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Performance and Reliability Improvement in Intercalated MLGNR Interconnects using Optimized Aspect Ratio

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ABSTRACT

In this work, aspect ratio of various intercalation doped MLGNR interconnects are optimized using a numerical approach to achieve improved performance and reliability. A numerical optimization method is presented to estimate optimized aspect ratio considering combined effects of performance, noise and reliability metrics for any arbitrary nano interconnect system. This approach is cost effective and will be extremely useful to industry for selection of aspect ratio of interconnects as it is a non-SPIICE method and reduces fabrication iterations for achieving desired performance and reliability. Our numerical method suggests that by minimizing the figure of merit (i.e. Noise Delay Power Product ($NPDP$) / Breakdown Power P_{BD} ratio), aspect ratio of $FeCl_3$ doped MLGNR interconnect is optimized at 0.987, 0.61 and 0.579 for local, intermediate and global level, respectively at 7 nm node. Comparing the optimized performance metrics in this work with the estimated metrics at prescribed aspect ratio by IRDS roadmap, delay, noise delay product (NDP), power delay product (PDP), PDP/P_{BD} ratio and figure of merit are improved by ($\sim 2\%$ and $\sim 25\%$), ($\sim 44\%$ and $\sim 50\%$), ($\sim 9\%$ and $\sim 48\%$), ($\sim 6\%$ and $\sim 48\%$) and ($\sim 49\%$ and $\sim 68\%$) for 10 μm and 1 mm long $FeCl_3$ doped MLGNR interconnect, respectively at 7 nm node. Increase in contact resistance leads to significant decrease in performance and increase in optimized aspect ratio of local $FeCl_3$ doped MLGNR interconnect. Scaling down from 10 nm to 7 nm node results in increase of optimized aspect ratio in all levels of interconnects. Even though the performance of MLGNR degrades with scaling down but when compared to copper, the performance improves with technology scaling. Finally, this study provides circuit designers a detailed guideline for selecting an optimized aspect ratio for achieving better performance, power efficiency and reliability in doped MLGNR interconnects.

Introduction

Copper interconnects have reached their performance limits due to high resistivity, grain boundary scattering effects and electromigration issues¹. Their current carrying capacity has reduced resulting in poor IC performance^{2,3}. Other alternative materials such as cobalt and ruthenium were proposed due to their higher EM reliability even though they have higher resistivity than copper^{4,5}. Graphene nanoribbons (GNRs) have proved to have high conductivity, great electromigration reliability and superior transport properties making them more suitable as an alternative interconnect material than copper^{6,7}.

Multilayer Graphene Nanoribbons (MLGNRs) are preferred over single layer graphene because of their lower resistivity. However, due to inter-sheet electron hopping, it suffers from decrease in conductivity. To solve this issue, intercalation doped MLGNRs were first proposed by Xu et. al.⁶. Sahoo et. al. analyzed the crosstalk and reliability effects in MLGNR interconnects in⁸. Liao et. al. in⁹ investigated high field transport in GNRs up to breakdown. In¹⁰, Jiang et. al. proposed $FeCl_3$ doped MLGNR for better performance and reliability to challenge copper as an interconnect. They showed that $FeCl_3$ doping is very efficient for diffusion in scaled MLGNRs, is stable at room temperature and shows excellent current carrying capacity ($> 200MA/cm^2$). But Jiang et. al. did not consider the effects of via and aggressor nets which is a pressing concern in IC design. Agashiwal et. al. in¹¹ engineered a CMOS-compatible solid-phase growth technique to yield large-area multilayer graphene on dielectric (SiO_2) and metal (Cu) substrates and subsequently demonstrating multi-level interconnects with metal vias. Also, Fischer and his team demonstrated an ingenious method in¹² to produce metallic GNRs based on the atomically precise bottom-up synthesis. These fabrication advancements have strengthened the claim of graphene nanoribbons as an effective alternative to commercial metals. Wang et. al. in¹³ also advertised graphene nanoribbon as a promising candidate for quantum electronic applications praising its high mobility and current-carrying capability. Nishad et. al. in¹⁴ optimized thickness of *Lithium* and *AsF₅* intercalated Top-Contact MLGNR (TC-MLGNR) interconnects and compared with copper and pristine interconnects. Both Jiang et. al. and Nishad et. al. have not shown any dimensional optimization for improved

Figure 1. Structural representation of doped MLGNR interconnect.

Figure 2. Electrical equivalent of MLGNR interconnect system.

performance and reliability issues which is a concerning factor to consider for commercialization of MLGNR interconnects in near-future VLSI circuits.

In this work, a numerical model is developed for optimization of aspect ratio (AR) by minimizing delay and FOM ($NPDP/P_{BD}$ ratio) for local, intermediate and global level MLGNR interconnects considering different intercalation dopants. This model is supported by the simulation results provided in section IV. Delay, $Delay/P_{BD}$, NDP and PDP , PDP/P_{BD} and $NPDP/P_{BD}$ are compared by considering AR prescribed by IRDS 2018 roadmap¹ and the optimized AR obtained from this work (for $FeCl_3$ doped MLGNR). Impact of scaling on optimization of AR is studied for two representative nodes, 7 nm and 10 nm. Effect of contact resistance on numerically optimized AR is shown which acts as an important factor in sub-10 nm technology nodes. Our study is in accordance with the trends observed in IRDS roadmap. A realistic model including the effects of crosstalk and vias is adopted which is not considered in¹⁰. Modeling of coupled three conductor line system shown in Fig. 3 is performed in Verilog-A. This proposed numerical methodology is applicable to all types of nano-interconnects making it a generalized model. We have validated this model with experimental data from¹⁰ and simulation data from¹⁴.

