Application of Molecular Electronics Devices in Digital Circuit Design

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Abstract. The Breit-Wigner resonance formula is used to model a class of molecular electronic devices, in order to establish an abstract model for exploration of their applicability in future nanoelectronic systems. The model is used to characterize molecular device I-V curves in terms of the coupling between the molecule and the leads, and demonstrate digital circuit functionality. Circuit metrics such as noise margin, speed and power are investigated.

Keywords: molecular electronics, circuit simulation, nanotechnology.

1 Introduction

Due to recent success in measuring the $I - V$ characteristics of individual or small groups of molecules, developing and controlling electronic molecules that can serve as the active elements in future nano-electronic circuits has become a current objective in this field [1,2,3,4]. Hence developing a hierarchy of device and interconnect models and an efficient simulation methodology is a key step in exploring the system capabilities of molecular device based circuits, as part of the search for miniaturization of devices beyond CMOS, as predicted by the ITRS[5]. In this paper, we propose a refinement of a compact model introduced by Purdue University [6,7,8] that describes the static or steady-state behaviour of a device. The extension allows the dynamic behavior of the device to be modeled and hence investigation of the potential performance impact that general molecular electronics device technology could have on Very Large Scale Integration (VLSI) circuit applications.

2 Device Model

Static Behavior. The transmitted current I through the metal-molecule-metal junction is proportional to the transmission probability $T(E)$ describing the ease with which electrons can scatter through the molecule from the source lead into the drain lead for a range of energy levels around the Fermi energy of the leads. From [9], the current is computed using

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$$I(V) = \frac{2e}{h}\int_{-\infty}^{\infty} T(E)\left(\frac{1}{\exp[E-\mu_s]/kT+1} - \frac{1}{\exp[E-\mu_d]/kT+1}\right)dE \qquad (1)$$

where e is the electron charge and h is Planck's constant. For symmetric molecules, the two electro-chemical potentials μ_s and μ_d (refering to the source and drain respectively) are defined to be $\mu_s = E_f + eV/2$ and $\mu_d = E_f - eV/2$, where V is the bias voltage applied between the source and drain, and E_f is the Fermi energy for the contacts. In the case of weak interaction between the leads and the molecule, it is well known [10] that the transmission probability can be approximated by the Breit-Wigner formula $T(E) = \frac{4\Gamma_1\Gamma_2}{(E-\epsilon_0)^2+(\Gamma_1+\Gamma_2)^2}$ where the variables Γ_1 and Γ_2 represent the broadenings of molecular levels by hybridization with the contacts and the molecular level ϵ_0 is related to the intrinsic chemistry of the molecule. A plot of this probability and corresponding I-V characteristics calculated using Eq.(1) is given in Fig.(1).

Dynamic Behavior. For the purpose of circuit performance investigation, knowledge of an equivalent time constant related to the physical description of the device is sufficient for its dynamic characterization. This time constant can be estimated by calculating the difference between the time spent by the electron in the region of scattering interaction and the time spent in the same region in the absence of scattering interaction.

The event of scattering is described using the scattering matrix $S(E)$ [11]. $S(E)$ is unitary and can be written as $S(E) = \exp(2i\delta)$, where $\delta(E) = -i\log S(E)$ is called the scattering phase shift. For narrow isolated resonance with a single open channel, $\delta(E)$ may be parameterized in terms of the resonance position ϵ_0 and width $\Gamma_1+\Gamma_2$ by the Breit-Wigner one-level formula $\tan[\delta(E)] = -\frac{(\Gamma_1+\Gamma_2)/2}{E-\epsilon_0}$ [10]. The definition of the phase shift $\delta(E)$ has a very intuitive physical meaning, as it is related to the Wigner delay time τ which is the additional time spent in the scattering process compared to free motion by $\tau \times |\frac{(\Gamma_1+\Gamma_2)}{E-\epsilon_0+i(\Gamma_1+\Gamma_2)/2}|^2 = 2\hbar(d\delta/dE)$. Hence under the weak coupling condition, the time constant of the

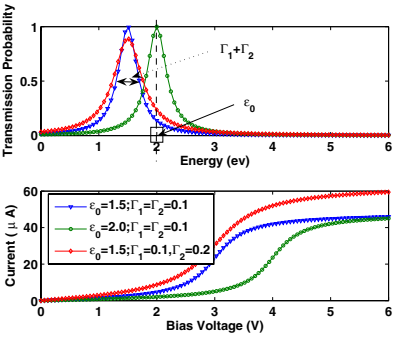

Fig. 1. The transmission probability as a function of molecular energy and corresponding $I-V$ characteristics for different coupling parameters

molecular device is expressed as $\tau = \frac{\hbar}{\Gamma_1+\Gamma_2}$ at $E = \epsilon_0$. We propose to use this time constant to describe the dynamic behavior of the device as an exponential decay; i.e. τ is the time taken to reach 63.2% of the final value of the step response of the device. The current through the device as a function of time can then be described as $I(t) = I_{sat}(1 - \exp(-t/\tau))$, where I_{sat} is the pulse amplitude calculated using the static model for a given voltage.

3 Implementation and Results

The model proposed in Sec.2 can be used to describe two terminal devices using resonance tunneling as a conduction mechanism. Such a device can be used as a two-terminal switch with the "on" or "off" states being a function of the terminal voltage. The device models have been implemented using the analog hardware description language VerilogA, allowing arbitrary circuit configurations to be simulated for static and dynamic behavior within the analog and mixed-signal simulation environment from Cadence that includes the Spectre circuit simulator.

