Analysis of Graphene, Molecular Wires and Inorganic Materials For Nanoelectronics and Low Power Integrated Circuits

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ABSTRACT

This paper studies some emerging and prospective materials along with possible solutions for envisioned high-performance nanoscale microelectronic devices and integrated circuits (ICs). To assess and evaluate the performance of *microscopic* and *macroscopic* (nanoscale and microelectronic) devices, we apply experimental results, perform quantum mechanical analysis, and use advanced numeric methods. We examine graphene, graphite and molecular chains (wires) which are, to some extent, compatible with well-developed silicon technology, processes and materials. Quantum mechanics is used to assess energetics, statistics and other quantitative quantities of interest for graphene, graphite and molecular chains.

***Keywords*:** Graphene, graphite, molecular wires

1. INTRODUCTION

Novel materials have extensively studied from various prospects, such as [1]:

1. Fundamentals and characteristics as related to device physics, performance and capabilities;
2. Compatibility and practicality;
3. Yield and affordability;
4. Fabrication processes and technologies (microelectronic, molecular and other), such as lithography, patterning, self-assembly, deposition, packaging, etc.

Materials must suit prospective and emerging devices in terms of device functionality, performance, density, interconnect, etc. Due to the material- and technology-defined scaling limits for silicon microelectronics [1], it can be expected that graphite layered compounds and graphene may provide some opportunities for microelectronics. These solutions may advance the planar conductor-insulator-semiconductor device topologies, as well as enable field-effect device physics of electrostatic solid-state devices. The following features may be achieved:

1. Mobility enhancement;
2. High carrier velocity;
3. High switching frequency;
4. Low power and losses;
5. High current density;
6. High thermal conductivity;
7. Multiple gating, etc.

2. MATERIALS AND SOLUTIONS FOR *MICROSCOPIC* AND *MACROSCOPIC* DEVICES

Graphene and graphite are the single- and multi-atomic planar layers of sp^2 carbon atoms with bond length in graphene ~0.142 nm [2]. Different processes and techniques, including epitaxial grow and chemical vapor deposition on various substrates, are available to make graphene, graphates and various compounds. Graphene on silicon carbide, metal and other substrates can be patterned using well-defined processes.

The electronic *macroscopic* properties of certain multilayered epitaxial graphenes and graphates are identical to graphite due to symmetry. In graphite, each carbon atom uses 3 of its 4 outer energy level electrons in covalently bonding to three other carbon atoms in a plane. Each carbon atom contributes one electron to a delocalized system of electrons which form the covalent bonds. The *delocalized* electrons are able to propagate throughout the plane. Thus, graphite conducts electricity along the planes of carbon atoms, but does not conduct in a direction at right angles to the plane.

The properties of graphene and graphate may be controlled using various dopants. These materials may ensure *material-by-design* capabilities through *engineered* composition, structure, morphology, properties, etc. Figure 1 documents a multilayered graphene compound with Ga^+. In addition to the *first-stage* layers with various +1 cations, other dopants can be used. One can affectively *engineer* complex graphene compounds which exhibit weak or strong complexing for carbon π-electrons, orbital mixing and other desired features.

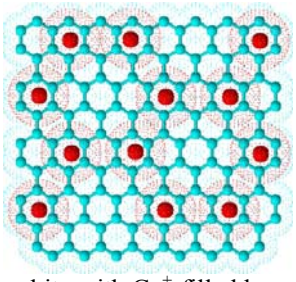

Figure 1. Graphite with Ga^+-filled hexagonal sites

3. Analysis of Materials and Structures in *Microscopic* and *Macroscopic* Devices

Analysis of *microscopic* "systems" (graphene, molecular wires and other *material-by-design* may be used as structures, insulators, interconnect or other) cannot be performed using conventional laws of physics. These *microscopic* systems exhibit quantum phenomena and must be examined quantum-mechanically departing from bulk-centric analyses [3, 4].

Solving the governing equations, one derives statistics, energetics and other descriptive features pertained to a *microscopic* system. The Schrödinger, Poison and Maxwell equation may be solved self-consistently using advanced numeric algorithms. The mathematical results must be substantiated by experiments.

To examine various problems, such as carrier velocity, energetics, conductivity and others, quantum mechanics is applied. Consider electrons in a one-dimensional periodic potential

$$\Pi(x+(a+b))=\Pi(x) \tag{1}$$

with the widths of the well and barrier denoted as a and b.

We consider a typifying potential in periodic lattices in order to obtain an analytic solution. Though (1) may not be absolutely accurate, this $\Pi(x)$ will allow us to analytically and numerically solve the problems under consideration. The results can be easily verified.

