Design Considerations for CdTe Nanotetrapods as Electronic Devices

S. L. Teich-McGoldrick,† M. Bellanger,‡ M. Caussanel,§ L. Tsetseris,¶,⊥
S. T. Pantelides,‖ S. C. Glotzer,* †,# and R. D. Schrimpf* ,∇

Department of Chemical Engineering, University of Michigan,
Ann Arbor, Michigan 48109-2136, INSA (Institut National des Sciences Appliquées) de
Toulouse, 135 Avenue de Rangueil, 31077 Toulouse Cedex 4, France, Laboratoire
ELIAUS, Universite de Perpignan Via Domitia, Perpignan Cedex, France,
Department of Physics, Aristotle University of Thessaloniki, GR-54124 Thessaloniki,
Greece, Department of Physics and Astronomy, Vanderbilt University,
Nashville, Tennessee 37235, Department of Materials Science and Engineering,
University of Michigan, Ann Arbor, Michigan, 48109-2136, and Department of
Electrical Engineering and Computer Science, Vanderbilt University,
Nashville, Tennessee 37235

Received January 9, 2009; Revised Manuscript Received February 16, 2009

ABSTRACT

We investigate the feasibility of using CdTe nanotetrapods as circuit elements using models and simulation at multiple scales. Technology computer-aided design tools are used to simulate the electrical behavior for both metal−semiconductor field-effect transistors and junction field-effect transistors. Our results show that by varying the doping concentrations and material composition, CdTe nanotetrapods have the potential to be useful circuit elements. Monte Carlo simulations provide insight into how control over interparticle and particle−substrate interactions can lead to the directed assembly of ordered arrays of electrically gated nanotetrapods.

In the last 40 years, the silicon-based microelectronics industry kept pace with Moore’s law by steadily decreasing transistor size and cost while increasing clock speed. As the limits of miniaturization of conventional technology are clearly on the horizon, new approaches are sought to complement or integrate traditional top-down fabrication of CMOS technology with bottom-up fabrication of unique nanoelectronic devices.1−4

The premise that bottom-up assembly could supplement top-down CMOS technology to achieve continued advances in chip speed and performance is based on recent investigations into nanoparticle synthesis, assembly, and characterization. An impressive variety of nanoscopic building blocks (NBB) of different shapes, sizes, and materials5−13 have been synthesized, and in some cases, their ability to self-assemble into unique desired structures on the basis of composition, geometry, and local environment14−19 has been demonstrated. The electrical properties of some of these individual nanoparticles have been characterized,3,20−23 demonstrating desirable $I−V$ characteristics. Indeed, many of the general components of CMOS technology are being realized on the nanoscale, created from nontraditional materials and in nontraditional functional forms21,24−26.

As of yet, the themes of synthesis and characterization of NBBs with respect to their electronic properties and the investigation of self-assembled architectures have proceeded in parallel, and largely within different communities. Progressing from a set of disjointed works to the end goal of nanocircuits for memory and logic applications requires a connection be established across disciplines. This work aims to establish such a connection and provides the first study that bridges computational modeling of NBB electronic characteristics and assembly toward this goal.

Nanotetrapods are an ideal model NBB for this study, since they are well studied experimentally. Recent studies of CdTe nanotetrapods have included fabricating particles with independent control over arm aspect ratio,27 using capillary interactions to deposit particles into lithographically defined spaces,28 and analyzing the particle’s electrical responses.20
Our investigation capitalizes on the natural anisotropy of nanotetrapods. Variation in material composition of tetrapod arms allows for a range of current–voltage responses, which can be used to construct working devices. Additionally, material asymmetry can be exploited and material-specific interactions tuned to direct the assembly of nanotetrapods into circuits.

In this work, we use technology computer-aided design (TCAD) tools to simulate the electrical behavior of a single CdTe tetrapod with varying physical characteristics. We report results for metal semiconductor field-effect transistor (MESFET) tetrapods and junction field-effect transistor (JFET) tetrapods. Analytical modeling of various two-terminal (here, two-arm) voltages is used to analyze the physical behavior of the tetrapod transistors and develop design equations. To capitalize on the use of nanotetrapods as field effect transistors, it is essential to direct their assembly into predesigned circuits. We carry out Monte Carlo simulations to determine the necessary requirements to achieve this assembly.