The remainder of the paper is organized as follows: Section II presents the equivalent electrical model of MLGNR interconnects. Section III proposes an numerical model for optimizing AR . Section IV presents the simulation results. Finally, Section V concludes this paper.

0.1 Circuit Modeling of MLGNR Interconnects - An Overview

The structural representation of MLGNR interconnect is shown in Fig. 1. Here, thickness and width are denoted by t and w , respectively and ht denotes the height of interconnect above ground plane. The spacing between two layers of MLGNR is represented by δ . The advantage of doping is that each layer of intercalated MLGNR can be understood as stacked single layer GNRs because these layers do not have any interaction with each other. So, every layer of MLGNR can be modeled as Equivalent Single Conductor (ESC) model as shown in Fig. 2.

Electrical equivalent model of MLGNR interconnect system is shown in Fig. 2 where driver and load (at active device level) are connected to the interconnect metal line through vias. Copper is chosen as the via material in this study whose dimensions are taken from IRDS 2018 roadmap.

The electrical circuit of MLGNR interconnect model consists of lumped resistance, ($R_{fix} = \frac{R_{con} + R_{qtm}}{2}$) where R_{con} is the

Figure 3. Electrical equivalent of three-line MLGNR interconnect system.

imperfect contact resistance (MLGNR to Nickel contact) which is taken as $6 \Omega - \mu m/W$ ¹⁰. R_{qtm} is the quantum resistance which is given by⁸,

$$R_{qtm} = \frac{\frac{h}{2q^2}}{N_{ch}N_{oL}} = \frac{12.94K\Omega}{N_{ch}N_{oL}} \quad (1)$$

where N_{oL} denotes the total number of layers present in MLGNR and N_{ch} represents number of conducting channels associated with each layer of MLGNR⁸.

The per unit length (p.u.l) distributed resistance of MLGNR as shown in Fig. 2 can be calculated as⁶,

$$R_{pul} = \frac{1}{G_{pul} * N_{oL}} \quad (2)$$

where G_{pul} represents the p.u.l conductance of a single layer MLGNR as expressed below⁶,

$$G_{pul} = \frac{2q^2}{h} f(i, \lambda_D, w) \frac{2w^2}{hv_F} 2KT \log \left(2 \cosh \left(\frac{E_f}{2KT} \right) \right) \quad (3)$$

where $f(i, \lambda_D, w)$ as expressed in⁶, is a function of specularly parameter where, $i = (1 - P)$, λ_D is the mean free path. P represents specularly index which is a measure of specularly of GNR edges. $P = 1$ means completely specular edges whereas $P = 0$ implies completely diffusive edges⁶.

The p.u.l capacitance (C_{pul}) is a series combination of quantum capacitance (C_{qtm}) and electrostatic capacitance (C_{elc}) as described below¹⁵.

$$C_{qtm} = N_{ch}N_{oL} \cdot \frac{4q^2}{h v_F} = N_{ch}N_{oL} \times 193.18 aF / \mu m \quad (4)$$

$$C_{elc} = C_{gnd} + C_{inter} + C_{intra} \quad (5)$$

where C_{gnd} , C_{inter} and C_{intra} are wire to ground capacitance, inter-layer capacitance and intralayer capacitance, respectively explained in detail in¹⁵.

The coupling capacitance between two interconnect lines as shown in Fig. 3 is given by⁸,

$$C_{cup} = \epsilon_0 \epsilon_r \left[1.14 \frac{t}{s} \left(\frac{ht}{ht + 2.06s} \right)^{0.09} + 0.74 \left(\frac{w}{w + 1.59s} \right)^{1.14} + 1.16 \left(\frac{w}{w + 1.87s} \right)^{0.16} \left(\frac{ht}{ht + 0.98s} \right)^{1.18} \right] \quad (6)$$

The p.u.l inductance (L_{pul}) of MLGNR is sum of p.u.l kinetic inductance (L_{kn}) and self inductance (L_{sf}) and is expressed as $L_{pul} \approx (L_{kn} + L_{sf})$ ¹⁵. L_{sf} and the electrostatic capacitance (C_{elc}) of MLGNR are considered same as of copper interconnect having equal dimensions¹⁰. Here, we have ignored the mutual inductance because the analysis is done for low/mid frequency range where effect of mutual inductance is negligible.

The capacitance model used for copper and cobalt interconnect is taken from⁸ and the resistance model is described in⁴ where 30% of the copper line is occupied by liner and cobalt has no liner.

Figure 4. Per unit length electrical resistance for (a) intermediate level ($L = 10 \mu\text{m}$) and (b) global level ($L = 1 \text{ mm}$) interconnects.

1 Formulation and Methodology

This proposed methodology provides a detailed numerical dimensional optimization procedure and is applicable to any generic nano-interconnect system. This numerical methodology can avoid costly simulators set-ups and expensive fabrication procedures for providing the dimensional design guidelines to achieve such improvement in performance. Aspect ratio (AR) optimization serves to be an effective dimensional optimization technique for achieving superior performance and reliability metrics. Here, dependence of the RLC parameters on AR is discussed in order to establish relation between AR of interconnect and its delay, noise induced effects, power consumption and breakdown power.

