DFT Analysis of Different Shaped Cu Nanowires for Interconnect Application

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Abstract

In the present work, Density functional theory (DFT) based comparative analysis has been implemented to analyze the structural stability, electronic and transport properties of Copper (Cu) nanowires with varied morphologies and diameters. The calculation of formation energy shows the stability of Cu nanowires increases with increasing the diameter. Further, from the transport properties analysis, it confirms that the rectangular morphology of Cu nanowire at 1.8 nm diameter shows linear I-V characteristics and significantly low interconnect parameters i.e. kinetic inductance and quantum capacitance in comparison to other morphologies and diameters of Cu nanowires, and which is good for interconnect perspective. Hence, it can be concluded that Cu nanowire with 1.8 nm diameter of rectangular morphology may be a possible candidate for interconnect application.

Keywords 1

Copper nanowires, Dynamical parameters, Interconnects, morphology

1. Introduction

Advances in integrated circuit technology require that the chip dimensions decreases in size, to satisfy the Moore's law of continuous miniaturization, which creates the need to scale down the size of the metallic interconnects too [1]. At nanoscale the scaling of interconnect dimensions leads to rise in Cu resistivity that causes performance degradation. The resistivity of a Cu wire increases with decreasing area of cross-section due to quantum effects, which become significant as the interconnect dimensions get closer in magnitude to the electron mean free path (~40 nm) around room temperature [1]. Cu faces two critical problems as a nanoscale interconnect material, first, its inability to carry high current densities, and increased resistivity [2] due to surface scattering of electrons and grain-boundary issues [3]. The increase in resistivity of the nanoscale Cu interconnects severely impacts the interconnect performance, in turn affecting adversely the performance of the nanoelectronic circuits incorporating them.

In spite of these problems, there are qualities that maintain Cu as the material of choice for making interconnects. First, Cu is reasonably inert under a variety of conditions. Other reason for choosing Cu is quite abundantly available making it lucrative from a commercial point of view. There are some experimental reports [3],[4] available which reveals that bulk Cu may be replaced with Cu nanowire as interconnects in future nanoscale devices due to various challenges in the bulk Cu.

The analysis of electronic, magnetic, thermoelectric, optical and transport properties of various nanowires like CdS, CdO, CdTe, Fe and Co have been recently reported elsewhere [5], [6], [7], [8] depending on the shape, geometry and applied pressure. In another report [9] the analysis of Pt, Rh, Ir nanowire, have been presented and compared their performance with bulk Cu, and concluded that

VI International Conference Information Technologies and High-Performance Computing (ITHPC-2021), September 14–16, 2021, Khabarovsk, Russia
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CEUR Workshop Proceedings (CEUR-WS.org)

CEUR-WS.org/Vol-2930/paper8.pdf

these nanowires are relatively better than Cu bulk structure for interconnect application. In another report on Cu nanowires, Ma et al. [10] have analysed the structural and electronic properties of Cu nanowires with different cross sections and concluded that number of channel increases as nanowires diameter increases. In [11], the structural and mechanical properties of nanowires have been compared with the experimental results. In spite of available reports on nanowires, this attempt of ours is probably for the first time to compute the structural electronic and transport properties of morphology dependent Cu nanowires for interconnect application. Reason being, the different morphologies and size of cu nanowires can be formed during the synthesis process.

In the present work, the performance of interconnects has been measured in terms of the structural stability, bandstructure, density of states, conductance, quantum capacitance and kinetic inductance. The quantum capacitance and kinetic inductance are calculated following the approach reported in [12, 13]. Further, analysing the interconnect parameters with different diameters, the relatively best morphology of Cu nanowires has been considered as a candidate for interconnect application.

2. Computational methods

The structures of the nanowires are created using the FCC crystal structure with bulk lattice constant of a = 3.61 Å for Cu. The wire axis is taken along the [100] lattice direction. Further, the electronic structure calculations are based on first principles density functional theory (DFT) using the Atomisticx-tool kit virtual nanolab (ATK-VNL) [14,15]. DFT calculations with generalized gradient approximation (GGA) [16] in form of Perdrew-Burke-Erenzhorf (PBE) functional are considered for ground state properties calculations. Mesh cut-off energy of 75 Hartee. Double zeta double polarized (DZDP)) basis set and brillouin zone integration with k-point Monkhorst-Pack sampling of 1 x 1 x 20 are selected for geometry optimization and electronic properties evaluation. Whereas 1 x 1 x 100 k points are selected for the computation of transport properties. Structures are relaxed until forces on each atom reaches to 0.05 eV/Å. To confine the dimension of nanowires along transverse direction with respect to longitudinal one (nanowire periodically growth) large cross section of super cell has been chosen to avoid mirror image interaction and to ensure negligible interaction between the wire and its replica, vacuum space of 15 Å is used.