**MESFET Tetrapods.** The MESFET tetrapod considered here is comprised of two CdTe arms with Ohmic contacts to the source and the drain and two metal arms connected to a backgate (Figure 1). As in the work by Cui et al.,20 the main gating mechanism is through the third tetrapod arm. This choice is supported by the findings of Cui et al. that direct electrostatic interaction from the metal electrode plays a less important role, which means it is not a good gating mechanism for a transistor. The semiconductor arms correspond to the conducting channel in conventional MESFET transistors. Each arm has a diameter of 20 nm and is 75 nm long. The metallic arms are composed of palladium and serve as backgates. Additionally they form a Schottky contact with the intrinsic CdTe ($\Phi_{\text{CdTe}} = 5.12$ eV). For the present electrical simulations, the tetrapods are made of a continuous macroscopic material without any internal interfaces. Considerations of crystal orientations and internal surfaces are beyond the scope of this paper, which seeks to provide a first understanding of how such devices might operate.

We assume that the TP arm surfaces are simply passivated by the surfactant so that the semiconductor extends unaltered up to the interface with the surfactant. In principle one can include the effect of charging on the surfactant, but to a good approximation the net effect would be a narrowing of the diameter of the conducting path. For the purposes of the present calculation, charging effects have been neglected in order to get a first description of a device with this kind of geometry.

For undoped CdTe arms, the drain current is very low and significant leakage current flows through the gate. This low current results from the very low intrinsic density of CdTe ($n_i \approx 10^{15}$ cm$^{-3}$) and the extension of positive space charge through the tetrapod, limiting the current from the source to the drain. Such intrinsic devices are therefore unsuitable for transistor applications.

We focus next on Schottky-gated structures in which the two current-carrying (CdTe) arms are doped n-type with concentrations, $N_D$, ranging from $10^{18}$ to $10^{20}$ cm$^{-3}$. These structures were simulated using the DESSIS simulator,31 which solves Poisson’s equation, along with the electron and hole continuity equations.

For the case of $N_D = 10^{18}$ cm$^{-3}$, the output drain current ($I_D$) is low and the gate pinch-off voltage, $V_{P,i}$, is approximately 0.5 V, as shown in Figure 2a. The entire...
The drain current is plotted vs drain voltage for different values of gate-arm doping concentrations (\(N_A\)) in Figure 3b. The current is higher for the gates with lower doping concentrations (Figure 3b), since the depletion region extends primarily into the gate rather than the channel. On the other hand, higher values of \(N_A\) increase the amount by which the drain current changes for a given change in the gate voltage (i.e., the transconductance). In these tetrapod devices, there is a good compromise only when both doping concentrations \(N_A\) and \(N_D\) have the same order of magnitude, with \(N_A\) slightly higher than \(N_D\) (maroon curve in Figure 3b).

**Carrier Transport.** The \(I–V\) characteristics of these devices are affected significantly by high field velocity saturation, since the simulations show that the electric field can exceed \(10^6\) V/cm in some regions of the tetrapod. TCAD simulations of the simpler plane-parallel structure, shown in Figure 4a, demonstrate that quantum effects (based on quantization of the density of states) are not significant for this tetrapod size. Quantum effects begin to be significant for an arm diameter below 10 nm, as shown in Figure 4b, although the effects are relatively minor for this arm diameter. Simulations of a MESFET tetrapod (\(N_D = 3 \times 10^{19}\) cm\(^{-3}\)), based only on electron current (no hole current) confirm that quantum effects are negligible for tetrapods with arm diameter of 20 nm. Single electron charging is not included in this model, and the tetrapod is modeled as a conventional device.
In addition to TCAD simulations, it is useful to develop analytical models that describe the electrical characteristics of tetrapods. We use a two-arm MESFET structure (Figure 5a) to approximate the $I-V$ characteristics of tetrapods as well as important parameters such as the gate pinch-off voltage ($V_{PO}$) and the saturation current ($I_{sat}$). This is a useful tool that can be used to aid in device design or for analyzing the physical phenomena observed in the simulation results.

