



Boundary Condition for Modeling Semiconductor Nanostructures

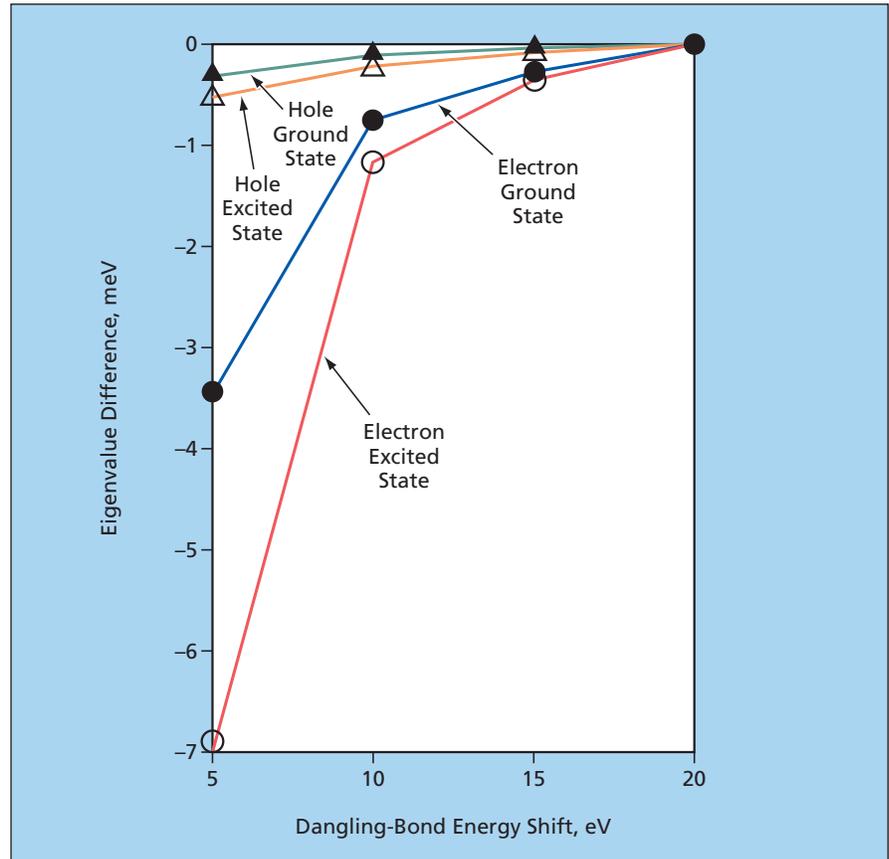
Simulation domains are truncated without introducing spurious surface quantum states.

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A recently proposed boundary condition for atomistic computational modeling of semiconductor nanostructures (particularly, quantum dots) is an improved alternative to two prior such boundary conditions. As explained below, this boundary condition helps to reduce the amount of computation while maintaining accuracy.

The electronic properties of semiconductor nanostructures (hereafter called “nanodevices”) are already utilized in sensors, lasers, memory circuits, and electro-optical and optoelectronic devices. The electronic properties of a nanodevice are sensitive to numerous parameters, including those pertaining to sizes, shapes, alloy compositions, and interfaces between different materials. Atomistic computational simulation of a nanodevice can help in the selection of optimal parameters in the huge design space inhabited by the parameters. However, until now, the computational burden posed by the large numbers of atoms in a nanodevice has made it necessary to limit computational modeling to a semi-classical, continuum approximation. The purpose served by the present boundary condition (and by the two prior boundary conditions with which the present boundary condition is compared) is to enable truncation of the simulation domain at an artificial boundary surface so that the domain can be made small enough that atomistic computational simulation becomes practical.

The truncation problem can be summarized as follows: Whereas, as its name suggests, a nanodevice can have characteristic dimensions of the order of nanometers, it is typically embedded within a larger semiconductor structure having characteristic dimensions of the order of micrometers. Therefore, in the absence of a means of truncation, the simulation domain must typically encompass all of the atoms contained within a micrometer-sized region. The key to truncation lies in recognition that a smaller electronically active region is



Eigenvalues of Quantum States in the band gap of a simulated InAs-in-GaAs quantum dot are already converged within a few meV at a dangling-bond shift of 5 eV, and converge further as the dangling-bond shift is increased to 20 eV.

defined by localization of the electron density in and near a potential well established by the energy-band offset between two adjacent semiconductor materials. However, without a proper boundary condition, simply drawing an artificial boundary surface around the electronically active region results in many spurious quantum states associated with dangling interatomic bonds at the boundary surface.

The present boundary condition effectively eliminates the spurious surface quantum states by artificially shifting their energy levels well above the energy band of interest, as though the dangling bonds were passivated by high-energy molecules. The size of the dangling-bond energy shift is not critical, as long

as it suffices to remove all spurious quantum states from the semiconductor band gap in the electronically active region of interest. For example, in the case of an InAs self-assembled quantum dot embedded in GaAs, a shift of 5 eV is sufficient to remove the spurious states and make electron and hole energies converge to within a few meV (see figure).