To compute the transport properties, we have designed a two probe setup has been modelled by extending the channel regions in electrodes, which can be explained through NEGF approach and computes the current using the Launder–Büttiker formula reported elsewhere[17]

$$I = \frac{2e}{h}\int_{\mu L}^{\mu R}(T(E)[\,\mathrm{F_L(E)} - \mathrm{F_R(E)}])\mathrm{dE} \quad (1)$$

$$\mathrm{T(E,V)} = \mathrm{Tr}(\Gamma_L(\mathrm{E,V})\mathrm{G^R(E,V)}\Gamma_R(\mathrm{E,V})\mathrm{G^A\,(E,V)}) \quad (2)$$

Here$\mu_R$and $\mu_L$represents the chemical potential of left and right electrode, respectively, with Fermi distribution functions $F_L(E)$ and $F_R(E)$. T(E) is total transmission probability of all the channels at applied voltage V and energy E. G^R and G^A are the retarded and advanced Green's function with Γ_L and Γ_R as coupling functions of left and right electrode self-energies.

3. Result and Discussion

The unit cell of Cu nanowires with three different diameters (1 nm, 1.4 nm and 1.8 nm) of tetragonal morphology have been optimized and shown in fig. 1(a), 2(a), 3(a) respectively. Further different morphologies of nanowires like rectangular, square and triangular of nanowires are created by removing the number of atoms with varied diameter of nanowires (shown in fig. 1(b-d), 2(b-d), 3(b-d)) and their structural, electronic and transport properties have been investigated. All the theoretical characterizations are done in terms of formation energy per atom, bandstructure, density of states, conductance, kinetic inductance, quantum capacitance and I-V characteristics.

3.1. Stability analysis

As the stability of any structure at nanoscale is a big challenge, especially for certain device application. The stability of structure has been analysed by examining the formation energy (E_{form}) per atom for each morphology using equation (3) and reported in table 1.

$$E_{form} = \frac{E_{\text{total}} - nE_{Cu}}{n} \quad (3)$$

Where E_{total} is the total energy of the unit cell of nanowire, E_{Cu} are the energy of isolated Cu atom, n represent the total number of atoms in periodic unit cell of the nanowire.

From the Table 1, it can be observed that as the diameter of nanowire increases, the stability also increases evaluated in terms of formation energy per atom. It is also observed that, analysis with varied diameters (1 nm, 1.4 nm and 1.8 nm), the tetragonal morphology has higher stability in comparison to its other counterpart. The modelled Cu nanowire geometry follows the similar trend i.e. tetragonal > rectangular> square > triangular, with an interesting fact that the triangular morphology at 1.4 nm diameter is unstable due to bond breaking.

Table 1

Formation energy/atom (eV) of nanowires with different morphologies

Morphology	Diameter 1 nm	Diameter 1.4 nm	Diameter 1.8 nm
Tetragonal	-2.02477	-2.2195	-2.37347
Rectangular	-1.87984	-2.15021	-2.33543
Triangular	-1.6571	-1.80474	NA
Square	-1.65708	-2.07072	-2.2951

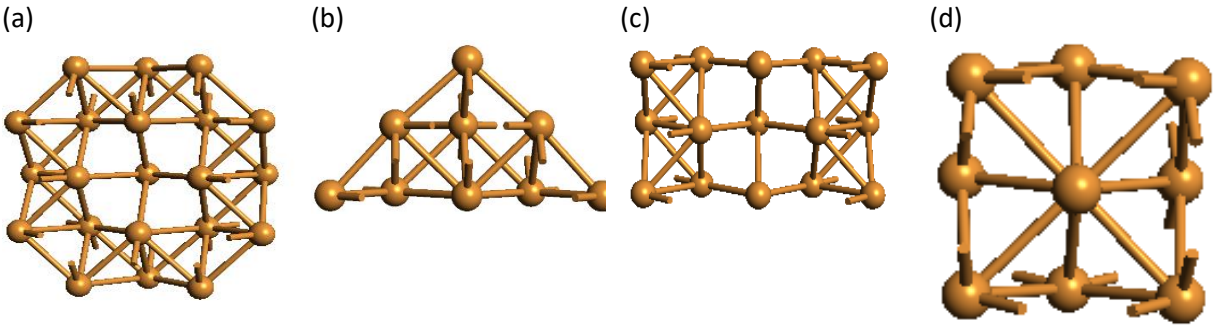


Figure 1: Optimized geometries of Cu nanowire with different morphologies at 1 nm diameter (a)Tetragonal (b) Triangular (c) Rectangular (d) Square