The output current $I_D$ is modulated by the width of the depletion region in the cylindrical gate region. We find that the $I-V$ characteristic has the following form (2)

$$I_D = G_0 \left\{ V_D + \frac{1}{2V_{PO}} [(V_D + V_{G}^{'})^2 - V_{G}^{'^2}] - \frac{4}{3\sqrt{V_{PO}}} [(V_D + V_{G}^{'})^{3/2} - V_{G}^{3/2}] \right\}$$

(2)

where $G_0$ is the transconductance and $V_{PO}$ is the gate pinch-off voltage.

The first term of eq 2 describes a linear dependence between the output current ($I_D$) and the applied voltage ($V_D$), whereas the second term describes the parabolic contribution to the behavior. The results obtained from these equations are compared to TCAD simulations in Figure 5b, illustrating very good agreement, especially for high values of $N_D$ ($N_D > 10^{19}$ cm$^{-3}$).

The analytical model assumes a single value for the mobility and does not include quantum effects. However, it is useful as a design tool for evaluating the effects of changes in the dimensions (length and diameter of the tetrapod) and the tetrapod material.

**Nanotetrapod Assembly.** In our investigation of nanotetrapod electronic behavior, each particle is individually addressed and backgated. To create complex circuits, it is desirable to assemble multiple particles into a single structure. Previously investigated methods based on capillary interactions are not material-specific and therefore do not offer precise control over nanoparticle placement. Here we consider directed assembly based on specific material interactions.

Figure 4. (a) Simulation structure used to analyze the significance of quantum effects in the current–voltage characteristics of a plane-parallel MESFET. The lines represent the mesh used for the finite-element simulations. (b) Output characteristic of a plane-parallel MESFET with an edge dimension of 10 nm.

Figure 5. (a) Theoretical two-arm equivalent of a backgated tetrapod. (b) Comparison of TCAD and theoretical results.
For computational expediency, we model a tetrapod as a rigid particle constructed of overlapping beads with the angle between the spherocylindrical arms set at 109.5° (Figure 6a).

Beads on different tetrapods interact through excluded volume interactions, while beads forming the tips of the four tetrapod arms have additional attractive, square-well interactions that mimic lock and key type interactions between tetrapod tips and electrodes or tetrapod tips and substrate.\textsuperscript{18,19} Specifically, the tips of two arms interact selectively with the electrodes, while the other two tips interact selectively with the floor of the trench, Figure 6b. Such selective interactions could be achieved through a different material deposited at the tip, or via short DNA oligonucleotides grafted to the tips and to the electrodes in such a way as to enhance, or at least not disrupt, the conduction path. The substrate, trench walls, and trench floors are all modeled as flat planes, and the electrodes are modeled as a series of beads joined together residing at the intersection of the trench wall and substrate, Figure 6b.

To study the self-assembled structures formed by systems of nanotetrapods, we perform Monte Carlo (MC) simulations in the NVT ensemble where \( N \) = number of tetrapods, \( V \) = volume, and \( T \) = temperature. Starting from an initial random configuration, we run different initial starting configurations, cooling cycles, and system sizes to ensure that the final observed structures are the most probable and not a result of the system becoming kinetically trapped in a metastable state.

Our simulations are performed in a rectangular box with the box walls being hard barriers to the tetrapod. The reduced units for length and energy are \( \sigma = 1 \) and \( \varepsilon = 1 \), respectively, where \( \sigma \) is taken to be the diameter of the beads making up the tetrapod and \( \varepsilon \) is the strength of the repulsion between tetrapods. The reduced temperature is defined as \( T^* = k_B T / \varepsilon \). In each MC step, a translation or rotation move is attempted for every tetrapod; the maximum translation and rotation moves allowable are 0.1 bead diameters to optimize the acceptance probability for moves. Smaller moves do not change the result; larger moves can produce unphysical overlaps and very low acceptance probabilities.

