Carbon-based nanoelectronics: nanoICs with fullerenes

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Abstract - Carbon-based electronic nanodevices can be utilized in interfaced, functional three-dimensional complexes that are able to perform computations, memories, information processing and other functions. The density of nanoICs fabricated using nanotechnology by millions of times exceeds the density of most advanced CMOS-based ICs. This paper reports design and analysis of nanoICs with fullerenes that proposed to be utilized as multi-terminal electronic nanodevices. Novel concepts to perform modeling, analysis and design of electronic nanodevices and 3DnanoICs are reported. High-fidelity modeling, heterogeneous simulation and data-intensive analysis are performed addressing 3DnanoICs CAD.

I. INTRODUCTION

Revolutionary carbon-based technology emerges in nanoelectronics. Optimistic evolutionary developments in scaling down microelectronics predict that FETs may be scaled down to 100 nm in the total size by 2010 if the 18 nm gate-length projection will be met. Currently, 65 nm technology is emerging to fabricate high-yield planar (two-dimensional) multi-layered ICs with billions of transistors on a single lcm² die. However, revolutionary developments are required utilizing nanotechnology. NanoICs will utilize novel nanodevices. Microelectronics can be expanded to nanotechnology-enhanced electronics which is not nanoelectronics. Electronic nanodevices and nanoICs are based on novel phenomena and unique functional utilization of those phenomena observed at nanoscale.

Devising design and fabrication of novel affordable high-yield nanoelectronics are critical. The projected progress towards nanoelectronics is reported in Figure 1 [1]. The power- and size-centered version of the Moore law for room-temperature mass-produced electronics is shown. Due to imminent fundamental and technological limits, microelectronics cannot sustain the envisioned rate [1, 2]. Microelectronics will be supported by the nanotechnology-enhanced microelectronics that will be replaced by nanoelectronics. High-yield nanoelectronics is projected to enter the market in 2010 ensuring superior performance, high-yield, affordability, multiplicity and robustness.

Tremendous progress has been accomplished in the fullerene-centered nanoelectronics [1, 2]. Utilizing 1 nm fullerenes as multi-terminal devices, there are \(1 \times 10^9\) networked and functional fullerenes can be packed in 1 mm³ volume. These 1,000,000,000,000,000,000 enhanced-functionality nanodevices packaged in the 1 mm³, as appropriately interfaced, can ensure the implementation of novel three-dimensional nanoIC architectures derived using logic design [1]. The fundamental developments and CAD must be coherently integrated with technologies.

As electronic nanodevices, fullerenes exhibit novel phenomena that can be uniquely utilized. Fullerenes and resulting 3DnanoICs are examined in this paper. There is a lack of the fundamental and applied research studying fullerenes as electronic nanodevices for nanoICs, and design of 3DnanoICs have not been thoroughly addressed. We report novel results in design, modeling, analysis, simulation and CAD.

II. FULLERENES FOR NANOELECTRONICS

Endohedral and doped fullerenes exhibit semiconducting properties at room temperature. Different techniques to fabricate interconnected fullerenes are reported in [1, 3]. It is possible to substitute carbon with the heteroatoms (alkali, alkaline earth metals, transition metals, etc.) in the carbon cages. For example, silicon fullerene complexes Si@C₆₀ have been demonstrated. Boron and nitrogen doped heterofullerenes C₆₀-B(N) can be utilized in the fullerene-centered nanoelectronics [1]. The B-N bond lengths are in the range from 1.4 to 1.5 Å. The C-C bond distance in fullerenes varies from 1.4 to 1.47 Å. For example, the C-C, C-N, C-B and B-N distances in the C₆₀B₅N are 1.45, 1.43, 1.4 and 1.41 Å. Other heterofullerenes that have been examined are C₆₀N₂₆, C₆₀B₁₂, etc. Those and other doped fullerenes that are kinetically stable can be uniquely utilized. The energy bandgaps, HOMO and LUMO energy levels, atomic charges and other important data are reported in [1-10].