From $N_{oL} = 1 + \lfloor \frac{L}{\delta} \rfloor$, we get $N_{oL} \propto AR$. And N_{ch} is a function of width of the interconnect. Therefore $R_{qtm} \propto (1/AR)$ as N_{ch} is constant and N_{oL} is a function of AR .

So, $R_{pul} \propto (1/AR)$ as shown in Fig. 4 because G_{pul} is a constant here as it is a function of width and N_{oL} is directly proportional to AR .

Similarly, C_{pul} is an increasing function of AR . C_{gnd} , C_{intra} and C_{inter} collectively adds to C_{elc} , where C_{inter} can be neglected¹⁵. They can be described as functions of AR as mentioned in Equations 7 and 8,

$$C_{gnd} \propto \left[\frac{1}{AR} + \left(\frac{1}{1+AR} \right)^{1.16} + 1 \right] \quad (7)$$

$$C_{intra} \propto \left[A \cdot R^{1.7} \left(\frac{1}{1+AR} \right)^{0.7} + 1 \left(\frac{AR}{1+AR} \right)^{0.8} + 1 \left(\frac{AR}{1+AR} \right)^{3.5} \right] \quad (8)$$

The dependence of C_{cup} on AR is described as,

$$C_{cup} \propto \left[AR^{1.09} \left(\frac{1}{1+AR} \right)^{0.09} + 1 \left(\frac{AR}{1+AR} \right)^{1.18} + 1 \right] \quad (9)$$

Noise and power consumption are a function of capacitance and hence they increase with increasing AR . However, delay is the dominating factor in NDP and PDP metrics. So, the expression of NDP and PDP leads to an optimized AR value.

1.1 Delay Centric Design

Propagation delay in an interconnect is basically a function of its RC product. With increasing AR , resistance decreases as shown in Fig. 4. But the capacitance increases, therefore an optimized value of AR is obtained for minimum delay point. The transfer function for the crosstalk delay or noise evaluation in the victim net will be denoted as $H(s)$. The second-order *Pade's* expansion of the transfer function is given by¹⁶:

$$H(s) \approx \frac{1}{1 + sb_1 + s^2b_2} \quad (10)$$

The two poles of the transfer function are:

$$s_{1,2} = \frac{-b_1 \pm \sqrt{b_1^2 - 4b_2}}{2b_2} \quad (11)$$

where b_1 and b_2 are functions of R,L,Cs provided in¹⁶. They can be defined as a function of AR as follows,

$$b_1 \propto \frac{c_1}{AR} + c_2 + c_3 A.R \quad (12)$$

$$b_2 \propto \frac{a_1}{AR} + a_2 \quad (13)$$

The coefficients a_1, a_2, c_1, c_2, c_3 are described as:

$$a_1 = \frac{2R_d C_d C_l R_{qtm} \delta + LC_l L_{qtm} \delta + 2LC_l R_{qtm}^2 C_{qtm} \delta}{N_{ch} w} + \frac{LC_l \delta R_{qtm} C_{qtm}}{G_{pul} w} + \frac{L^3 C_l C_{qtm} N_{ch} \delta}{6G_{pul}^2 w} \quad (14)$$

$$a_2 = \frac{L^2 L_{qtm} C_{qtm}}{2} + \frac{L^4 C_{qtm}^2 N_{ch}^2}{24.G_{pul}^2} + \frac{L^2 R_d (C_d + C_l) C_{qtm} N_{ch}}{2G_{pul}} + \frac{L^3 R_{qtm} C_{qtm}^2 N_{ch}}{6G_{pul}} + LR_d (C_d + C_l) R_{qtm} C_{qtm} + \frac{L^3 R_d C_{qtm}^2 N_{ch}^2 w}{6G_{pul} \delta} \quad (15)$$

$$c_1 = \frac{2C_l R_{qtm} \delta}{N_{ch} w} + \frac{LC_l \delta}{G_{pul} w} \quad (16)$$

$$c_2 = LR_{qtm} C_{qtm} + \frac{L^2 C_{qtm} N_{ch}}{2G_{pul}} + R_d (C_d + C_l) \quad (17)$$

$$c_3 = \frac{LR_d C_{qtm} N_{ch} w}{\delta} \quad (18)$$

The step response, which is the inverse Laplace transform of $\frac{1}{H(s)}$, is given by:

$$v(t) = V_0 \left[\frac{1-s_2}{s_2-s_1} \exp(s_1 t) + \frac{s_1}{s_2-s_1} \exp(s_2 t) \right] \quad (19)$$

The 50% propagation delay (τ) is given by¹⁶,

$$0.5 - \frac{s_2}{s_2-s_1} \exp(s_1 \tau) + \frac{s_1 s_2 - s_1}{\exp} (s_2 \tau) = 0 \quad (20)$$

$$\tau = \frac{b_2}{b_1} \left[\ln(0.5) + \ln \left(\frac{b_1}{\sqrt{b_1^2 - 4b_2}} - 1 \right) - \ln \left(\frac{b_1}{\sqrt{b_1^2 - 4b_2}} + 1 \right) \right] \quad (21)$$