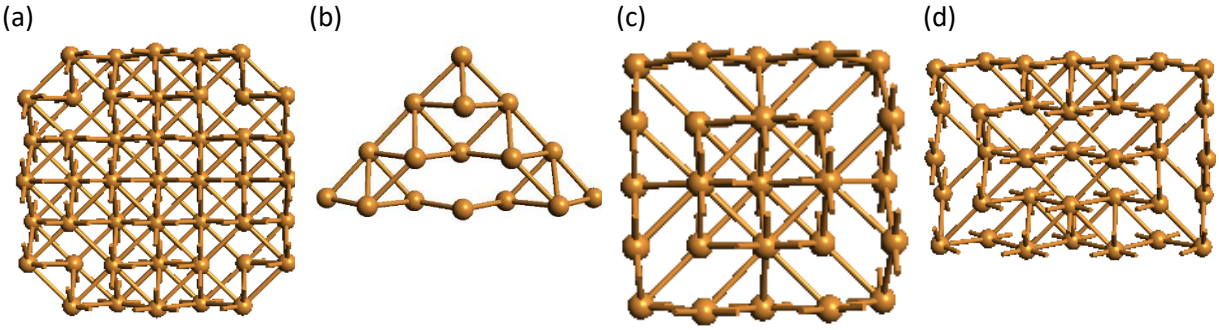


Figure 2: Optimized geometries of Cu nanowire with different morphologies at 1.4 nm diameter (a) Tetragonal (b) Triangular (c) Rectangular (d) Square

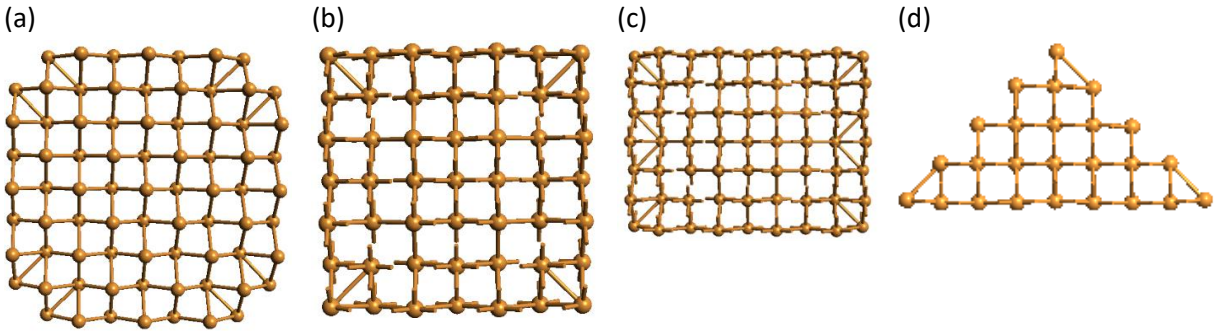


Figure 3: Optimized geometries of Cu nanowire with different morphologies at 1.8 nm diameter (a) Tetragonal (b) Rectangular (c) Square (d) Triangular

3.2. Electronic Properties

To analyze the electronic properties, the bandstructure and density of states profiles have been computed and shown in fig S1(a-d), S2(a-d), and S3(a-d) for 1 nm, 1.4 nm and 1.8 nm diameter respectively, in the supplementary information. From the bandstructure and density of states profile, it is clear that all the nanowires with different morphologies and different diameters shows metallic behaviour. As the diameter increases the metallicity also increases, number of bands at the Fermi level increases resulting in dense bandstructure with increase in diameter. From the bandstructure (E-K diagram) the Fermi velocity of each morphology has been calculated using equation (4) reported elsewhere [18]

