOS technology due to the fairy low resistivity. Another variant of tungsten such as its subsidiary oxides are used commonly in semiconductor and nanotechnology-based applications. The research potential in WO_x can be seen as early as the 17th century, when people began studying the different properties of $LiWO_3$ and were searching for methods to grow compounds like WO_3 and $NaWO_3$. Along with the progress of nanotechnology, the fabrication of Tungsten and its oxide have become increasingly prominent as nanostructures of W and WO_x have better performance. Nano-structured WO_x is exceptionally versatile and offers a wide range of unique characteristics when it comes to VLSI design. In comparison to other oxides such as TiO_2, ZnO, NiO, WO_x exhibits much more advanced electrical properties and also being employed as material which can be used in nano-sensing [23-25]. Thus, it has been observed that the Tungsten and its oxides can be used for interconnect in integrated circuits design.

In this paper, an attempt is made and the various existing materials as well as Tungsten oxides in the form of nanowires has been simulated using the COMSOL software. Moreover,

the detailed characteristics of simulated nanowires has been studied.

TABLE I. THEORETICAL NANOWIRE PROPERTIES OF EXISTING INTERCONNECT MATERIALS

Parameters	Aluminium (Al)	Copper (Cu)	Gold (Au)	Silver (Ag)	Silicon (Si)
Molecular Wt.	26.98	63.55	196.97	107.87	28.086
Melting Point (^{0}C)	660.37	1085	1064	961.8	1414
Boiling Point (^{0}C)	2467	2562	2700	2162	3265
Density (g/cm^3)	2.7	8.96	19.3	10.49	2.33
Resistivity	2.6548 μΩ-cm	1.673 μΩ-cm	24.4 nΩ-cm	15.9 nΩ-cm	64 mΩ-cm
Electronegativity	1.5	1.90	2.54	1.93	1.9
Heat of Fusion (kJ/mol)	10.79	13.26	12.55	11.3	50.55
Heat of Vaporization (kJ/mol)	293.4	300.4	334.4	250.58	384.22
Poisson's Ratio	0.35	0.34	0.42-0.44	0.337	0.22
Specific Heat (kJ/kg K)	0.900	0.390	0.129	0.240	0.710
Thermal Conductivity (Wm^{-1} K)	205	401	310	406	150
Coefficient of Thermal Expansion (μm-m^{-1} K^{-1})	23.1	16.5	14	18	2.6
Vicker Hardness (MPa)	167	369	216	251	9630
Young's Modulus (GPa)	0	110-128	79	85	130-180
Tensile Strength (MPa)	40-700	210	80-700	100-200	20-170

III. EXPERIMENTATIONS AND OBSERVATIONS

Before you begin to format your paper, first write and save the content as a separate text file. Complete all content and organizational editing before formatting. Please note sections A-D below for more information on proofreading, spelling and grammar. In this experiment, the various experimentation is carried out using COMSOL Multiphysics Modelling on the system which has Intel(R) Core (TM) i7 CPU with 2.4 GHZ frequency processor and 8 GB RAM.

In the first experiment, the Aluminium, Coper and Silver wire has been simulated with the various parameters. Here, the "Electric Currents" module on COMSOL version 5.3a has been used to simulate the particular wire. The available quantities such as resistance, reference impedance, terminal voltage, terminal current, total electrical energy as shown in Table 2. Moreover, the current of $1\mu A$ through the wire with dimension radius 0.5nm, and length 10nm is considered for the evaluation. Table 3 shows the calculated values of resistivity, conductivity and current density, respectively. The details of simulation of Aluminium, copper and silver using COMSOL software is shown in Fig 1.

TABLE II. OPERATIONAL VALUES FOR ALUMINIUM, COPPER AND SILVER

Parameters	Aluminium	Copper	Silver
Resistance (Ω)	370	233	226.52
Electrical Energy (J)	4.337×10^{-29}	1.717×10^{-29}	-2.48×10^{-28}
Reference Impedance (Ω)	50	50	50
Terminal Voltage (V)	3.69×10^{-4}	2.326×10^{-4}	2.26×10^{-4}

TABLE III. CALCULATED VALUES OF RESISTIVITY, CONDUCTIVITY AND CURRENT DENSITY

Parameters	Al	Copper	Silver
Resistivity (Ω-m) $\rho = RA/l$	2.91×10^{-8}	1.83×10^{-8}	1.78×10^{-8}
Conductivity (S/m) $\sigma = 1/\rho$	3.4×10^{7}	5.46×10^{7}	5.6×10^{7}
Current density (A/m^2) $J = I/A$	3.82×10^{12}	3.82×10^{12}	3.82×10^{12}