Delay in terms of AR can be defined as:

$$\tau = \left(\frac{a_1 + a_2.AR}{c_1 + c_2.AR + c_3.AR^2} \right) \left[\ln(0.5) + \ln \left(\frac{c_1 + c_2.AR + c_3.AR^2}{\sqrt{q_1 + q_2.AR + q_3.AR^2 + q_4.AR^3 + q_5.AR^4}} - 1 \right) - \ln \left(\frac{c_1 + c_2.AR + c_3.AR^2}{\sqrt{q_1 + q_2.AR + q_3.AR^2 + q_4.AR^3 + q_5.AR^4}} + 1 \right) \right] \quad (22)$$

Setting the derivative of delay with respect to AR to zero, we can obtain the optimized AR at which delay is minimum:

$$\frac{\partial \tau}{\partial AR} = 0 \quad (23)$$

$$\tau = u * v \implies \frac{\partial \tau}{\partial AR} = u * \frac{\partial v}{\partial AR} + v * \frac{\partial u}{\partial AR} = 0 \quad (24)$$

where u , v , $\frac{\partial u}{\partial AR}$ and $\frac{\partial v}{\partial AR}$ are described as:

$$u = \left(\frac{a_1 + a_2 \cdot AR}{c_1 + c_2 \cdot AR + c_3 \cdot AR^2} \right) \quad (25)$$

$$v = \left[\ln(0.5) + \ln \left(\frac{c_1 + c_2 \cdot AR + c_3 \cdot AR^2}{\sqrt{q_1 + q_2 \cdot AR + q_3 \cdot AR^2 + q_4 \cdot AR^3 + q_5 \cdot AR^4}} - 1 \right) - \ln \left(\frac{c_1 + c_2 \cdot AR + c_3 \cdot AR^2}{\sqrt{q_1 + q_2 \cdot AR + q_3 \cdot AR^2 + q_4 \cdot AR^3 + q_5 \cdot AR^4}} + 1 \right) \right] \quad (26)$$

$$\frac{\partial u}{\partial AR} = \left[\frac{a_2(c_1 + c_2 \cdot AR + c_3 \cdot AR^2) - (a_1 + a_2 \cdot AR)(c_2 + 2c_3 \cdot AR)}{(c_1 + c_2 \cdot AR + c_3 \cdot AR^2)^2} \right] \quad (27)$$

$$\begin{aligned} \frac{\partial v}{\partial AR} = & \left(\sqrt{q_1 + q_2 \cdot AR + q_3 \cdot AR^2 + q_4 \cdot AR^3 + q_5 \cdot AR^4} \cdot (c_2 + 2c_3 \cdot AR) \right) \\ & - \left[(c_1 + c_2 \cdot AR + c_3 \cdot AR^2) \left(\frac{q_2 + 2q_3 \cdot AR + 3q_4 \cdot AR^2 + 4q_5 \cdot AR^3}{2\sqrt{q_1 + q_2 \cdot AR + q_3 \cdot AR^2 + q_4 \cdot AR^3 + q_5 \cdot AR^4}} \right) \right] \end{aligned} \quad (28)$$

The constant coefficients q_1, q_2, q_3, q_4, q_5 are described here as follows,

$$q_1 = c_2^2 \quad (29)$$

$$q_2 = 2c_1c_2 - 4a_2 \quad (30)$$

$$q_3 = c_1^2 + 2c_2c_3 - 4a_1 \quad (31)$$

$$q_4 = 2c_1c_3 \quad (32)$$

$$q_5 = c_3^2 \quad (33)$$

Equation (23) can be numerically solved (here Newton Raphson is used) to obtain the optimized AR value at which delay is minimum. The initial guess value of AR was taken as 1 and the equation converged in less than 8 iterations giving optimized AR value of 1.418, 1.3329 and 1.213 for intermediate level AsF_5 , $FeCl_3$ and *Lithium* doped MLG NR interconnects, respectively. Global level AsF_5 , $FeCl_3$ and *Lithium* doped MLG NR interconnects optimized at AR of 1.06, 0.87 and 0.76, respectively.

1.2 FOM centric design

Similar approach is adopted to obtain the optimized AR at minimum FOM. We define Figure of Merit (FOM) as:

$$FOM = \tau * N_{peak} * Power / P_{BD} \quad (34)$$

where τ is given in equation (5), peak noise voltage (N_{peak}) is given by^{17,18},

$$N_{peak} = \frac{C_{cup}}{s_2} \left(\frac{s_2}{s_1 - s_2} \right) \left[\left(\frac{s_1}{s_2} \right)^{\frac{-s_2}{(s_1 - s_2)}} - \left(\frac{s_1}{s_2} \right)^{\frac{-s_1}{(s_1 - s_2)}} \right] \quad (35)$$

The total power consumed in the interconnect is mainly because of the power consumed by driver and load buffers which is given by¹⁹,

$$P_{total} = (N_{opt} + 2)(P_{switch} + P_{short} + P_{leak}) \quad (36)$$

where P_{switch} , P_{short} and P_{leak} are switching, short circuit and leakage power of a repeater, respectively. The definition of various parameters are specified in detail in²⁰. Switching power dominates the equation thus is considered for further calculation for simplicity¹⁹.