$$V_f = \frac{1}{h}\frac{dE}{dK} \quad (4)$$

Where 'h' is the Planck constant and 'dE/dK' is the slope of the E-K diagram. From the equation (4) [18] it can be seen that Fermi velocity is proportional to the slope of E-K diagram. The Fermi velocity has been calculated at the Z point of brillouin zone. The table 2 confirms that Fermi velocity follows the order,(abbreviations:-Cu_radius in Å_Morphology) Cu_5_squ > Cu_7_rec > Cu_5_tetra > Cu_9_squ >Cu_9_rec > Cu_9 >Cu_7_tetra > Cu_7_squ > Cu_5_rec > Cu_7_tri > Cu_5_tri, which conclude that the Cu nanowires at 1nm diameter have slightly higher fermi velocity in comparison to that of 1.4 and 1.8 nm diameters, due to the higher slope of bandstructure profile of Cu nanowires. The calculated Fermi velocity will be used in the analysis of dynamical parameters.

Table 2
Fermi Velocity (m/s) of nanowires with different morphologies

Morphology	Diameter 1 nm	Diameter 1.4 nm	Diameter 1.8 nm
Tetragonal	1.86x10^4	8.38x10^3	8.48X10^3
Rectangular	5.78x10^3	1.87x10^4	9.83X10^3
Triangular	1.34x10^4	3.86x10^2	NA
Square	2.37x10^4	6.97x10^3	1.2X10^4

3.3. Transport properties

Transport properties of nanowires has been analysed using two probe approach. A two-probe model has been designed by repeating the unit cell of nanowire by 3 times and extending the channel region into the electrode region.

3.3.1. Conductance analysis

The conductance of all the varied diameter and morphologies of Cu nanowires computed by calculating the transmission spectrum. From the bandstructure analysis, it has been confirmed that as the diameter increases metallicity increases, hence conductance also increases with increasing diameter as shown in Fig. 4. From the fig. 4, it is observed that the conductance increases with increase in diameter and at each diameter 1 nm, 1.4 nm and 1.8 nm diameters, tetragonal morphologies show higher conductance in comparison to other considered morphologies. Other morphologies (rectangular and square) also show good conductance with a smaller number of atoms as compared to tetragonal morphology.

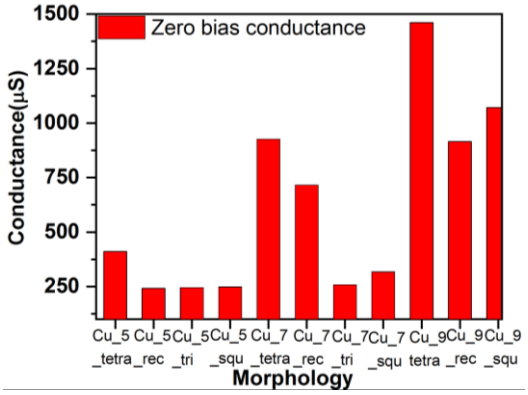


Figure 4: Zero bias conductance of different morphologies of Cu nanowires at 1 nm, 1.4 nm and 1.8 nm diameters (abbreviations: - Cu_radius in Å_morphology)

3.3.2. I-V Characteristics

Further the I-V Characteristics of the different morphologies of nanowires at different diameters have also been computed and shown in fig. 5 (a-d). The I-V characteristics of simplest natural structures i.e. Linear Atomic Chains (LAC) of all the popular metals are also computed for the comparison of results with the Cu nanowires and shown in Fig. 5(e).

At 1 nm diameter with different morphologies of Cu nanowire, current is highest in tetragonal morphology up to 0.5 V, however, beyond 0.5 V it shows decrease in current. Whereas, in case of rectangular morphology the current is highest in the voltage range 0.5 V to 1 V. The triangular and square morphologies show monotonically increasing I-V characteristics in the bias range 0-1 V.

At 1.4 nm diameter, current is lowest in triangular morphology and highest in tetragonal morphology with monotonously increasing trend. Whereas, in the rectangular morphology, current is linear with (constant slope) in the applied voltage range of 0-1 V, hence, this morphology can be a good candidate for interconnect application. Further, increasing the diameter to 1.8 nm, all the stable morphologies show monotonically increasing I-V characteristics and rectangular morphology shows linear current with almost constant slope i.e. constant resistance, hence, these can be a potential candidate for interconnect application.