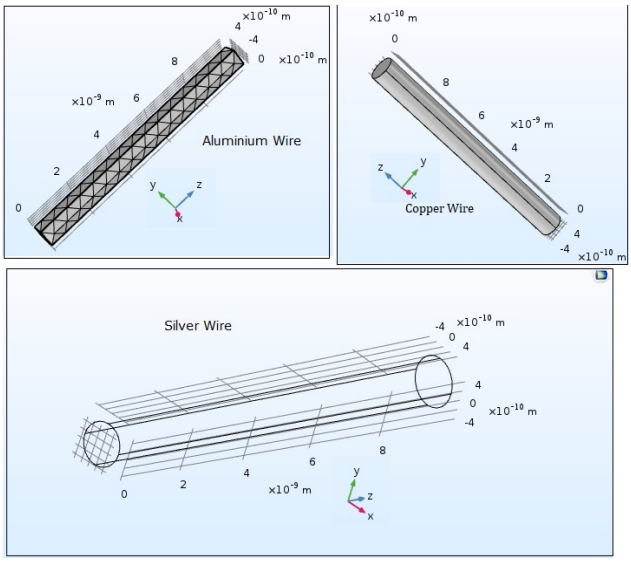

Fig. 1. Simulation of Aluminium, Copper and Silver wire.

In second experiment, the normal tungsten with same dimensions as previous experiment has been simulated and various parameters are obtained. The resistivity ($6.1\text{x}10^{-8}$

Ωm), conductivity (1.64x10^7 S/m), and current density (3.82x10^{12}A/m^2) which is better than the other materials such as Aluminium, copper and silver. The simulation of Tungsten nanowire is shown in Fig. 2.

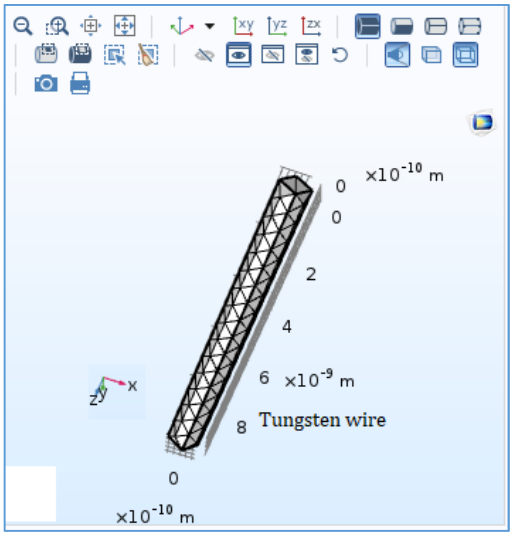

Fig. 2. Simulation of Tungsten Nanowire

From the study of Aluminium, copper, silver and Tungsten, it cannot be concluded whether Tungsten material is viable as an interconnect. Therefore, it has been decided to study the different types of Tungsten Alloy in COMSOL to find the suitable material nanowire interconnect. Following materials are considered and simulated in COMSOL:

- Tungsten [CVD <001>, tested at 293K, 9500/s]
- Tungsten [CVD <011>, tested at 293K, 6600/s]
- Tungsten [gas]
- Tungsten [liquid]
- Tungsten [MEMS]
- Tungsten [powder metallurgy, tested at 293K, 4000/s, annealed at 2873K]
- Tungsten [rod, tested at 3073K]
- Tungsten [sheet,1.5 mm sheet, strain relieved at 1423K]
- Low Carbon Steel Tungsten Steel
- Tungsten [swaged bar, tested at 1033K]
- Tungsten [Built in]

There are mainly two parameters in the COMSOL material contents toolbar, without which the simulation will not run properly. The first is relative permittivity of 6.2438 and 22.254 and second is electrical conductivity 1.79×10^7 *S/m*. These both values have been obtained from online databases and verified. We have simulated all of tungsten available in the COMSOL material library and a separate file is prepared for each material to ensure no discrepancies in the observed values. Following values of parameters has been used in each calculation:

- Nanowire Radius: 0.5 *nm* or 0.5×10^{-9} *m*
- Nanowire height: 10 *nm* or 10×10^{-9}*m*
- Current: 1*nA*
- Electrical conductivity: 1.79×10^7 or 1.79×10^7 *S/m*
- Relative permittivity: ε_1= 6.2438, ε_2 = 22.254.

The resistivity of the materials has been calculated using the formula:

$$\rho = \frac{RA}{L} \tag{1}$$

where, *R* is resistance, *A* area of cylindrical wire and *L* is the length per height of the wire. The various simulations have been carried out using COMSOL for different Tungsten variant. The simulation has been shown in Fig. 3. The simulation results are summarized in Table 4. The simulated tungsten wires for a nanowire yielded a resistivity of 6.8×10^{-8} in most of the cases. However, this is insufficient information as to whether top-down manufacture will influence the resistivity of the metal. Since we had to provide the values of conductivity and the relative permittivity values in each case, we found that the former had a bigger impact on the resistance value in each case rather than the latter. The tungsten liquid has a higher resistance in liquid which is attributed to the fact that tungsten is covalent in nature and considering the fact that ionic solutions have higher conductivity. The Tungsten [MEMS] structure shows a slightly lower resistance as compared to the built-in Tungsten. This value also corresponds to the theoretical obtained resistivity value.

