

peratures, and the s values of $\text{Mo}_3\text{Sb}_{5.4}\text{Te}_{1.6}$ were compared with those of other state-of-the-art thermoelectric materials (see figure). The ZT values of both $\text{Mo}_3\text{Sb}_{5.5}\text{Te}_{1.5}$ and $\text{Mo}_3\text{Sb}_{5.4}\text{Te}_{1.6}$ were found to increase with temperature up to 1,050 K, which is just below the decomposition temperature. The fact that ZT for $x = 1.6$ exceeds that for $x = 1.5$ might be taken as a hint that one could increase ZT by increasing x , except for the observation

that attempts to synthesize $\text{Mo}_3\text{Sb}_{7-x}\text{Te}_x$ having $x > 1.6$ resulted in specimens that appeared to be multiphase. Hence, other approaches to doping may be more promising.

The s value of $\text{Mo}_3\text{Sb}_{5.4}\text{Te}_{1.6}$ was found to increase from about 1 V^{-1} at 300 K (room temperature) to about 2 V^{-1} at 1,000 K. This doubling of s indicates poor self-compatibility of $\text{Mo}_3\text{Sb}_{5.4}\text{Te}_{1.6}$ over the affected temperature range. However, $\text{Mo}_3\text{Sb}_{5.4}\text{Te}_{1.6}$

could be suitable for segmentation: for example, a $\text{Mo}_3\text{Sb}_{5.4}\text{Te}_{1.6}$ segment (which can withstand a temperature $> 800 \text{ K}$) could be joined to a lower-temperature PbTe segment at an interface temperature at or slightly below 800 K, where their s values are equal.

This work was done by G. Jeffrey Snyder, Frank S. Gascoin, and Julia Rasmussen of Caltech for NASA's Jet Propulsion Laboratory. For more information, contact iaoffice@jpl.nasa.gov. NPO-43862

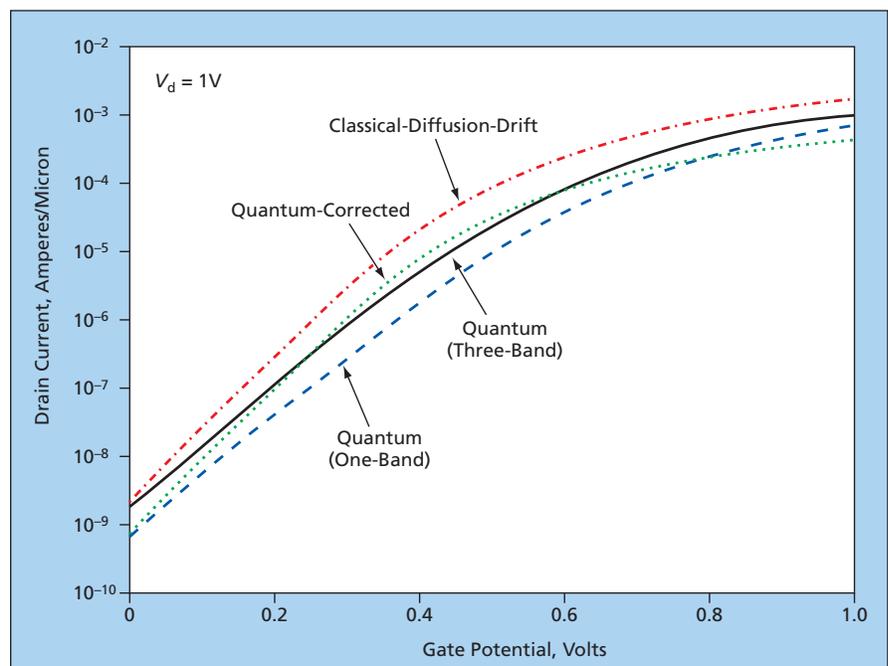
Two-Dimensional Quantum Model of a Nanotransistor

Quantum effects that become important at the nanoscale are taken into account.

