Application of Artificial Neural Network Surrogate Models for Efficient Signal Integrity Analysis in Emerging Graphene-Based Interconnects

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***Abstract* — With advancing technology nodes, conventional copper on-chip interconnects are becoming more susceptible to different scattering mechanisms such as sidewall scattering, surface roughness scattering and grain boundary scattering. These scattering mechanisms increase the per-unit-length resistance of the interconnects, thereby leading to increased signal attenuation, latency, and power losses. In order to address these limitations of conventional copper interconnects, more advanced interconnect technologies such as carbon nanotubes and hybrid copper-graphene interconnects are currently being investigated. These newer technologies exploit the enhanced electrical and material properties of novel 2D materials such as graphene to improve the overall conductive properties of the interconnects. However, in order to model the electrical properties of graphene-based interconnects, highly complicated equivalent circuit models are required, the solution of which are extremely time consuming. One approach to mitigate the high computational costs of modeling such novel interconnects is by using artificial neural network models. In this article, we review the current state-of-the-art in artificial neural networks to efficiently model the transient responses of the aforementioned emerging graphene-based interconnects.**

***Index Terms* — Artificial neural networks (ANNs), design space exploration, copper-graphene interconnects, transient response, signal integrity analysis.**

I. Introduction

With the sustained device scaling below the 22-nanometer mark, on-chip copper interconnects are becoming highly vulnerable to various scattering mechanisms such as sidewall and top/bottom surface scattering, surface roughness scattering, and grain boundary scattering [1]. These scattering mechanisms collectively decrease the mean free path of electrons travelling in the copper conductors. This, in turn, significantly increases the per-unit-length (p. u. l.) resistance of the interconnects beyond their nominal bulk value. The increased p. u. l. resistance results in increased signal attenuation, greater signal propagation delay, and increased power losses [1]-[3]. Moreover, with the decrease in transistor feature sizes, the roughness of the copper conductors become more pronounced. This increase in surface roughness leads to greater effective surface area between the conductors themselves and between the conductor and ground, which in turn results in increased parasitic capacitances. The increase in the parasitic capacitance result in greater crosstalk noise and even larger signal propagation delays [3]-[5]. Therefore, copper on-chip interconnects are nearing their performance and reliability limits within the 22nm technology node.

In order to address the above limitations of copper on-chip interconnects, investigations into newer 2D materials such as graphene are currently underway [5], [6]. In particular, the following interconnect technologies based on graphene have been suggested in the literature [6].

(i) Carbon nanotubes (CNTs): Carbon nanotubes can be of two kinds – single-walled carbon nanotubes (SWCNTs) and multi-walled carbon nanotubes (MWCNTs). SWCNTs comprise of a single graphene sheet rolled up as shown in Fig. 1(a) [7] while MWCNTs consist of multiple graphene sheets rolled up as shown in Fig. 1(b) [7]. Of these, currently MWCNTs are preferred because not only can they carry higher current through the multiple graphene sheets but their growth process is also easier to control [7]. Moreover, statistically speaking, only a third of SWCNT shells in a bundle exhibits metallic conductor properties due to their chirality while the rest exhibit semiconductor properties [7]. This is in contrast to MWCNTs where due to the increasing diameters of the outer shells, almost all shells exhibit metallic conduction even if they are of semiconductor chirality [7].

Both SWCNTs and MWCNTs exploit the significantly higher mean free path of graphene compared to copper at room temperatures [8]. This ensures that CNT interconnects offer much smaller scattering resistance than their conventional copper counterparts. Moreover, MWCNTs also possess much higher current carrying capacity, higher thermal conductivity, and higher mechanical strength than copper interconnects [7]-[9]. As a result, MWCNTs can support extremely high signal speeds (in the range of THz as opposed to GHz), exhibit much smaller propagation delay (in the order of picoseconds instead of nanoseconds), and are far less susceptible to thermal and structural breakdown compared to conventional copper interconnects [9].

