Extended Abstracts of the 1998 International Conference on Solid State Devices and Materials, Hiroshima, 1998, pp. 198-199

Theory of Collective Behavior and Single Electron Processes in Coupled Nanowire Arrays

A. J. Bennett and J. M. Xu
Department of Electrical and Computer Engineering, Toronto, Ontario, Canada, M5S 3G4
Phone: 416-978-8935, Fax: 416-971-2626, Email: bennett@ecf.utoronto.ca

1. Introduction

We present an analytical continuum model of collective behavior in the charge distribution in a coupled array of nanostructures, for single electron tunneling in the high-bias/elastic tunneling regime. The results of the model suggest that charge density oscillations of short spatial wavelength persist longer than those of long wavelength. Such charge distributions and their lifetimes might be measurable by scanning probe microscopic techniques. This brings new insights to help us to the long-sought goal of extracting computational functions from collective behavior of nanoelectronic arrays.

2. Background

Recently, progress was made in the non-lithographic fabrication of close-packed nanostructure arrays, which exhibit single-electron charging effects[1]. Due to their potential applications in novel optical devices or nanoscale electronic circuits, it is of interest to study the large scale electronic properties of such nano-arrays. However, conventional Monte-Carlo techniques used for individual tunneling junctions or small circuits are not feasible for an 2D array of $\sim 10^{10}$ coupled junctions. Thus, a new analytical approach was required.

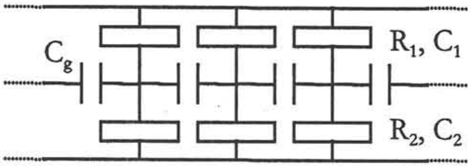

Figure 1. Schematic of the model system. The islands are capacitively coupled to one another by capacitance C_g, and to the electrodes by tunnel junctions 1 and 2.

We sought to model the behavior of these arrays on a macroscopic scale, using the small-scale characteristics of the individual nanostructures as parameters for the macroscopic model. For metal wires, the screening length is short, and a nearest-neighbor approximation is appropriate. The coupling between wires was thus modeled by a capacitance between the "islands".

3. Derivation of the continuum model

First-principles arguments suggest that nearest-neighbor coupling yields an exponential potential change with distance $\Delta V(x_j)$ or ΔV_j for an electron added to an island i; this was confirmed by self-consistent Monte-Carlo calculations on a long array of coupled double junctions[2]. These potential changes contribute to ΔE, the net energy change seen by the tunneling electron.

$$\Delta E_i^k = \tfrac{1}{2}e(V_i^k \mp \Delta V_{ii}) \mp \tfrac{1}{2}e\sum_j n_j \Delta V_{ij} \quad (1)$$

In (1), V_i^k is the pre-tunneling potential across junction k of wire i, ΔV_{ij} is the potential shift of wire j due to an excess electron on wire i, and n_j is the number of electrons on wire j. The signs denote tunneling onto (-) or off the island (+).

In turn, ΔE governs the rate of electron tunneling through the conventional expression

$$\Gamma_i^k = \frac{\Delta E_i^k}{e^2 R} \quad (2)$$

which applies to elastic tunneling at T=0, where no electron energy is transferred to excitations in the circuit, or to the lattice[3].

The discrete model is inconvenient for an analytical approach, and is replaceable with a continuum model. The summation becomes an integral

$$\Delta E(r) = \int_{-\infty}^{\infty} \phi_0 \exp(-|r+\delta|/a_0) n(r+\delta) d\delta \quad (3)$$

where ϕ_0 is the voltage change seen on an island with one added electron. Eqn. (3) is the energy change for an electron tunneling into the array at position r, assuming that a_0 is small.

In order to perform the integral, we expand $n(r+\delta)$ in series and integrate term by term, yielding

$$\Delta E(r) = (ea_0\phi_0)(1 - 2a_0{}^2 \frac{\partial^2}{\partial r^2})^{-1} n(r) \quad (4)$$

as the exact sum of the series. This requires

$$a_0{}^2 \frac{\partial^2 n(r,t)}{\partial r^2} < n(r,t) \quad (5)$$

for the series to converge.

The island electron density is governed by the tunneling rate through each junction in the following way

$$\frac{\partial n(r,t)}{\partial t} = \vec{\Gamma}_1(n(r,t),V) - \vec{\Gamma}_2(n(r,t),V) \quad (6)$$

where for simplicity we set $T=0$ and thus need only use the forward rates. $\vec{\Gamma}_1$ and $\vec{\Gamma}_2$ are determined by equations (3) and (5), and the complete rate equation is given by

$$(1 - a_0{}^2 \frac{\partial^2}{\partial r^2})\frac{\partial n(r,t)}{\partial t} = c_1 - c_2 n(r,t) \quad (7)$$

where $c_1 = (V_1{}^0 - \phi_0)/2eR_1 - (V_2{}^0 - \phi_0)/2eR_2$ and $c_2 = (a_0\phi_0/2e)(R_1^{-1} + R_2^{-1})$; V_i^0 is the voltage across junction i (1,2) in the absence of charges on the island. Eqn. (7) assumes continuity of $n(r,t)$ in time, and is applicable only over time scales in which many single-electron tunneling events occur.

3. Solution of the equation

Equation (7) has a steady state solution in which there is no spatial variation in $n(r,t)$. This solution may be subtracted out to examine the spatial and temporal behavior of perturbations.

The perturbation equation is solved by a trial solution of the form $n(r,t) = A(t)\exp(ikr)$. From this we obtain $A(t)$, and the general solution

$$n(r,t) = \sum_k A_k \exp(-\frac{c_2 t}{1 + a_0{}^2 k^2}) e^{ikr}. \quad (8)$$

The terms are spatial waves which decay in time, but with a wavevector-dependent time constant. This suggests that rapidly-varying charge distributions persist longer than more gradually varying distributions. An cutoff of a_0^{-1} is established for the summation over k by the convergence condition (6).

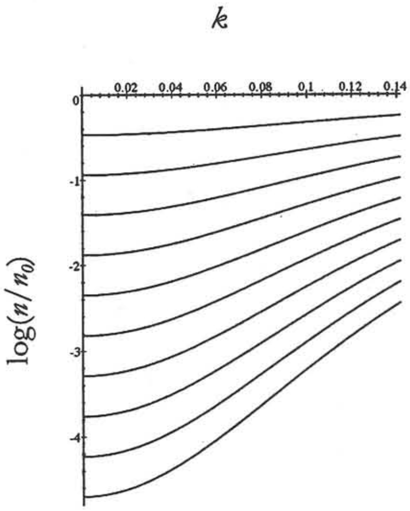

Figure 3. Plot of $\log(n/n_0)$ vs. wavevector k up to the wavevector cutoff, beginning with uniform perturbation n_0 The curves are for different times from $t=0$ (k-axis) to $t=2\cdot10^{-10}$ (lowest curve). (parameters: $R_1=R_2=10^6\ \Omega$, $C_1=C_2=10^{-16}$ F)

4. Conclusions

We have described a continuum model of coupling and collective behavior in nanostructure arrays. The model predicts spatial-wavevector dependent evolution of charge distributions in the arrays which could be detected through scanning probe techniques.

References

1. D. Routkevitch, T. Bigioni, M. Moskovits and J. M. Xu, *J. Phys. Chem.*, **100** (1996) 14307.
2. C. B. Whan, J. White, and T. P. Orlando, *Appl. Phys. Lett.*, **68** (1996) 2996.
3. G.-L. Ingold, and Yu. V. Nazarov, in *Single Charge Tunneling in Nanostructures*, Plenum: New York (1992) ch. 2.