The considered potential (1) is applicable to graphene, graphite and other materials. In a perfectly arranged lattice, one examines the electron wave function, energy discontinuities, energy levels, etc. The dependence of the energy band on a, b and the barrier potential Π_0 are studied.

The solutions for the time-independent Schrödinger equation

$$-\frac{\hbar^2}{2m}\frac{d^2\Psi}{dx^2}+\Pi(x)\Psi=E\Psi\,, \tag{2}$$
$$\Pi(x)=\begin{cases}0 \text{ for } 0\le x\le a\\ \Pi_0 \text{ for } a<x<b\end{cases},$$

are found for $E<\Pi_0$ and $E>\Pi_0$.

In particular, for $E<\Pi_0$ we have the following equation

$$\frac{\kappa_b^2-k_a^2}{2k_a\kappa_b}\sin(k_a a)\sinh(\kappa_b b)+\cos(k_a a)\cosh(\kappa_b b)=\cos\big(k(a+b)\big), \tag{3}$$
$$k_a^2=\frac{2m}{\hbar^2}E\,,\ \kappa_b^2=\frac{2m}{\hbar^2}(\Pi_0-E)\,,\ k_a^2+\kappa_b^2=\frac{2m}{\hbar^2}\Pi_0\,,$$

where k is the wave numbers, $k=2\pi/\lambda$; λ is deBroglie wavelength, $\lambda=h/p$.

For $E>\Pi_0$ we obtain

$$-\frac{k_a^2+k_b^2}{2k_a k_b}\sin(k_a a)\sin(k_b b)+\cos(k_a a)\cos(k_b b)=\cos\big(k(a+b)\big), \tag{4}$$
$$k_b^2=\frac{2m}{\hbar^2}(E-\Pi_0) \text{ and } k_a^2-k_b^2=\frac{2m}{\hbar^2}\Pi_0\,.$$

For electrons, which could be tightly bound, free or in an intermediate state, the discontinuities in E occur at $\cos(ka)=\pm1$. That is, when the wave numbers are

$$k=n\pi/a,\ n=1,2,3,\ldots\,. \tag{5}$$

At these $k=n\pi/a$ ($\pm\pi/a,\pm2\pi/a$, …), a small increase in electron momentum will result in the energy of an electron increasing discontinuously from one allowed band to the next band.

The group velocity of an electron wave packet in a given band is

$$\langle v_k\rangle=\frac{1}{\hbar}\frac{d}{dk}\langle H_k\rangle=\frac{1}{\hbar}\frac{dE(k)}{dk}\,, \tag{6}$$

where $E(k)$ is the energy values in the band, and eigenenergies are periodic with a period $2\pi/(a+b)$, $E(k)=E(k+\frac{2\pi}{a+b}n)$; H_k is the Hamiltonian operator.

The $E(k)$ curves for the studied $\Pi(x)$ are examined. The discontinuous energy-wave number relationship, given by a discontinuous $E(k)$, is described by the free-particle energy curve

$$E(k)=\frac{\hbar^2}{2m}\left(k+\frac{2\pi}{a+b}n\right)^2,\ n=0,\pm1,\pm2,\ldots \tag{7}$$

4. Quantum-Mechanical Analysis of Graphene and Graphite

We perform quantum-mechanical analysis on graphene and graphite. To examine the baseline physical quantities, one solves the time-dependent Schrödinger equation

$$-\frac{\hbar^2}{2m}\nabla^2\Psi(t,\mathbf{r})+\Pi(t,\mathbf{r})\Psi(t,\mathbf{r})=i\hbar\frac{\partial\Psi(t,\mathbf{r})}{\partial t}\,. \tag{8}$$

To mathematically examine properties, capabilities and performance of various microstructured *engineered* materials, equation (8) must be solved to derive the wave function $\Psi(t,\mathbf{r})$. The wave function is affected by inherent material characteristics which define the potential energy function $\Pi(t,\mathbf{r})$. In section 3, the problem was solved for periodic one-dimensional potentials $\Pi(x)$ as given by (2).

Using the Hamiltonian operator H, one explicitly derives the evolution of the expectation value for the observable b. Using the operator B, one has

$$\langle b\rangle=\int \Psi^*(t,\mathbf{r})B\Psi(t,\mathbf{r})dV\,. \tag{9}$$

Thus, the expectation value for the velocity, momentum, energies and other quantities are derived.

5. Quantum-Mechanical Analysis and Numerical Results

Consider a graphene lattice. Our goal is to derive the electron velocity in ~10×10 nm graphene using the quantum-mechanical approach and results reported.