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A mathematical model, and software to implement the model, have been devised to enable numerical simulation of the transport of electric charge in, and the resulting electrical performance characteristics of, a nanotransistor [in particular, a metal oxide/semiconductor field-effect transistor (MOSFET) having a channel length of the order of tens of nanometers] in which the overall device geometry, including the doping profiles and the injection of charge from the source, gate, and drain contacts, are approximated as being two-dimensional. The model and software constitute a computational framework for quantitatively exploring such device-physics issues as those of source-drain and gate leakage currents, drain-induced barrier lowering, and threshold voltage shift due to quantization. The model and software can also be used as means of studying the accuracy of quantum corrections to other semiclassical models.

The present model accounts for two quantum effects that become increasingly important as channel length decreases toward the nanometer range: quantization of the inversion layer and ballistic transport of electrons across the channel. Heretofore, some quantum effects in nanotransistors have been analyzed qualitatively by use of simple one-dimensional ballistic models, but two-dimensional models are necessary for obtaining quantitative results. Central to any quantum-mechanical approach to modeling of charge transport is the self-consistent solution of a wave equation to describe the quantum-mechanical aspect of the transport, Poisson's equation, and equations for statistics of the particle ensemble.



Drain Current Versus Gate Potential in a conceptual 25-nm-gate-length MOSFET commonly used as an example for testing MOSFET-simulating software was calculated by means of a three-band and a one-band version of the present quantum-based model. For comparison, the plot also shows results from a classical diffusion-drift model and a quantum-corrected model embodied in a commercial MOSFET-simulation computer program. A drain bias of 1 V and a gate oxide thickness of 1.5 nm were used in the simulations.

Non-equilibrium Green's function (NEGF) formalisms have been successful in modeling steady-state transport in a variety of one-dimensional semiconductor structures. The present model for the two-dimensional case includes the NEGF equations, which are solved self-consistently with Poisson's equation. At the time of this work, this was the most accurate full quantum model yet applied to simulation of two-dimensional semiconductor devices. Open boundary conditions (in which the nar-

row channel region opens into broad source, gate, and drain regions) and tunneling through oxide are treated on an equal footing. Interactions between electrons and phonons are taken into account, causing the modeled transport to deviate from ballistic in a realistic manner. Electrons in the wave-vector-space ellipsoids of the conduction band are treated within the anisotropic-effective-mass approximation.

Self-consistent solution of the Poisson and NEGF equations is computa-

tion-intensive because of the number of spatial and energy coordinates involved. Therefore, parallel distributed computing is imperative: the software that implements the model distributes the computations, energy-wise, to the

various processors. Initial simulations were performed using, variously, between 16 and 64 processors of an SGI Origin multiprocessor computer. The figure presents an example of results of one set of simulations.

This work was done by T. R. Govindan and B. Biegel of Ames Research Center and A. Svizhenko and M. P. Anantram of Computer Science Corp. Further information is contained in a TSP (see page 1). ARC-15471-1

Scanning Miniature Microscopes Without Lenses

Polarization-sensitive and multicolor versions should also be possible.

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The figure schematically depicts some alternative designs of proposed compact, lightweight optoelectronic microscopes that would contain no lenses and would generate magnified video images of specimens. Microscopes of this type