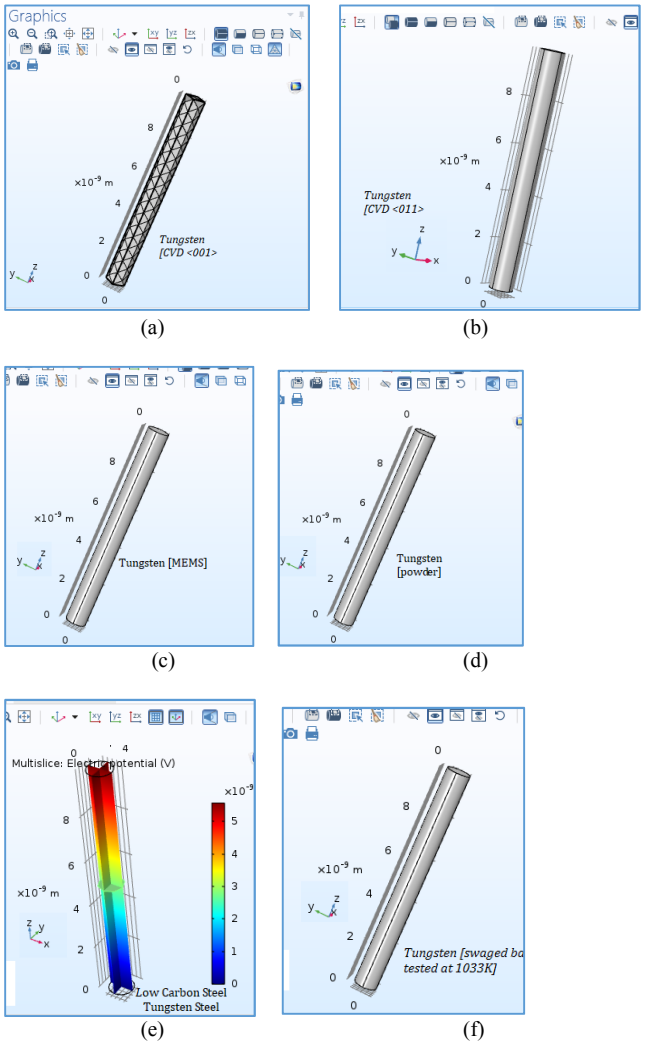

Fig. 3. Simulation of Tungsten Nanowire; (a) Tungsten [CVD <001>], (b) Tungsten [CVD <011>], (c) Tungsten [MEMS], (d) Tungsten [Powder], (e) Low Carben Steel Tungsten Sheet, (f) Tungsten (Swaged).

TABLE IV: CALCULATED VALUES OF RESISTIVITY, CONDUCTIVITY AND CURRENT DENSITY

Material	Electrical Parameters					
	Resistance (Ω)	Total Energy (J)	Reference Impedance (Ω)	Terminal Voltage (V)	Resistivity (Ω)	Conductivity (S/m)
Aluminium	370	4.3×10^{-29}	50	3.6×10^{-4}	2.91×10^{-8}	3.4×10^{7}
Copper	233	1.7×10^{-29}	50	2.3×10^{-4}	1.83×10^{-8}	5.4×10^{7}
Silver	226.52	-2.48×10^{-28}	50	2.2×10^{-4}	1.78×10^{-8}	5.7×10^{7}
Tungsten	775	1.91×10^{-28}	50	7.7×10^{-7}	6.1×10^{-8}	1.6×10^{7}
Tungsten (CVD 001)	780	4.3×10^{-33}	50	7.8×10^{-7}	6.123×10^{-8}	1.63×10^{7}
Tungsten (CVD 011)	779	1.2×10^{-33}	50	7.7×10^{-7}	6.1×10^{-8}	1.6×10^{7}
Tungsten (Gas)	779	4.29×10^{-33}	50	7.8×10^{-7}	6.1×10^{-8}	1.6×10^{7}
Tungsten (Liquid)	18209	2.34×10^{-30}	50	1.8×10^{-5}	1.43×10^{-6}	7×10^{5}
Tungsten (MEMS)	690	3.4×10^{-33}	50	6.97×10^{-7}	5.4×10^{-8}	1.85×10^{7}
Tungsten (Powder)	779	4.29×10^{-33}	50	7.8×10^{-7}	6.1×10^{-8}	1.6×10^{7}
Tungsten (Rod)	779	4.29×10^{-33}	50	7.8×10^{7}	6.1×10^{-8}	1.6×10^{7}
Tungsten (Sheet)	779	4.29×10^{-33}	50	7.8×10^{-7}	6.1×10^{-8}	1.6×10^{7}
Tungsten (Steel Alloy)	5.6	9.8×10^{-33}	50	5.58×10^{-9}	4.4×10^{-10}	2.3×10^{9}
Tungsten (Swaged Bar)	779	4.29×10^{-33}	50	7.8×10^{-7}	6.1×10^{-8}	1.6×10^{7}