$$P_{switching} = S_f(S_r(c_d + c_l) + L_{rep}C_{pul})V_{DD}^2f_{clk} \quad (37)$$

where V_{DD} is power supply voltage, f_{clk} is the clock frequency, L_{rep} is the inter repeater stage length, S_r is the ratio of buffer size to minimum sized buffer and S_f is the switching factor, which is the fraction of repeaters on a chip that are switched during an average clock cycle. It can be taken as 0.15²⁰. P_{switch} as a function of AR can be defined as:

$$\begin{aligned} P_{switch} = & \left[\frac{1}{AR} + \left(\frac{1}{1+AR} \right)^{1.16} + AR \left(\frac{AR}{1+AR} \right)^{0.7} + \left(\frac{AR}{1+AR} \right)^{0.8} + \left(\frac{AR}{1+AR} \right)^{3.5} \right] \\ & \left[\sqrt{AR^2 + AR(1+AR)^{1.16} + AR + (1+AR)^{0.8} + \left(\frac{(1+AR)}{AR} \right)^{0.7} + (1+AR)^{3.5} + 1} \right] \end{aligned} \quad (38)$$

Table 1. Calibration of our results ($FeCl_3$ doped interconnect) with¹⁰ at 11 nm technology node

Performance metrics	Results ¹⁰	Our results
Delay ($p - sec$)	5.5	5.236
Energy ($\times 10^{-16} J$)	2.80	2.648
Power ($\mu W/mm$)	20.8	19.49

In order to have an understanding of reliability, we need to calculate and analyse the power consumed at the point where GNR interconnects breakdown and is given by^{9,21},

$$P_{BD} = gL(T_B - T_A) \left[\frac{\cosh(\frac{L}{2L_{TH}}) + gL_{TH}R_T \sinh(\frac{L}{2L_{TH}})}{\cosh(\frac{L}{2L_{TH}}) + gL_{TH}R_T \sinh(\frac{L}{2L_{TH}}) - 1} \right] \quad (39)$$

where L_{TH} is defined as the thermal healing length of the metal line²¹. Breakdown power as a function of AR can be defined as:

$$P_{BD} \propto \left[\frac{\cosh(\frac{1}{\sqrt{AR}}) + \sqrt{AR} \sinh(\frac{1}{\sqrt{AR}})}{\cosh(\frac{1}{\sqrt{AR}}) + \sqrt{AR} \sinh(\frac{1}{\sqrt{AR}}) - 1} \right] \quad (40)$$

Setting the derivative of FOM with respect to AR to zero, we can obtain the optimized AR at which FOM is minimum:

$$\frac{\partial FOM}{\partial AR} = 0 = \frac{P_{BD} \left(\frac{\partial \tau}{\partial AR} N_{peak} P_{sw} + \frac{\partial N_{peak}}{\partial AR} \tau P_{sw} + \frac{\partial P_{sw}}{\partial AR} \tau N_{peak} \right) - \tau N_{peak} P_{switch} \frac{\partial P_{BD}}{\partial AR}}{(P_{BD})^2} \quad (41)$$

This equation is numerically solved (here Newton Raphson is used) to obtain optimized AR value which minimizes the FOM. Here the initial guess value of AR was taken as 0.5 and the equation converged in 11 iterations giving optimized AR value of 0.633, 0.61 and 0.583 for intermediate level AsF_5 , $FeCl_3$ and *Lithium* doped MLGNR interconnects, respectively. Global level AsF_5 , $FeCl_3$ and *Lithium* doped MLGNR interconnects optimized at AR of 0.585, 0.579 and 0.481, respectively. And local level AsF_5 , $FeCl_3$ and *Lithium* doped MLGNR interconnects optimized at AR of 1.08, 0.987 and 0.623, respectively.

1.3 Validation With Existing Results

For calibration of the electrical model, we have estimated delay, energy and power consumption in $FeCl_3$ doped MLGNR at 11 nm technology node utilizing the models described in this work (refer section II) and compared them with results obtained by Jiang et. al.¹⁰. The comparison is shown in Table 1. All the dimensional parameters are taken from¹⁰ for comparison.

Also to validate our numerical model, comparison is shown in Table 2. Optimized AR estimated using our numerical model is compared with that obtained from existing works^{10,14}. All the dimensional parameters are considered to be same as in respective papers for a fair comparison.

2 Results and Discussion

The simulations are carried out in Cadence Virtuoso, version IC 6.1.6-64B.5004 under standard desktop environment. The coupled three conductor model as described in Fig. 3 is modeled using Verilog-A including the effects of vias and crosstalk. IRDS 2018 roadmap¹ is considered for extracting the parameters used in the calculations. 7 nm technology node is used for intermediate and global level interconnects.

Length of local level (Metal line 1), intermediate level (Metal level 2) and global level (Metal level 6) interconnects are considered as 500 nm, 10 μm and 1 mm, respectively. Fermi levels are 0.2 eV for neutral and 0.6 eV, 0.68 eV, 1.5 eV for AsF_5 , $FeCl_3$ and *Lithium* doped MLGNR interconnect. Nearly specular (i.e. $P = 0.8$) MLGNR interconnects is considered for all the calculations. Properties of various intercalated MLGNR interconnect materials are described in Table 3.

Aspect ratio is varied from 0.4 to 3.2 for intermediate level and 0.4 to 3.4 for global level interconnects. Width of local level (Metal line 1) interconnects is considered as w_{min} as specified in IRDS roadmap¹ for 7 nm and 10 nm nodes. It is taken as 1.5 times the w_{min} for intermediate level and 5 times the w_{min} for global level as specified in IRDS roadmap¹ to reduce delay and power consumption²⁴.