The endohedral mono-, di-, tri- and other high-order metallofullerenes M@C₆₀ are fabricated by the direct-current discharge. For La@C₆₀ core rods are packed with a mixture of graphite and either pure La, La₂O₃, or other composite rod under helium flow at high pressure. The graphite rods can be filled with La₂O₃ with a metal concentration doping from 1 to 5%. The electronic configurations of metallofullerenes are distinct [1], and for Sc@C₆₀ we have Sc⁺⁺ @ C₁₂, Sc⁺⁺⁺ @ C₁⁴⁺ and Sc⁺⁺⁺ @ C₁⁴⁺. The scandium cluster is encapsulated in the C₆₀ carbon cage with the average inner fullerene diameter 5.3 Å. The outer Sc@C₆₀ metallofullerene diameter is 8.28 Å. The distances between the center of the Sc, trimer and carbon atoms, and the Sc-C distances are 3.4 Å and 2.52 Å. Other functional fullerenes such as Er₂Sc₂N@C₆₀, Er₂Sc₅N@C₆₀, Er₃N@C₆₀ as well as other lanthanide derivatives R₂@[N@C₆₀] and R₁@[N@C₆₀] exist. Fullerenes react with the carbon...
derivatives resulting in functional fullerenes complexes, for example $\text{Sc}_3\text{N}@\text{C}_{80}$-$\text{ClO}_3$-$\text{O}$. Fullerenes, utilized as functional multi-terminal electronic nanodevices, can provide one with a viable solution for nanoelectronics. However, fullerenes have not been coherently examined and characterized. The electronic structure of fullerenes is very complex, and fundamental - applied - experimental research must be performed with the ultimate objective to model, analyze and assess fullerenes at the devise-level in future nanoICs. The proposed concept in mathematical modeling is based on high-fidelity modeling of complex phenomena using quantum mechanics integrated with tensor calculus and numerical techniques. As fullerenes are assessed, the efforts are directed to develop the CAD components for nanoICs.

The interactive CAD is aimed to fully support synthesis, analysis, design and optimization of 3DnanoICs [11]. This CAD is based on unique phenomena, enhanced functionality, novel architectures and advanced topologies. Correspondingly, coherent synthesis, analysis, design and optimization paradigms must be developed. As shown in Figure 2, the core CAD themes are integrated within four domains: 1) devising (synthesis), 2) modeling-analysis-simulation, 3) design-optimization, and 4) fabrication. The synthesis of nanoICs and electronics nanodevices is represented as a bi-directional X-flow-map [1].

III. MODELING OF FULLERENES

Fundamental and applied research, as well as experiments, have been carried out to understand and utilize unique electronic, optical and chemical properties of individual molecules, molecular assemblies, clusters and fabrics. These developments range from application of the Schrodinger equation and density functional theory to spectroscopy. Electronic nanodevices are examined using the quantum mechanics and other methods. Many paradigms are based on the energies and examine kinetic and potential energies, as well as Fermi energy ($E_F$), energy level broadening ($E_B$) and charge density [1, 12-14].

Figure 3 illustrates a multi-terminal electronic nanodevice that comprise the carbon molecule with atomic interconnects to sources and drains. We consider the application of the Schrödinger concept [1] and the Green function method [1, 12-14]. Using notations reported in [1], we have the following expression for the Green function

$$G(E) = (E - E_v + iE_B)^{-1}.$$ 

The total number of electrons $N$ and $N_0$ are found using the trace operator as $N = \text{tr}(\rho S)$ and $N_0 = \text{tr}(\rho_{\text{equilibrium}} S)$. Using the overlap identity matrix $S$, the Green function is found to be

$$[G(E)] = \frac{1}{2\pi} \sum_{\nu, \mu} \int (E, \nu V_{\nu\mu}) [G(E)] [E_{\nu\mu}, (E)] [G^*(E)] dE.$$ 

The current between two junctions is found to be

$$I = \frac{2e}{h} \int \text{tr}(E_{\nu\mu} G(E_{\nu\mu}) G^*(E_{\nu\mu})) [f(E_v, V_{\nu\mu}) - f(E_v, V_{\nu\mu})] dE.$$ 

Taking note of the Green function, the density of state $D(E)$ is given as $D(E) = \frac{1}{\pi} \text{Im}(G(E))$. The non-equilibrium density matrix is

$$[\rho(E)] = \frac{1}{2\pi} \sum_{\nu, \mu} \int (E, \nu V_{\nu\mu}) [G(E)] [E_{\nu\mu}, (E)] [G^*(E)] dE.$$ 

Using the transmission matrix $T(E) = \text{tr}(E_{\nu\mu} G(E) E_{\nu\mu} G^*(E))$, the current between two junctions is found to be

$$I = \frac{2e}{h} \int \text{tr}(E_{\nu\mu} G(E) E_{\nu\mu} G^*(E)) [f(E_v, V_{\nu\mu}) - f(E_v, V_{\nu\mu})] dE.$$ 

The current–voltage characteristics for fullerenes are obtained by self-consistently solving the coupled transport - capacitive Poisson's equation [1, 12-14]. We also applied the Schrödinger equation

$$E(x, y, z, t) \psi(x, y, z, t) = -\frac{\hbar^2}{2m} \nabla^2 \psi(x, y, z, t) + \Pi(x, y, z, t) \psi(x, y, z, t)$$

in order to perform data-intensive analysis of fullerenes.