(ii) Graphene Nanoribbons (GNRs): Graphene nanoribbons consist of either single or multiple ultra-thin layers of graphene conductors stacked vertically [10]. Figure 1(c) illustrates the vertical stacking of multiple graphene layers to form multilayered graphene nanoribbon (MLGNR) interconnects. MLGNR interconnects, by virtue of having multiple graphene layers has far higher conductivity than single layer graphene nanoribbon interconnects. The MLGNR interconnects can be of the top contact variety (i.e., the MLGNR is connected to the electrode through a metal contact present on the top graphene layer only) or of the side contact variety (i.e., the MLGNR is connected to the electrode through a metal contact deposited over the near and far-end

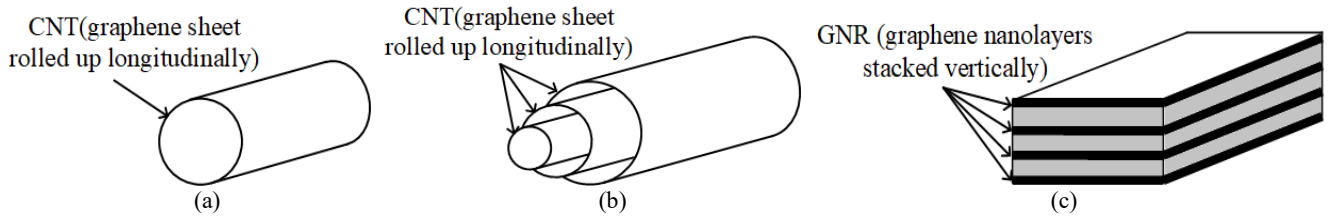

Fig. 1 Cross-sectional view of emerging graphene-based interconnects. (a) Cross-sectional view of SWCNT interconnect (b) Cross-sectional view of MWCNT interconnects (c) Cross-sectional view of MLGNR interconnects

sides of the entire stack). In these interconnects, once again, the lower scattering resistance, the higher thermal conductivity, higher current carrying capacity, and higher mechanical strength of graphene compared to copper is exploited to ensure better electrical performance [10]-[12]. Once possible drawback of MLGNRs is the possibility of inter-sheet electron conduction (i.e., current conduction in the transverse direction) that can reduce the overall current conduction along the length of the conductor (i.e., in the longitudinal direction). To mitigate this issue, intercalation doping is used to improve the Fermi level of the MLGNRs and thus, their overall conductivity.

(iii) Copper-Graphene Hybrid Interconnects: Another issue with conventional copper on-chip interconnects is the diffusion of copper ions from the conductor into the dielectric layer. This increases the dielectric conductivity and leakage losses while introducing discontinuities into the interconnects [13]. As a remedy for the diffusion of copper ions, a barrier layer of tantalum (Ta) or tantalum nitride (TaN) is generally placed around the copper conductor [13]. However, explorations into alterative barrier layer materials have led to the use of graphene nanoribbons as barrier layers around the copper interconnects [14]. Due to the lower scattering resistance of graphene compared to copper, the graphene barrier layers possess better conductive properties than the copper conductor. The presence of these barrier layers significantly lowers the equivalent resistance of the conductor plus the barrier layers [15]. Moreover, graphene barrier layers being ultra-thin, they can stop diffusion of copper ions into the dielectric without significantly reducing the effective cross-sectional area (i.e., the conductance) of the interconnect. Finally, graphene barrier layers possess good thermal stability at very high temperatures.

II. Modeling of Emerging Graphene-Based Interconnects

Despite the many advantages of graphene-based interconnects, all of these emerging interconnects are highly sensitive to fabrication process variations and manufacturing tolerances [16]. Therefore, thorough and detailed design space exploration, design optimization, and variability analysis of such interconnects are required as a precursor to their fabrication. Typically, such analyses of interconnects are performed using thousands of repeated SPICE simulations of the interconnects [16]. The key problem with the SPICE simulations is that the equivalent circuit models of MWCNT, MLGNR, and copper-graphene hybrid interconnects are highly complicated and cumbersome, thus making even a solitary SPICE simulation computationally prohibitive, let alone thousands of simulations. In the following subsections, the details regarding the circuit models of different emerging interconnects are discussed.

A. Equivalent Circuit for MWCNT and MLGNR Interconnects

The MWCNT and MLGNR interconnects are longitudinally divided into small sections where each section is represented using equivalent lumped resistance-inductance-conductance-capacitance (RLGC) circuit elements as shown in Fig. 2. It is noted from Fig. 2 that the equivalent circuit models of these interconnects consist of individual RLGC models of each conducting shell or nanoribbon making up a conductor which are then coupled together using parasitic circuit elements (e.g., the tunneling conductances, quantum capacitances, and inter-shell capacitances) [7], [17]. Therefore, for realistic MWCNT and MLGNR interconnects consisting of a large number of conducting shells or nanoribbons, the overall equivalent circuits are usually massive. These massive equivalent circuits are directly represented in SPICE using a massive coupled modified nodal analysis (MNA) system of equations. This massive MNA system of equations is then directly solved in SPICE to derive the transient response of the near and far-ends of the interconnects - in other words, the signal integrity quantities of the interconnects are probed in SPICE. Unfortunately, the solution of these massive coupled system of MNA equations require massive computational time and memory costs.