For a *delocalized* electron, the quantum-mechanical problem is simplified by using the molecular orbital theory. We solve the matrix eigenvalue equation

$$\mathbf{Hc}=\mathbf{\Lambda Ic},\ H_{ij}=\langle \Phi_i \,|\, H^{nlm} \,|\, \Phi_j\rangle \tag{10}$$

with the eigenvalue matrix $\mathbf{\Lambda}$.

The overlap matrix is

$$\mathbf{I}=\langle \Phi_i \,|\, \Phi_j\rangle=\delta_{ij}. \tag{11}$$

For the electric field $\mathcal{E}$ intensities 100, 1000, 10000 and 100000 V/cm, we found the average carrier (electron) velocities to be ~1.4×10^4, 1.35×10^5, 6.5×10^5 and 7.9×10^5 m/sec, respectively.

The numeric results indicate that in graphene, the electron may not exceed the maximum velocity (the saturational velocity is used to analyze bulk semiconductors). Advanced algorithms are applied to achieve robust numerical solutions, avoiding singularity issues occurring at high $\mathcal{E}$.

The electron mobility μ_e cannot be estimated as

$$\mu_e=|e|t_a/m. \tag{12}$$

Using the quantum-mechanical analysis, under the bulk-centric assumptions, we obtain that the *effective* mobility reaches ~14,000 cm^2/V-sec. This estimate is derived from

$$\boldsymbol{v}_e=-\mu_e\boldsymbol{\mathcal{E}}. \tag{13}$$

However, expression (13) is obscure from the quantum mechanics viewpoint, and, even in *macroscopic* analysis of solid-state devices, one recalls the nonlinear dependence $\mu_e(\mathcal{E})$. Recall that equation

$$\langle v_k\rangle=\frac{1}{\hbar}\frac{d}{dk}\langle H_k\rangle=\frac{1}{\hbar}\frac{dE(k)}{dk} \tag{14}$$

gives the expectation value of a group velocity of an electron wave packet in a given band.

For intrinsic Si,

$$\rho=1/\sigma=3.33\times10^5\ \Omega\text{-cm},\ \sigma=3\times10^{-6}\ \Omega^{-1}\text{-cm}^{-1},$$

and the intrinsic carrier density n_i is ~1×10^{10}/cm^3.

This leads to the electron and hole mobilities μ_n and μ_p as ~1350 and 500 cm^2/V-sec, respectively.

For a *bulk* graphite,

$$\rho=1/\sigma=5\times10^{-3}\ \Omega\text{-cm, and, } \sigma=200\ \Omega^{-1}\text{-cm}^{-1}.$$

Using Avogadro's number $N_A=6.022\times10^{23}$, graphite density $\rho_G=2.1$ g/cm^3 and atomic weight $A_{rG}=12.01$ g/mole, one obtains the number of atoms per unit volume

$$N=N_A\rho_G/A_r=1.05\times10^{23}\ \text{atoms/cm}^3.$$

The derived N agrees with the atomic density of graphite 1.14×10^{23}/cm^3. However, this N may not be used as an estimate for free electron density in the expression,

$$\sigma=N|e|\mu_e. \tag{15}$$

In fact, the use of N in (15) this yields a very low mobility 0.012 cm^2/V-sec. Though one may refine these results using results of quantum mechanics, it was demonstrated that quantum-mechanical analysis can be performed in order to reduce the number of simplifications and assumptions. Furthermore, quantum mechanics eliminates discrepancies and inconsistencies.

In silicon at 300K, the electron and hole mobilities significantly decrease as the total impurity concentration N_T increases. In silicon, μ_n and μ_p sharply decrease from 1400 to 100 and from 500 to 70 cm^2/V-sec, as N_T increases from ~1×10^{14} to ~1×10^{21}/cm^3.

In graphene, the electron mobility 15000 cm^2/V-sec at 300K is reported in [5]. Furthermore, the mobility was found to be the same for variations of temperature from 10K and 100K [6]. The mobility estimate 200000 cm^2/V-sec at 300 K and a carrier density of 10^{12} cm^{-2} are derived in [7, 8]. We were unable to achieve those estimates. It is unlikely that graphene may ensure properties significantly different when compared to graphite with a few layers.

Our results are consistent with the quantum mechanics and supported by experimental data. As was emphasized,

one should cautiously apply *macroscopic*-centric analysis. In general, *macroscopic* premises may be found inapplicable or inaccurate for *microscopic* devices, structures and materials.

6. CONCLUSIONS

We reported quantum-mechanical analysis for emerged and prospective *engineered* materials and structures. These *microscopic* materials are applicable for high-performance, low-power microelectronic devices and ICs. It was illustrated that quantitative quantum-mechanical analysis must be performed to assess and evaluate the characteristics, performance and capabilities of graphene, graphite and molecular wires. Our fundamental, analytical and numerical results comply with experimental data providing evidence of accuracy and correctness.

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