Table 2. Validation of our numerical model (section III) with¹⁰ and¹⁴

Optimization Parameters	Optimized AR (Existing Works)	Optimized AR (Numerical Model)
Minimizing Delay of $FeCl_3$ doped MLGNR interconnect	0.8 ¹⁰	0.88
Minimizing Delay of AsF_5 doped TC-MLGNR interconnect	0.958 ¹⁴	1.04
Minimizing Delay of <i>Lithium</i> doped TC-MLGNR interconnect	0.802 ¹⁴	0.871
Minimizing EDP of AsF_5 doped TC-MLGNR interconnect	0.479 ¹⁴	0.52
Minimizing EDP of <i>Lithium</i> doped TC-MLGNR interconnect	0.37 ¹⁴	0.415

Table 3. Electronic Properties of different intercalated MLGNR interconnects

Properties	Neutral ⁶	AsF_5 ²²	$FeCl_3$ ^{10,22}	<i>Lithium</i> ^{14,23}
Stage of Intercalation	NA	Stage 1	Stage 2	Stage 1
Mean free path (μm)	0.42	1.03	1	1.76
Fermi level (eV)	0.2	0.6	0.68	1.5
Avg layer Spacing (nm)	0.34	0.575	0.47	0.37

Figure 5. Optimized AR at minimum crosstalk induced delay in (a) intermediate level ($L = 10 \mu m$) and (b) global level ($L = 1 mm$) interconnects.

Figure 6. Optimized AR at minimum noise delay product in (a) intermediate level ($L = 10 \mu\text{m}$) and (b) global level ($L = 1 \text{ mm}$) interconnects.

Figure 7. Comparison of power consumption in interconnects at (a) intermediate level ($L = 10 \mu\text{m}$) and (b) global level ($L = 1 \text{ mm}$) interconnects.

2.1 Optimizing AR by minimizing various metrics

Fig. 5 shows the optimized AR in AsF_5 , FeCl_3 , *Lithium* doped MLGNR, neutral MLGNR, cobalt and copper interconnects. Intercalated MLGNR experiences very low delay when compared to neutral MLGNR and conventional metals irrespective of interconnect length for smaller AR. The AR for intermediate level, AsF_5 , FeCl_3 , *Lithium* doped MLGNR optimizes at 1.4, 1.4 and 1.2 for intermediate level and at 1.0, 1.0 and 0.8 for global level interconnects. Delay in neutral MLGNR and copper interconnect saturates for higher AR. Also it can be observed that copper and cobalt interconnects outperform all the doped MLGNRs after reaching an AR value of 1.4 and 1.8, respectively for intermediate level. Also, copper performs better than FeCl_3 doped MLGNR for an AR value of 2.0 or higher for global level interconnects. AR of global level interconnects optimizes at larger value as compared to intermediate level because of higher resistance as implied by Fig. 4 and this trend matches with the IRDS suggestion.

Optimized AR at minimum NDP is shown in Fig. 6. AsF_5 , FeCl_3 , *Lithium* doped MLGNR is optimized at 0.8, 0.8 and 0.6 for intermediate level and at 0.6 for global level interconnects. Intermediate level copper and cobalt cut all the doped MLGNR at AR value of 1.6 and 2, respectively. Hence, intermediate level MLGNR interconnects are more prone to noise for higher AR as compared with copper and cobalt as shown in Fig. 6 (a). But Fig. 6 (b) shows that this is not the case for global level interconnect.

Figs. 7 (a) and 7 (b) show power consumption in cobalt, copper, neutral and various doped MLGNR interconnects for intermediate and global level respectively. Switching power is the dominating factor in total power consumed by the repeaters. P_{switch} increases as AR increases. So, interconnects with large AR consume more power as inferred from Fig. 7. Cobalt interconnect consumes least power among others as it has lower capacitance and higher resistance value.

The least PDP is obtained at AR value of 1.0, 1.0 and 0.6 for intermediate level AsF_5 , FeCl_3 , *Lithium* doped MLGNR

Figure 8. Optimized AR at minimum power delay product in (a) intermediate level ($L = 10 \mu\text{m}$) and (b) global level ($L = 1 \text{ mm}$) interconnects.

Figure 9. Variation of breakdown power versus aspect ratio for $10 \mu\text{m}$ long interconnects.

interconnects but copper and cobalt beats them at even lower AR as shown in Fig. 8 (a). Fig. 8 (b) shows optimization at 0.8 which is also the crossing point after which copper exceeds all the doped MLGNR interconnect.

Fig. 9 shows the variation of breakdown power with respect to aspect ratio of interconnects. Here, we can see an increasing curve of breakdown power as the aspect ratio increases. Thermal healing length increases with an increase in AR. Breakdown power is a function of thermal healing length for intermediate level when L_{TH} is comparable to GNR length. doped MLGNRs appear to be the most reliable candidates among all as they have large breakdown power.

The optimization of AR by minimizing the metric ($Power * Delay / P_{BD}$) is shown in Fig. 10. The optimization for AsF_5 , $FeCl_3$, $Lithium$ doped MLGNR interconnects are obtained at 1.0, 1.0 and 0.6. In case of cobalt and copper interconnects, the metric decreases with increasing AR.