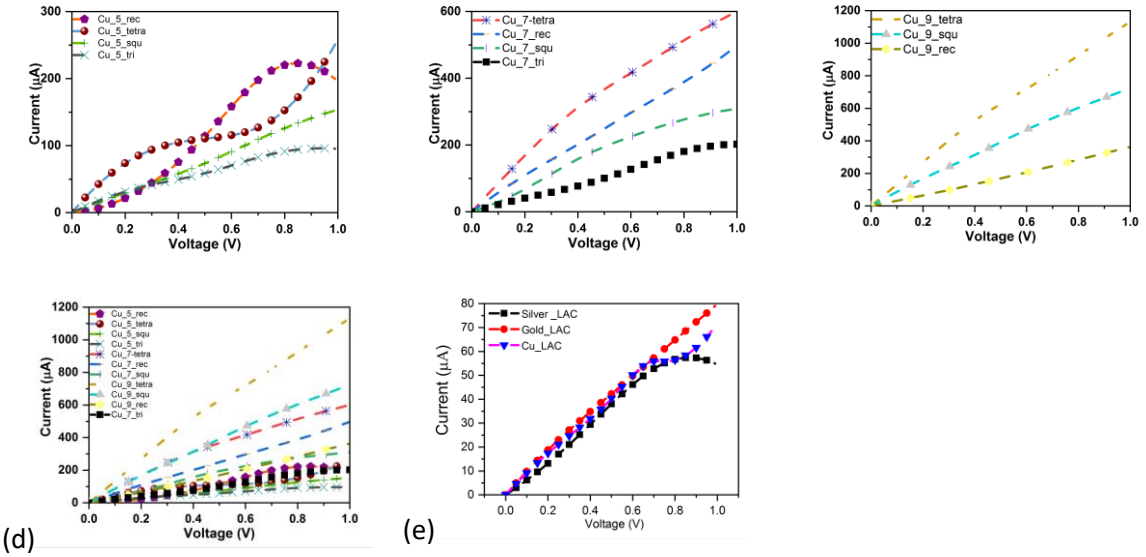
When the I-V characteristics of all the morphologies with varied diameters are being compared, then the morphologies at 1.8 nm diameters shows relatively better conductance. The I-V characteristics of these nanowires are also compared with the natural linear atomic chains of metals i.e. gold, silver and copper (as shown in fig. 5(d)), From the results it can be observed that these metallic chains show maximum current of 80 μA, whereas the tetragonal morphology of Cu nanowires have maximum current up to 1200 μA at 1.8 nm diameter, which is almost 15 times higher than the metallic LACs.

From the above observations and comparison of I-V characteristics at different diameter and different morphologies, it is observed that although the current is highest with monotonously increasing trend in tetragonal morphology of Cu nanowire at 1.8 nm diameter, suffers its linear behaviour. Rectangular morphology gives linear current with increases in the bias voltage range 0-1 V

which is desired for interconnect application. For much better understanding of the properties of nanowires, transmission eigen values or transmission channel (Nch) of each nanowires has also been computed and observed that number of channel increases with increase in diameter, which is in agreement with reports [10].

Further, the tensile stress in the periodic direction has also been computed and given in table 3. From the stress analysis, it has been observed that the proposed Cu nanowires of 1 nm and 1.4 nm have higher stress in the optimized geometries. However, the rectangular, square morphology at 1 nm diameter and rectangular, square and triangular morphology at 1.4 nm diameter, retain almost linear current voltage characteristics under stressed condition up to certain bias voltages.

(a) (b) (c)



(d) (e)

Figure 5: I-V characteristics of Different nanowire with different morphologies (a) At diameter of 1 nm (b) 1.4 nm diameter (c) 1.8 nm diameter (d) Comparison of both 1 nm, 1.4 nm and 1.8 nm diameter (e) I-V characteristics of metallic atomic chains

Table 3
Stress (eV/Å^3) in different geometries of nanowires at different diameters

Morphology	Diameter 1 nm	Diameter 1.4 nm	Diameter 1.8 nm
Tetragonal	0.01206921	4.63018388e-3	-4.08972570e-03
Rectangular	0.08139395	1.47867e-3	-0.00114492
Triangular	0.02471341	3.83135199e-3	NA
Square	0.0043406	2.62136173e-3	1.27405730e-03

3.4. Dynamical parameter analysis

For the interconnect point of view, the dynamical parameters like Resistance, kinetic inductance and quantum capacitance also play important role, especially the challenges of interconnects at nanoscale, [1, 19, 20, 21], as these parameters are responsible for interconnects delay. Interconnect delays are proportional to kinetic inductance and quantum capacitance, for lower interconnect delays these quantities should be low. Further these parameters have been computed by using the equations given by (5) and (6) for analysing the possible interconnects performance and shown in fig. 6.