B. Equivalent Circuit for Hybrid Copper-Graphene Interconnects

Hybrid copper-graphene interconnects include a combination of the electrical properties of both copper and graphene. The effective electrical characteristics of each hybrid conductor can be expressed using the Telegrapher's partial differential equations and the effective p. u. l. parameters [18]. Importantly, the effective p. u. l. parameters of such heterogeneous interconnects are extracted from a quasi-TEM approximation of the interconnect structure,

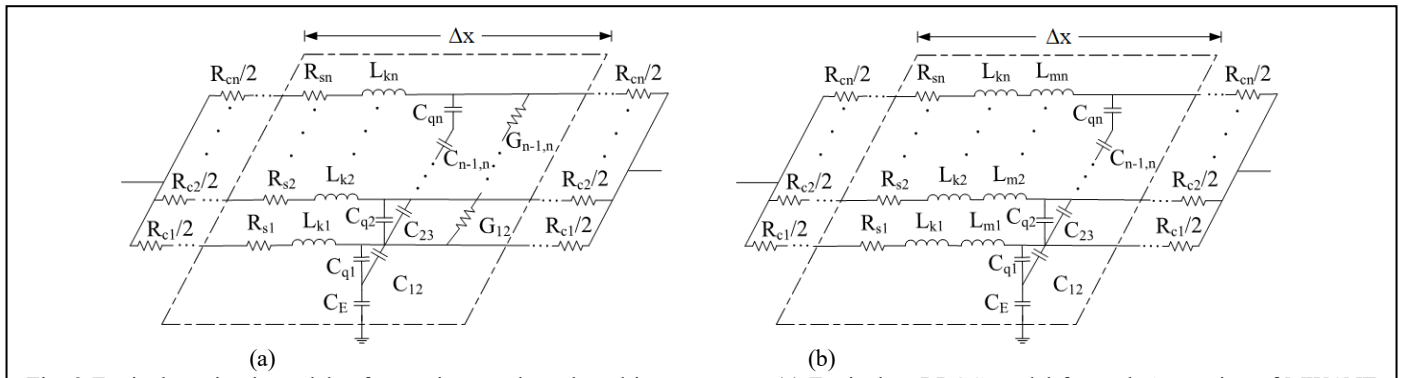

Fig. 2 Equivalent circuit models of emerging graphene-based interconnects. (a) Equivalent RLGC model for each Δx section of MWCNT interconnects (b) Equivalent RLGC model for each Δx section of MLGNR interconnects

usually using full-wave electromagnetic (EM) solvers. For example, a quasi-static 2D EM solver based on the finite element method (FEM) technique is used to calculate the p. u. l. capacitance parameters of the interconnects while a quasi-static 3D EM solver using the method of moments (MoM) technique is used to calculate the p. u. l. inductance parameters [19]. Once, the p. u. l. parameters are extracted, multiconductor transmission line (MTL) models can be used to represent the hybrid interconnects in a SPICE framework. These MTL models can be directly solved in SPICE to probe the transient response of the network. Unfortunately, for hybrid interconnects, the very first step of extracting the p. u. l. parameters using full-wave EM techniques is extremely time consuming [20], [21]. Thus, even for hybrid copper-graphene interconnects, performing SPICE-based design space exploration and variability analysis of these interconnects still remains a major computational challenge.

III. Application of Artificial Neural Networks for Signal Integrity Analysis

A. History of Application of ANNs to Interconnect Modeling

One of the most effective ways to reduce the computational cost of modeling, simulating, and analyzing high-speed interconnects is by using surrogate models. Surrogate models or metamodels are closed-form mathematical expressions that are trained to emulate the input-output relationship of a system under test [22]. Once trained, the metamodels act as analytic functions that are far more numerically efficient to solve compared to simulating the system under test based on the fundamental governing physics equations as done in conventional EM and circuit solvers (e.g., SPICE). These metamodels can be stored and repeatedly used to probe the output results for different values of the input parameters. Hence, their advantage over conventional physics-based solvers is even more profound where the system under test needs to be simulated repeatedly (e.g., in design explorations, parametric sweeps, or Monte Carlo bases statistical analysis).