The Tungsten steel alloy had different results. Typically, alloys have to exhibit physical, chemical and electrical constants in relation to their parent metal. It has to be in between both the metals or closer to the base metal as per principle. The experiment started with 2.5×10^{6} S/m as the first value of electrical conductivity in order to obtain resistance and other parameters. The obtained resistance value is 780Ω, which is similar to the resistance of tungsten. When the conductivity is increased to 10^{7}-10^{8}, the resistance remains the same, which indirectly implies that Tungsten is the base metal. However, once we used 2.3×10^{9}, the resistance dropped to approximately 6Ω. Hence in order to get a lower resistivity, an alloy should be used to of a metal to reduce the resistivity or increase the conductivity. This intuition can be used to determine an alloy would serve as a better interconnect material. Another observation which plays a large role in design of Interconnects is the down scaling of the wires. The presented experimental data indicates that the resistivity in metal based thin films and wires in the nanometre dimension which is inversely related to the width/diameter. This is mainly attributed to the electron scattering which has increased due to Grain Boundaries (GB) and the roughness of the metal Surface Roughness (SR) of the wire boundaries. In simple words, if size decreases, resistance increases and vice versa. This in turn, has an effect wherein the wire dimensions have the constraint of scaling down along with the IC or Transistor size, and this scaling down of resistivity also gives rise to other shortcomings like higher heating issues, increased power consumption and delay in signal transmission. If this increase in resistivity is not kept in check, the interconnects will serve as the main issue during the fabrication of next generation ICs. Existing experimental data available tells us that the resistivity of these wires in the nanoscale agree with the Fuchs-Sondheimer (FS) and Mayadas-Shatzkes (MS) models and these models specifically utilize the fitting parameters and along with approximation of semi-classical mechanics. However, these models fail to provide the data about the domain of quantum mechanics when it comes to scattering, confinement and a well-defined and mapped structures of SRs and GBs. These models make use of fitting parameters and semi-classical approximations and do not provide further insight in the quantum-mechanical effects of scattering, confinement and the detailed structure of the GBs and SR. From studies, however, there has been a marginal decrease in the resistance. When the transition from the microscale to the nanoscale is considered, the classical mechanics will be replaced by the principles of quantum mechanics. The effect on the resistance and other physical properties need to be studied more in detail as COMSOL provides a limited insight. Since these properties cannot be altered, it is necessary to find a suitable alloy or mixture of tungsten which can exhibit the expected characteristic. It has been observed that tungsten alloys have extremely high corrosion resistance on par with Titanium when it comes to corrosion and stress. Moreover, it is highly durable with higher melting point (3422^{0}C) and boiling point (5555^{0}C).

IV. CONCLUSIONS

In this work, an extensive study has been carried out on the different materials for the nanowire's applications in integrated circuits design. The Tungsten and its variants are considered in this study and their electrical characteristics has been calculated using the various simulations. The obtained results are compared with mostly used materials like Aluminium, Copper, Silver, Silicon and Gold. It has been observed that the Tungsten alloy has better conductivity and resistivity as compared to the existing materials. Thus, the Tungsten alloys can be used as an interconnect in integrated circuits.

As a future scope for thsese studies, it can be further investigated tungsten to come to a more conclusive result. After noticing the properties of tungsten and silver, the research is being focused towards coming up with a tungsten-silver alloy as the next generation interconnect material. The alloy can be formed by either mixing both the molten metals and allowing alloy formation or powder metallurgy which

involves the sintering of powders of both metals. Theoretically, the resistivity of the metal should be close to the base metal, or in between both the metals, based on the percentage of each metal used in the alloy. The alloy may be having a proportion of 35-70% of each metal so as to not lose the base properties of the other. Tungsten and Silver together can overcome each one of the other's drawbacks. Although getting a conductivity close to the value of 2.3×10^9 as seen in Table IV is nearly impossible considering the current technology, working on an alloy which can provide a conductivity closer to Ag is very much possible. It can increase the inertness, melting point, boiling point and even the corrosion resistance of Silver, whereas Ag in turn can increase the conductivity, malleability and ductility of tungsten.

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