Fig.(2a) shows the generic circuit arrangement for an individual device, the simplest arrangement that suffices for illustration of circuit operation. A 3-D plot that shows the voltage across the device and the current through the device for different values of R is shown in Fig.(2b). Operating points for different values of R are shown in black on the plot, where $\Gamma_1 = \Gamma_2 = 0.1$ and $\epsilon_0 = 1.5$. The value of the pull-up (and pull-down) resistors in a more complex circuit will thus determine the DC bias point of the molecular device, and establish the regime of operation in which the device operates. Shown in Fig.(2c) is a three-input AND-OR gate implemented in a cross-bar architecture [12] and the DC simulation of V_{out} for various input combinations. The connectivity between nodes is established by molecular devices, while the horizontal and vertical lines represent nanowires.

The inputs are labeled alphabetically. For this logic gate, a low input is held at ground, and a high input is held at $+1V$. The schematic shows pull-up and

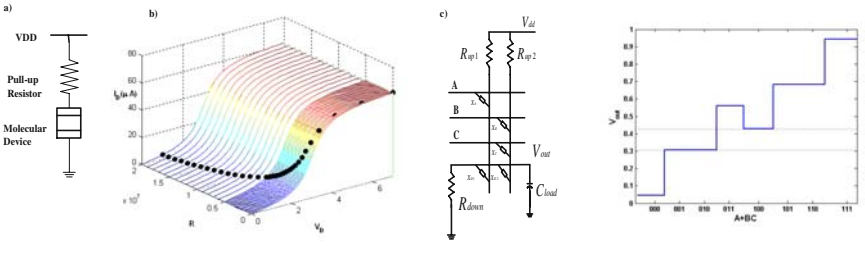

Fig. 2. *a*) A generic cross-bar circuit that utilizes a molecular device; *b*) black dots show how the DC operating point changes with the value of the biasing resistor; *c*) Circuit layout for the AND-OR gate; Derived truth table

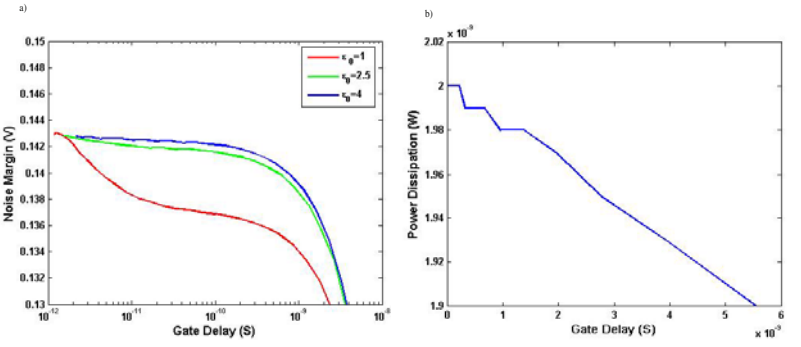

Fig. 3. *a*) The relationship between the speed and the noise margin of the gate for different values of ϵ; *b*) Trade-off between the power dissipation and speed of the gate

pull-down resistors labeled R_{up1}, R_{up2} and R_{down}. The gate uses five molecular devices X_A,X_B,X_C,X_{D1}, and X_{D2}. In the first instance we set the coupling values for all devices as 0.1 while $R_{up1} = R_{up2} = R_{down} = 1G$ and $C_{load} = 100aF$. The plot in Fig.(2c) is a truth table where the output is given as a voltage level. The output voltages of $V_{out} = 0.42V$ and $V_{out} = 0.56V$ are interpreted as binary "1" while voltages less than $0.3V$ are interpreted as logic "0". It can be seen that the circuit acts as a three-input AND-OR gate.

One of the most important metrics of interest in characterizing static behavior is the DC noise margin, which is a function of the separation between the high and low voltage levels, and is defined as $(V_{high} - V_{low})$ here for convenience. As mentioned, the delay time of the functional gate is a function of the coupling parameters. Hence a relationship can be established between the noise margin and the rise time of the step response. This relationship is shown in Fig.(3a).

Power dissipation results in heating that could have a particularly negative cumulative impact in an ultra-dense molecular electronic system with many closely-spaced wires, switches, gates, and functions. It is also crucial to estimate the power for a system that has a complexity similar to that of of a representative digital system such as a processor. The static and dynamic models proposed in this paper and our simulation methodology allows the calculation of such quantities. The gates constructed in this PLA type architecture have static power dissipation, on the order of tens to hundreds of nanowatts per complex gate. the I-V curve will influence the power dissipation, and this can be captured by the plot of Fig.(3b), which shows the variation of static power dissipation with gate delay. The static power dissipation will depend on the state the gate is in, and a representative average for this 3-input AND-OR gate is around 2nW. This translates to a total static power consumption of around 0.002W for a system of 1 million gates, which can be up to several orders of magnitude improvement on a state of the art CMOS implementation in a 50nm technology.

4 Conclusion

The Breit-Wigner formula for resonant conductance is used to extract current-voltage curves for a generic molecular electronic device, based on fundamental physical constants related to the electronic structure of the molecule. The Wigner delay time derived from the scattering matrix is used as the time constant to characterize the dynamic behavior of the device. Using the composite model, digital logic behaviour was demonstrated for a molecular-device-based circuit, and a comprehensive analysis of performance metrics of interest including noise margin, speed and power dissipation was carried out. The study reveals a separation between distinct logic levels that is several orders of magnitude greater than the thermal noise induced voltage at room temperature, and an equivalent output impedance of a few M ohms, resulting in a relatively slow (dis)charging time constant for sub fF loads that dominates the internal charging time of the device itself. Due to the logic architecture, the power consumption has an input-patter-dependent static component(a few nW for the 3-input AND-OR gate considered in the study) in addition to the familiar CMOS type dynamic component, that depends on the load and switching frequency. The general viability of molecular-based electronics for ultra dense low-power applications based purely on their functional capability and performance metrics appears to be promising.

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