Recently, machine learning (ML) techniques have garnered significant interest for their ability to construct metamodels that can emulate highly nonlinear input-output relationships [22], [23]. There currently are a variety of machine learning techniques available such as such as artificial neural networks (ANNs), support vector machines (SVMs), and Gaussian processes (GPs) [24], [25]. All of these techniques have already been applied to a variety of modeling and simulation problems within the general field of electronic design automation as well as the more specific field of electronic packaging and interconnect modeling [26]-[29].

Of the various ML techniques, ANNs have had a rich history of being used to model the performance of a variety of interconnect structures including but not limited to conventional copper interconnects [20], [21]. Indeed, ANN metamodels have already been reported for extracting the p. u. l. parameters of copper interconnects as analytic functions of the geometrical, physical, and material parameters of the interconnect structures [26], [27]. These metamodels being closed-form in nature, they can analytically predict the p. u. l. parameters of the interconnects for any arbitrary values of the geometry and layout at a fraction of the time and memory costs required by full-wave EM solvers [20], [21]. Similarly, in the works of [30], recurrent neural networks (RNNs) predicting the transient response of copper interconnects as analytic functions of the geometrical, physical, and material parameters of the interconnects have also been developed. In these works, it is possible to analytically predict the transient response and from them, directly extract the signal integrity quantities of interest while avoiding solving a large system of MNA coupled equations in SPICE at high time costs. In the following section, we will look at how ANNs can be adapted for modeling and simulating the transient response of emerging graphene interconnects.

B. ANNs for Emerging MWCNT and MLGNR Interconnects

The SPICE simulation of MWCNT and MLGNR interconnects involve solving a massive system of coupled MNA equations corresponding to the large RLGC circuit models of Fig. 2. The outputs of interest of such SPICE

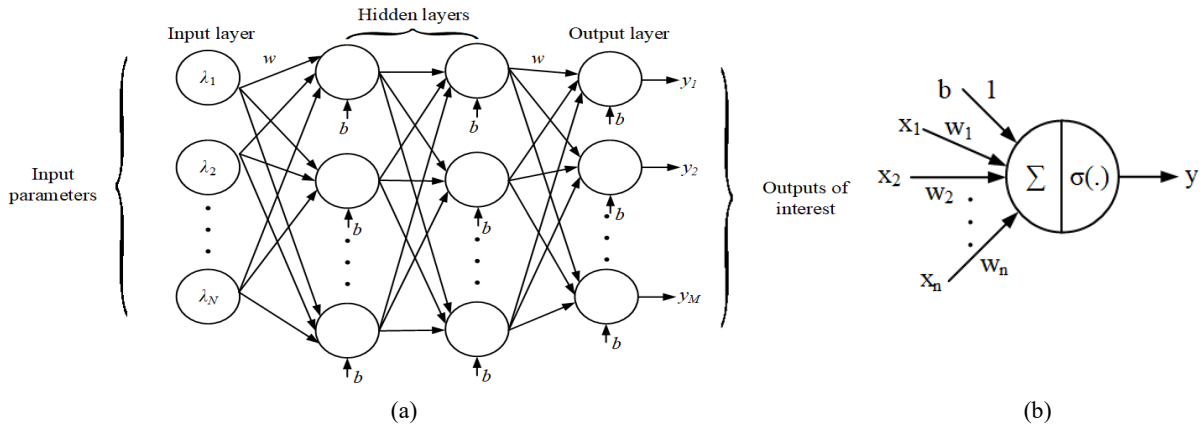

Fig. 3 (a) Basic MLP architecture of ANNs (b) Single neuron from the MLP architecture

simulations are the transient near-end and far-end responses of the interconnects. From the transient responses, signal integrity (SI) quantities such as 50% signal delay, peak crosstalk, eye height and eye width are extracted. Note that the values of all of these SI quantities will change as the values of the geometrical, material, and physical parameters of the interconnects change. Therefore, ANNs can be used to emulate the relationship between the geometrical, physical, and material parameters of the interconnects (inputs) and the corresponding values of the SI quantities (outputs).

In order to emulate the above input-output relationships, the architecture of ANNs take the form of multilayer perceptrons (MLPs) as shown in Fig. 3(a). In this architecture, the first layer on the left-hand side is called the input layer. This input layer accepts the normalized values of the geometrical, material, and physical parameters of the interconnects. These values are then processed and propagated through multiple layers of neurons referred to as the hidden layers (see Fig. 3(a)). Finally, the outputs of the hidden layers are again processed and propagated through the rightmost layer (i.e., the output layer) to yield the values of the SI quantities.