The resistance of the two-probe system can be modelled by the equation (7) shown in the following [22]:

$$C_Q = \frac{4e^2}{hv_f} N_{ch} \quad (5)$$

$$L_K = \frac{h}{4e^2 v_f}\frac{1}{N_{ch}} \quad (6)$$

$$R_Q = \frac{1}{G_Q} = \frac{h}{2e^2}\frac{1}{N_{ch}} \quad (7)$$

Where 'R_Q' is defined as the quantum of resistance and 'G_Q' is quantum of conductance defined for very small lengths. 'e' represents electronic charge, 'h' represents Planck's constant, and 'N_{ch}' represents the number of transmission channels. From the equation (7) the dependence of resistance on the number of transmitting channel (N_{ch}) can be observed. Here the transmission modes/transmission channel are number of half wavelength that can travel in a given width. From the table 4, it is observed that the dynamical parameters of Cu nanowires are lowest at 1nm diameters, with poor I-V characteristics and less stability. Whereas, at 1.8 nm diameter Cu nanowire shows acceptable dynamical parameters with linear as well as monotonically increasing I-V characteristics with higher stability and hence can be defended as a potential candidate for interconnect application.

Table 4

Number of transmission channel (N_{ch}), quantum capacitances (C_Q), kinetic inductance (L_K) and resistance (R_Q) of different morphologies of Cu nanowires at different diameter

Diameters	Cu nanowire morphologies	N_{ch}	C_Q(F/m)	$L_{K(H/m)}$	R_Q(kΩ)
1 nm	Cu_Tetragonal	10	8.3087E-08	3.48E-02	1.29
	Cu _Rectangular	5	1.3369E-07	2.24E-01	2.58
	Cu _Triangular	4	4.6132E-08	1.21E-01	3.225
	Cu _Square	5	3.2604E-08	5.46E-02	2.58
1.4 nm	Cu_Tetragonal	17	3.1351E-07	4.54E-02	0.758824
	Cu _Rectangular	17	1.4049E-07	2.04E-02	0.758824
	Cu _Triangular	4	1.6015E-06	4.19E+00	3.225
	Cu _Square	13	2.8824E-07	7.14E-02	0.992308
1.8 nm	Cu_Tetragonal	46	8.3832E-07	1.66E-02	0.280435
	Cu _Rectangular	32	5.0309E-07	2.06E-02	0.403125
	Cu _Square	32	4.1211E-07	1.69E-02	0.403125

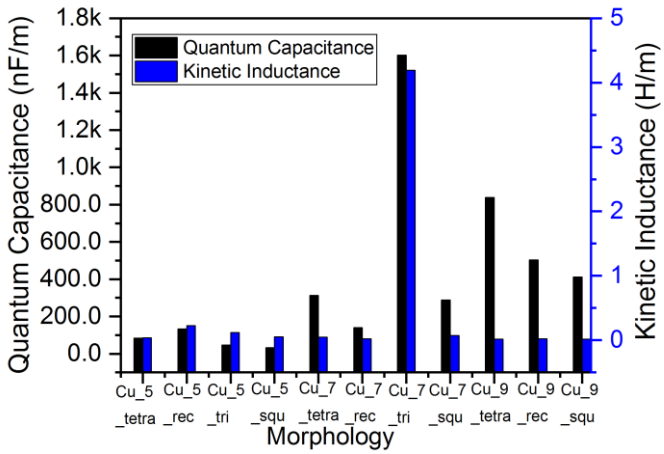


Figure 6: Dynamical parameters (quantum capacitance and kinetic inductance) of different morphology of Cu nanowires at different diameters

4. Conclusion

On analyzing the electronic and transport properties of Cu nanowires with three different diameters and four different morphologies. It is observed that the stability of Cu nanowires increases with increase in diameter. The transport of Cu nanowire with rectangular morphology at 1.8 nm diameter is better as compared to other counterparts, due to its linear I-V characteristics, with higher current than LACs as well as higher number of transmission channel. The kinetic inductance and quantum capacitances values of rectangular morphologies are 503.09 nF/m and .0206 H/m, respectively. From all the above observations it can be concluded that Cu nanowire with rectangular morphology at 1.4 nm diameter may be a potential candidate for interconnect application.

5. Acknowledgement

The authors are thankful to Computational Nanoscience and Technology Laboratory, ABV-IIITM Gwalior for providing infrastructure support and one of us S.A. is thankful to Ministry of Education for the Ph.D. fellowship.

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