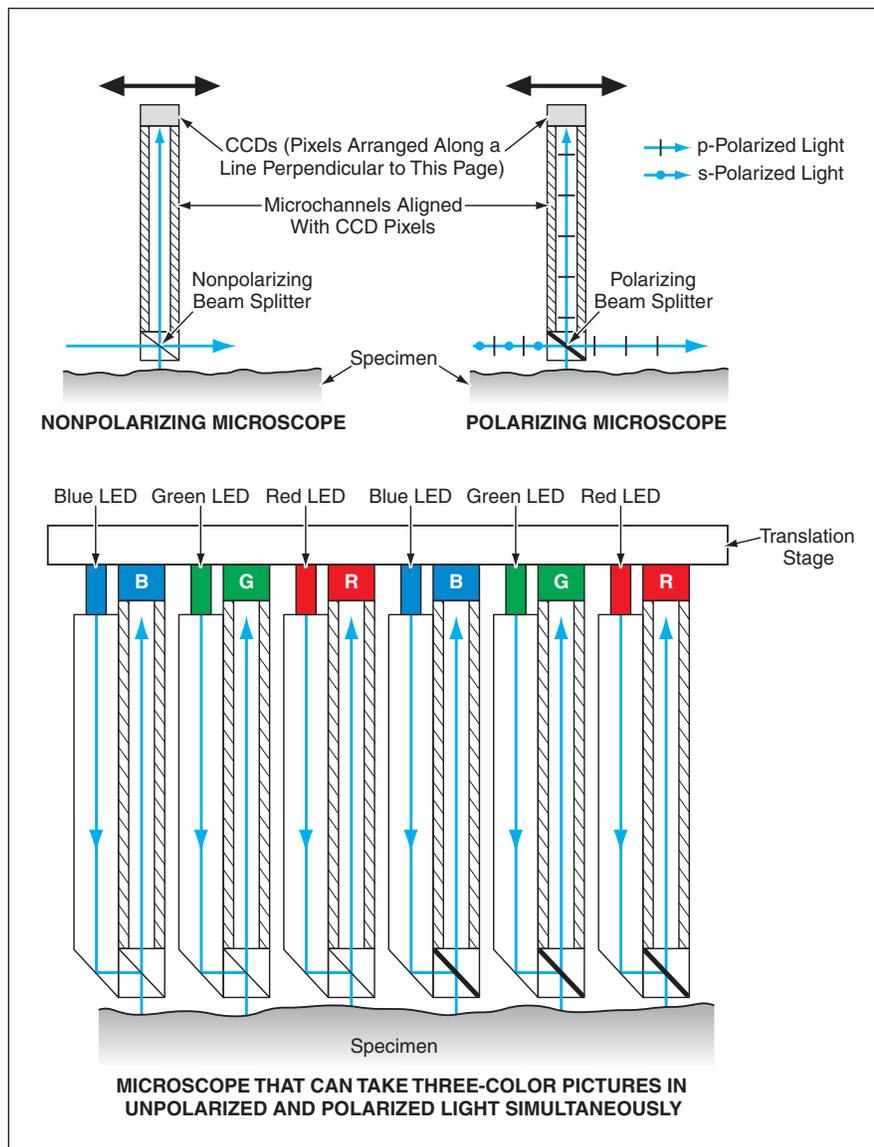
were described previously in "Miniature Microscope Without Lenses" (NPO-20218), *NASA Tech Briefs*, Vol. 22, No. 8 (August 1998), page 43 and "Reflective Variants of Miniature Microscope Without Lenses" (NPO20610), *NASA Tech*

Briefs, Vol. 26, No. 9 (September 1999), page 6a. To recapitulate: In the design and construction of a microscope of this type, the focusing optics of a conventional microscope are replaced by a combination of a microchannel filter and a charge-coupled-device (CCD) image detector. Elimination of focusing optics reduces the size and weight of the instrument and eliminates the need for the time-consuming focusing operation.

The microscopes described in the cited prior articles contained two-dimensional CCDs registered with two-dimensional arrays of microchannels and, as such, were designed to produce full two-dimensional images, without need for scanning. The microscopes of the present proposal would contain one-dimensional (line image) CCDs registered with linear arrays of microchannels. In the operation of such a microscope, one would scan a specimen along a line perpendicular to the array axis (in other words, one would scan in "pushbroom" fashion). One could then synthesize a full two-dimensional image of the specimen from the line-image data acquired at one-pixel increments of position along the scan.

In one of the proposed microscopes, a beam of unpolarized light for illuminating the specimen would enter from the side. This light would be reflected down onto the specimen by a nonpolarizing beam splitter attached to the microchannels at their lower ends. A portion of the light incident on the specimen would be reflected upward, through the beam splitter and along the microchannels, to form an image on the CCD.

If the nonpolarizing beam splitter were replaced by a polarizing one, then the specimen would be illuminated by s-polarized light. Upon reflection from the specimen, some of the s-polarized light would become p-polarized. Only the p-polarized light would contribute to the image on



Scanning Lensless Microscopes of various degrees of complexity and capability would be made from line-imaging CCDs, the pixels of which would be aligned with microchannels.