The power of ANNs arises from the nonlinear processing ability of each individual neuron in the MLP architecture [26], [28]. To better explain this, an arbitrary neuron from the MLP architecture is showed in detail in Fig. 3(b). The input to the neuron is the linear combination of the outputs of the previous layer with an added bias term. This linear combination term is then passed through a nonlinear activation function. This processing of the linear combination term through the activation function allows the ANN to be able to emulate highly complex nonlinear input-output relationships. Common activation functions include the hyperbolic tangent function, sigmoid function, arctangent function besides possible user defined functions [26]. The output of the ANNs depend on the values of the linear weights and bias terms used in each neuron. Therefore, the values of these weights and bias terms are tuned such that the error between the values of the SI quantities predicted by the ANN and the true values obtained from SPICE simulations are minimized over the entire input parameter space. This task of tuning the ANN weights and bias terms is referred to as the training of the ANN. The training of the ANN can be performed using well-known optimization algorithms (e.g., stochastic gradient descent and Levenberg-Marquardt with back-propagation [26], [28].

It is observed that in order to train the ANN, the true values of the SI quantities of the MWCNT or MLGNR interconnects have to be first extracted from repeated SPICE simulations. These true values are necessary to calculate the error loss term of the ANN which is to be minimized. The cost of the required repeated SPICE simulations of the interconnects will be typically high. However, this task needs to be done only once – in effect, the associated time cost is a one-time cost. Once the ANN has been trained, the input-output relationship modeled by the ANN will allow us to directly (i.e., analytically) predict the values of the SI quantities for any arbitrary values of the geometrical, material, and physical parameters of the interconnects at negligible computational time and memory costs compared to SPICE simulations.

C. ANNs for Hybrid Copper-Graphene Interconnects

For hybrid copper-graphene interconnects, the main computational effort is in extracting the p. u. l. parameters of these heterogeneous structures using full-wave EM solvers. Here, ANNs of the MLP architecture can be used to reduce this computational effort. For this purpose, the inputs of the ANNs will remain the same as before – the normalized values of the geometrical, material, and physical parameters of the interconnects. However, the outputs will now change to the p. u. l. resistance, inductance, conductance, and capacitance parameters of the interconnects including all mutual inductance terms and coupling capacitance terms. As in the case of MWCNT and MLGNR interconnects, the ANNs can be trained in a similar manner with the exception being that the error function that is to be minimized will now be the error between the p. u. l. parameter values predicted by the

ANN and the true values extracted from full-wave EM solvers spanning the entire input parameter space [20], [21]. Therefore, repeated simulations of the full-wave EM solver will be required to extract the true values of the p. u. l. parameters when calculating the error function. Just as before, this will be a one-time cost.

Now, once the ANN has been trained to accurately emulate the relationship between the geometrical, material, and physical parameters of the interconnects and the corresponding p. u. l. parameters, it will facilitate the repeated yet extremely fast prediction of the p. u. l. parameters followed by SPICE simulation of the MTL model of the hybrid interconnects during design space explorations, iterative design optimization, and Monte Carlo based statistical analysis. Importantly, during such analysis, the time-consuming simulations of the structure using full-wave EM solvers will be avoided entirely. One disadvantage of the above approach is that while the need for using the full-wave EM solvers will be eliminated, we will still need to perform the repeated SPICE simulations of the MTL models of the interconnects. This disadvantage can be eliminated if the ANN is modified to directly emulate the transient response of the interconnects instead of the intermediate p. u. l. parameters. This is possible if the MLP architecture is replaced by a recurrent neural network (RNN).

V. Conclusion

As new interconnect technologies such as those based on graphene (e.g., MWCNT, MLGNR, and hybrid copper-graphene interconnects) emerge, the SPICE-based transient analysis of such interconnects will be significantly more computationally intensive than for conventional copper interconnects. This is because the emerging interconnects possess significantly more complicated structures involving multiple conducting shells and nanoribbons not seen in conventional copper interconnects. In such scenarios, machine learning techniques in general and ANNs in particular have the capacity of emulating the nonlinear relationships between the geometrical, material, and physical parameters of the interconnects and its transient responses. These ANNs can be used as analytic functional maps to precisely predict the transient responses of the emerging interconnects for any arbitrary values of the geometrical, material, and physical parameters without resorting to time consuming SPICE or full-wave EM simulations. As a result, ANNs will enable the extremely fast design space exploration, optimization, and statistical analysis of the interconnects at a small fraction of the expected time costs.

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