We have considered the metric ($Noise * Delay * Power / P_{BD}$) as the Figure of Merit (FOM) which gives a measure of performance, noise, power consumption and reliability effects. The optimization of AR by minimizing this FOM for intermediate level interconnects is shown in Fig. 11. Here, we get an optimization AsF_5 , $FeCl_3$, $Lithium$ doped MLGNR interconnects at 0.6, 0.6 and 0.5, respectively. The FOM first decreases and then saturates with increasing AR for neutral MLGNR. It keeps decreasing with increasing AR for cobalt and copper interconnects. Doped MLGNRs are far better candidates considering an overall performance and reliability aspect specially at lower AR. Although *Lithium* dopant gives the highest advantage but *FeCl₃* is explored more in experimental literature's. Fig. 12 (a) and (b) show the optimization for global and local level interconnects, respectively. FOM for global level AsF_5 , $FeCl_3$, $Lithium$ doped MLGNR interconnects are minimum at AR of 0.6, 0.6 and 0.5, respectively. And for local level it is 1.0, 1.0 and 0.6, respectively. Doped MLGNR interconnect outperforms all other candidates by having minimum FOM at all metal levels as shown in Figs. 11 and 12. Thus we propose swapping all the metal lines (conventional copper lines) with any doped MLGNR interconnect in order to achieve performance as well as

Figure 10. Optimized AR at minimum (power delay product/breakdown power) for 10 μm long interconnects.

Figure 11. Optimized AR at minimum (noise power delay product / breakdown power) for 10 μm long interconnects.

Figure 12. Optimized AR at minimum (noise power delay product / breakdown power) in (a) global level ($L = 1\text{ mm}$) and (b) local level ($L = 500\text{ nm}$) interconnects.

Table 4. Comparison of our results (considering $FeCl_3$ doped MLG NR interconnect) with IRDS 2018 Roadmap suggestion of Aspect Ratio (for copper interconnect)¹ at 7 nm technology node

Performance metrics	IRDS specs	Our results	% decrease
Intermediate level (L=10 μm)	(AR = 2.1)		
Delay ($p - sec$)	104	102 (optimized AR = 1.4)	1.92
NDP ($pV - sec$)	1.75	0.975 (optimized AR = 0.8)	44
PDP ($aW - sec$)	3.36	3.07 (optimized AR = 1.0)	8.63
PDP/ P_{BD} ratio ($f - sec$)	0.46	0.43 (optimized AR = 1.0)	6.28
NPDP/ P_{BD} ratio ($aV - sec$)	7.765	3.97 (optimized AR = 0.6)	48.85
Global level (L=1 mm)	(AR = 2.3)		
Delay ($n - sec$)	0.531	0.397 (optimized AR = 1.0)	25.2
NDP ($nV - sec$)	0.088	0.044 (optimized AR = 0.6)	50.45
PDP ($fW - sec$)	0.467	0.243 (optimized AR = 0.8)	48
PDP/ P_{BD} ratio ($f - sec$)	0.142	0.074 (optimized AR = 0.8)	48
NPDP/ P_{BD} ratio ($aV - sec$)	23.51	7.541 (optimized AR = 0.6)	68

Table 5. Impact of contact resistance on optimized AR and FOM $FeCl_3$ doped MLG NR interconnects at 7 nm technology node.

Contact resistance	Optimized AR (FOM value)		
	Local	Intermediate	Global
5 $K\Omega$	0.87 (0.567 aV-sec)	0.617 (3.97 aV-sec)	0.58 (7.541 pV-sec)
10 $K\Omega$	1.02 (0.765 aV-sec)	0.62 (4.01 aV-sec)	0.582 (7.547 pV-sec)
15 $K\Omega$	1.09 (1.07 aV-sec)	0.626 (4.07 aV-sec)	0.586 (7.556 pV-sec)
20 $K\Omega$	1.18 (1.8 aV-sec)	0.633 (4.2 aV-sec)	0.591 (7.57 pV-sec)

reliability.

2.2 Comparison with IRDS roadmap suggestion

Table 4 shows a comparison between our results (considering $FeCl_3$ doped MLG NR interconnect) and results obtained using IRDS roadmap guidelines. Here, the minimum delay, NDP and PDP are calculated and compared considering the optimized AR obtained in our work and the AR prescribed by IRDS 2018 roadmap¹. It can be observed that there is insignificant advantage in intermediate level interconnect performance but when it comes to global level, a substantial improvement is registered. This improvement in global metal line becomes more substantial because, effect of via is more dominant in global metal path. It should be noted that our results show improved performance in $FeCl_3$ doped MLG NR interconnect for optimized value of AR as compared to IRDS roadmap 2015 prescribed AR. Also the improvement in FOM metric is significant indicating lower AR should be adopted considering overall performance and reliability.

2.3 Impact of Contact Resistance

Table 5 gives us an understanding of effect of contact resistance on numerically optimized AR and FOM. Here we have varied the contact resistance from 5 $K\Omega$ to 20 $K\Omega$ ²⁵. As we can see, intermediate and global lines are not affected by it. But when it comes to local lines, increase in contact resistance leads to significant decrease in performance and increase in optimized AR. With a 75% increase in contact resistance, $\sim 66\%$, $\sim 5.5\%$ and $\sim 0.4\%$ degradation in FOM of local, intermediate and global level $FeCl_3$ doped MLG NR interconnect, respectively is witnessed. Optimized AR also experiences an increase of $\sim 26\%$, $\sim 2.5\%$ and $\sim 1.8\%$ in local, intermediate and global level, respectively. This infers that when the contact resistance increases, then in order to compensate for the decrease in performance, AR can be increased (which will lead to increase in number of layers and thus decrease in contact resistance). So the performance of MLG NR interconnects will not improve beyond a certain limit.