Simulations with 15 tetrapods and 5 electrodes were performed, first assuming no particle–particle interactions other than excluded volume. We find that tetrapods align between every electrode within the trench and multiple

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure6.png}
\caption{(a) An individual tetrapod. The red tips are attracted to the electrodes while the white tips are attracted to the floor of the trench. (b) A single tetrapod in a trench. The electrodes are shown in yellow, the floor of the trench in light brown and the substrate surface in green/gray. (c) Multiple tetrapods aligning within a trench with no particle–particle interactions other than excluded volume.}
\end{figure}

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure7.png}
\caption{(a) Fifteen tetrapods aligned within a trench with repulsive interactions. (b) Region of assembly for tetrapods with varying interaction strengths (indicated on axes) and screening lengths (indicated on plot). The shaded region indicates the region of assembly for screening length \( \kappa \sigma = 0.5 \), while the black line indicates the region of assembly for \( \kappa \sigma = 1.0 \).}
\end{figure}
particles contact electrodes and each other (Figure 6c). In a working circuit this would result in a short, and therefore the addition of a repulsive interaction between beads forming different tetrapods was investigated. We choose to model this repulsion with a standard Yukawa potential (eq 3) used to model charged colloidal systems.22 Here ε is the strength of the repulsion, κ⁻¹ is the inverse screening length, and r is the separation between beads. After evaluating a range of potential cutoffs, r_c, we chose a cutoff leading to no more than 4% energy loss. This cutoff is both computationally efficient and does not produce errors from neglected particle interactions.

\[ U(r) = \begin{cases} \frac{\varepsilon \exp(-\kappa (r/\sigma - 1))}{r/\sigma} & \text{for } r > \sigma, r < r_c \\ 0 & \text{for } r < \sigma \end{cases} \]  

(3)

Realistically, CdTe nanoparticles are known to be charged in solution due to the ionization of the capping agent and interact through screening lengths between 1 and 10 particle diameters depending on solvent. Both the charge and screening length could be tuned through the addition of salt to the solvent.

Systems with 15 or 30 tetrapods were run in simulation boxes containing 5 electrodes or 10 electrodes, respectively. We investigated the effects of changing the relative strengths of the Yukawa potential and the square-well interaction between the tetrapods and floor or electrodes. The well depth of the square well attraction chosen between tetrapod tips and the substrate ranged between 0.5 and 10.0 \( \varepsilon_{\text{YUKAWA}} \), the depth of the square-well defining the interaction between tetrapod tips and the electrodes ranged from 0.5 and 6.0 \( \varepsilon_{\text{YUKAWA}} \), and the screening length (\( \kappa \sigma \)) varied between 0.5 and 4.0. Upon cooling to \( \varepsilon_{\text{Yukawa}}/k_B T = 0.1 \), it was found that tetrapod assembly is sensitive to screening length and only occurred for \( \kappa \sigma = 0.5 \) and 1.0. A typical system of assembled tetrapods with repulsive interactions is shown in Figure 7a, and Figure 7b shows the regions of assembly for screening lengths \( \kappa \sigma = 0.5 \) and 1.0. The shaded region indicates values of interaction strengths where assembly occurs for screening length \( \kappa \sigma = 0.5 \). Upon change of the screening length to \( \kappa \sigma = 1.0 \), the assembly region shrinks to the area represented by the black line.

These MC studies indicate assembly could be achieved in real systems by correctly choosing system attributes. Experiments conducted in solution would allow for the Brownian motion our simulations mimic and which is essential to particle arrangement via thermodynamically driven assembly. Attractive, short-range interactions could arise through lock-and-key interactions such as those arising between complementary strands of DNA or RNA, and both attractive and repulsive interactions could be achieved through solvent selectivity and appropriate choice of tip material.

**Conclusions.** In conclusion, tetrapods show promising results as MESFET and JFET structures. The use of nanotetrapods as simple logic circuit elements is conceivable, and we should focus now on more complex logic circuit elements derived from their assemblies. This conclusion is further supported by the results of our directed assembly simulation studies. When material specific interactions are tuned, systems of nanotetrapods can be backgated and aligned between electrodes, thus presenting an avenue to achieve logic circuits. A range of particle parameters lead to assembled structures, and exact material interactions should be determined by the required system tolerance. Future work will center on the electronic modeling of specific tetrapod circuit elements and devising self-assembly schemes for the resulting device.

**Acknowledgment.** The authors acknowledge joint funding by the Department of Energy under Grants DE-FG02-03ER46094 and DE-FG02-03ER46096. S.L.T.-M. also acknowledges the Graduate Fellowship Program of the National Science Foundation. S.T.P. also acknowledges the McMinn Endowment at Vanderbilt University.

**References**

(31) V. B. D. S. ISE TCAD Release 10.0, Integrated Systems Engineering, Zurich, Switzerland, 2004 (now part of the Synopsys tool suite).

NL9000794