The Schrödinger equation can be solved utilizing numerical methods, and the first difference for Laplacian is used. The Hamiltonian in the Schrödinger equation $H \psi = E \psi$ is expressed using the molecular energetics, electron effective mass, interatomic distances, etc. For $H$, the eigenvalues and eigenvectors can then be calculated numerically using MATLAB. These values represent the energies of the waves and their corresponding wavefunctions. The probability of finding an electron within a volume $V$ is $\int \psi^*(r) \psi(r) dV$. Using the probability, the $I-V$ and $G-V$ characteristics result. These results are demonstrated through illustrative examples. $G_{6,2}(\text{BN})$, Heterofullerene and $N@C_{59}$ Endohedral $N@C_{60}$ Fullerene. Consider these fullerenes that offer promising technological solutions for nanoICs. Using the specified potential barrier profiles for different values of $V_g$, $\text{sc}$.
and $V_{ds}$, the $I-V$ and $G-V$ characteristics are obtained. Some numerical results are reported in Figure 4.

![Figure 4. I-V characteristics for fullerenes](image)

IV. MODELING OF 3D-NANOICs AND NANNETWORKS

We develop the modeling concept for 3D-nanoICs that is based on nonlinear model of $N-K-M$ nanonetworks that integrate multi-terminal electronic nanodevices. NanoICs are defined as a 3D array of $N-K-M$ distinct nanodevices arranged in a spatial grid. Thus, nanoICs integrate $N-K-M$ nanodevices $B(i,j,g)$ in the locality $L(i,j,g)$ satisfying

$L(i,j,g) = \{l(n,k,m), 1 \leq n \leq N, 1 \leq k \leq K, 1 \leq m \leq M\}$

The state-space model with constrained control and outputs is given by a set of equations

1. state 3DnanoICs equation

$$x_{ij}(t) = \sum_{l(i,j,g), \epsilon(g)} F_i(t, x_{ij}, r_{ij}, d_{ij}, u_{ij}),$$

$$u_{ij}(t) \leq u_{ij} \leq u_{ij,\text{max}},$$

$$y_{ij}(t) = x_{ij,\text{max}},$$

2. output 3DnanoICs equation

$$y_{ij} = C(t, x_{ij}), y_{ij,\text{min}} \leq y_{ij} \leq y_{ij,\text{max}},$$

3. event 3DnanoICs equation

$$e_{ij} = E(t, x_{ij}, y_{ij}, r_{ij}, d_{ij}, u_{ij}, F_i, F_{ij}, C),$$

where $t$ is the time, $x_{ij}, y_{ij}, r_{ij}, d_{ij}$ are the state, control, output, input, disturbance (noise) and event vectors; $F_i, F_{ij}$ and $C$ are the nonlinear parametric-template maps that are defined by the devices dynamics (transient and steady-state behavior), nanoICs architecture, aggregation and topology, as well as parameter variations $y_{ij}$; $E$ is the nonlinear events map that is a function of the nanonetwork variables and parametric-template maps.

V. 3D-NANOICs CAD

The proposed 3DnanoICs CAD, shown in Figure 5, must be developed to attain a feasible cost-effective solution in coherent synthesis, design and analysis of nanoICs. This CAD must guarantee rapid prototyping with performance/assessment analysis and outcome prediction.

Rapid prototyping and technologies assessment will be supported without costly and time consuming design - fabrication - test - characterize - assess - refine - optimize solution. The CAD will provide the concurrent support to fundamental, applied and experimental research transfer and technologies developments.

![Figure 5. 3D-NanoICs CAD will solve fundamental, applied, and experimental problems for 3D-NanoICs with technology transfer](image)

VI. CONCLUSIONS

Proposed electronic nanodevices and 3DnanoICs allow one to increase the computing speed by a factor of millions compared with the existing CMOS-based ICs. Carbon-based electronic nanodevices ensure super-high density, superior bandwidth, high switching frequency, low power, and other desired characteristics. Novel methods to perform three-dimensional synthesis, design and analysis were addressed and developed. New synthesis, design and optimization fundamentals for high-performance nanoelectronics were developed from the system-level addressing technological considerations.

REFERENCES