Figure 13. Impact of scaling on $FeCl_3$ doped MLGNR interconnect of length $10 \mu m$ (Intermediate level).

Figure 14. Impact of scaling on $FeCl_3$ doped MLGNR interconnect considering FOM at local, intermediate and global level.

2.4 Impact of Scaling

The Impact of scaling (from $10 nm$ node to $7 nm$ node) on optimized AR value of $10 \mu m$ long $FeCl_3$ doped MLGNR interconnect is shown in Fig. 13. Here, we can observe that scaling leads to an increase in optimized AR value along with degradation in performance and reliability for intermediate level interconnects following IRDS trends. When compared to copper with cobalt liner (considering IRDS suggested dimensions), Improvement in FOM of $FeCl_3$ doped MLGNR interconnect (calculated at optimized AR) is $\sim 54\%$, $\sim 93\%$ and $\sim 98\%$ at local, intermediate and global levels, respectively for $7 nm$ and for $10 nm$, it is $\sim 43\%$, $\sim 85\%$ and $\sim 91\%$ at local, intermediate and global levels, respectively. The point to be noted here is that even though the performance of MLGNR degrades with scaling but when compared to copper, the performance increases with decreasing technology node. Fig. 14 gives an understanding on effect of scaling on local, intermediate and global level $FeCl_3$ doped MLGNR interconnect considering the FOM. Scaling down from $10 nm$ to $7 nm$ node leads to degradation in FOM in $FeCl_3$ doped MLGNR interconnect by 2.6% and 22.6% in intermediate and global level, respectively even though we increase the AR from 0.4 to 0.6 . But in case of local level, FOM is improved while scaling down by 8% if we increase the AR from 0.8 to 1.0 . It is evident that with scaling there is a need of increase in AR in order to improve performance and reliability. The optimized (recommended) aspect ratio in this paper is less than 1.0 . Although scaling down from $10 nm$ to $7 nm$ leads to an increase in optimized AR, but still it is lower as compared to IRDS suggestions ($AR > 2$). Jiang et. al. have fabricated $FeCl_3$ doped MLGNR interconnect with aspect ratio of 0.4 and 0.6 ¹⁰, which strengthens our claim from manufacturing point of view.

3 Conclusion

This work focuses on numerically determining optimum aspect ratio in order to improve performance, reliability and minimize noise effects and power consumption. This approach will be extremely useful to industry for selection of AR of interconnects as it is a non-SPICE method. Our approach provides a detailed guideline for the Aspect ratio optimization and reduces fabrication

cost to achieve high performance and reliability MLGNR interconnects by reducing iterations during fabrication process for achieving desired performance. The optimized AR of AsF_5 , $FeCl_3$, *Lithium* doped MLGNR interconnects by minimizing delay is obtained at 1.4, 1.4 and 1.2 for intermediate level and 1.0, 1.0 and 0.8 for global level interconnects, respectively. Intermediate level, AsF_5 , $FeCl_3$, *Lithium* doped MLGNR interconnects have an optimized AR of 1.0, 1.0 and 0.6 and global levels have an optimized AR of 0.8 at which minimum PDP is registered. PDP/P_{BD} ratio is minimized at an aspect ratio of 1.0, 1.0 and 0.6, respectively. The FOM is minimized at an aspect ratio of 1.0, 1.0 and 0.6 for local level and 0.6, 0.6 and 0.5 for intermediate and global level AsF_5 , $FeCl_3$, *Lithium* doped MLGNR interconnects, respectively. Increase in contact resistance leads to significant decrease in performance and increase in optimized AR of local $FeCl_3$ doped MLGNR interconnect. As we scale down, the optimized AR increases with decrease in performance and reliability for intermediate and global levels. But while scaling down, increase in optimized AR leads to better FOM in local level doped MLGNR interconnect. When compared to copper (considering IRDS suggested dimensions), Improvement in FOM of $FeCl_3$ doped MLGNR interconnect (calculated at optimized AR) is $\sim 54\%$, $\sim 93\%$ and $\sim 98\%$ at local, intermediate and global levels, respectively for 7 nm and for 10 nm, it is $\sim 43\%$, $\sim 85\%$ and $\sim 91\%$ at local, intermediate and global levels, respectively. When compared to IRDS suggestion, the estimated delay in intermediate level $FeCl_3$ doped MLGNR interconnect is improved by $\sim 2\%$, NDP by 44%, PDP by $\sim 9\%$, the PDP/P_{BD} is improved by $\sim 6\%$ and FOM by $\sim 49\%$. Similarly in global level, delay, NDP , PDP , PDP/P_{BD} and FOM is improved by 25%, 50%, 48%, 48% and 68%, respectively. This study has systematically formulated a numerical optimization methodology and guideline for selecting an optimized Aspect ratio to achieve improved performance and reliability for doped MLGNR interconnects.

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Author contributions statement

B.K. and M.S. conceived the idea. B.K. designed the proposed method and conducted the simulations. Finally, B.K. wrote the manuscript based on the input from all authors. R.S. and M.S. supervised the project and reviewed the manuscript.

Competing interests

The authors declare no competing interests.

Additional information

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