The present boundary condition is a refined version of one of the two prior boundary conditions in which the orbital energies of surface atoms are raised. Whereas the prior boundary condition does not differentiate among such details of the surface atoms as the numbers and directions of their dangling bonds, the present boundary condition does. The present boundary con-

dition is more physically realistic because, unlike in the prior boundary condition, the connected-bond energy of the surface atoms is kept unchanged and, hence, there is no extra energy penalty for electrons to occupy the con-

nected bonds of surface atoms. The other prior boundary condition is a periodic one and, hence, not well suited to modeling a nanodevice that has an irregular shape or is subjected to a non-periodic externally applied potential.

This work was done by Seungwon Lee, Fabiano Oyafuso, Paul von Allmen, and Gerhard Klimeck of Caltech for NASA's Jet Propulsion Laboratory. Further information is contained in a TSP (see page 1). NPO-41155

Miniature Distillation Column for Producing LOX From Air

This column is only about a hundredth as high as an industrial one.

John H. Glenn Research Center, Cleveland, Ohio

The figure shows components of a distillation column intended for use as part of a system that produces high-purity liquid oxygen (LOX) from air by distillation. (The column could be easily modified to produce high-purity liquid nitrogen.) Whereas typical industrial distillation columns for producing high-purity liquid oxygen and/or nitrogen are hundreds of feet tall, this distillation column is less than 3 ft (less than about 0.9 m) tall. This column was developed to trickle-charge a LOX-based emergency oxygen system (EOS) for a large commercial aircraft.

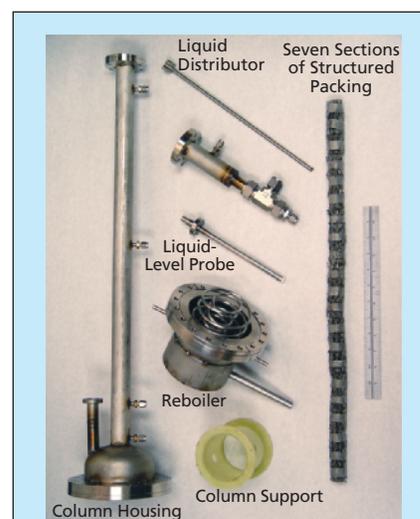
A description of the industrial production of liquid oxygen and liquid nitrogen by distillation is prerequisite to a meaningful description of the present miniaturized distillation column. Typically, such industrial production takes place in a chemical processing plant in which large quantities of high-pressure air are expanded in a turboexpander to (1) recover a portion of the electrical power required to compress the air and (2) partially liquefy the air. The resulting two-phase flow of air is sent to the middle of a distillation column. The liquid phase is oxygen-rich, and its oxygen purity increases as it flows down the column. The vapor phase is nitrogen-rich and its nitrogen purity increases as it flows up the column. A heater or heat exchanger, commonly denoted a reboiler, is at the bottom of the column. The reboiler is so named because its role is to reboil some of the liquid oxygen collected at the bottom of the column to provide a flow of oxygen-rich vapor. As the oxygen-rich vapor flows up the column, it absorbs the nitrogen in the down-flowing liquid by mass transfer. Once the vapor leaves the lower portion of the column, it interacts with down-flowing nitrogen liquid that has been condensed in a heat exchanger, commonly denoted a condenser, at the top of the column. Liquid oxygen and liquid nitrogen products are obtained by

draining some of the purified product at the bottom and top of the column, respectively.

Because distillation is a mass-transfer process, the purity of the product(s) can be increased by increasing the effectiveness of the mass-transfer process (increasing the mass-transfer coefficient) and/or by increasing the available surface area for mass transfer through increased column height. The diameter of a distillation column is fixed by pressure-drop and mass-flow requirements. The approach taken in designing the present distillation column to be short yet capable of yielding a product of acceptably high purity was to pay careful attention to design details that affect mass-transfer processes.

The key components in this column are the structured packing and the distributor. The structured packing is highly compact. Each section of packing is about 1 in. (about 2.5 cm) in diameter and 3 in. (about 7.6 cm) long. The column contains a total of seven sections of packing, so the total length of packing in the column is 21 in. (about 53 cm). The packing promotes transfer of mass between the up-flowing vapor and the down-flowing liquid. The liquid distributor, as its name suggests, helps to distribute the liquid as nearly evenly as possible throughout the cross section of the column so as to utilize the packing to the fullest extent possible and thereby maximize the mass-transfer effectiveness of the column.

In operation, saturated air at a pressure of 70 psia (absolute pressure of 0.48 MPa) enters the reboiler and partially condenses. The air is then fully condensed by an external refrigeration source, such as a small cryocooler. The air then goes through a pressure drop of about 50 psi (about 0.34 MPa) in a throttling valve and thereby becomes partially vaporized. This pressure drop sets the column pressure at about 20 psia (about 0.14 MPa). This column pressure is required to obtain a signifi-



COMPONENTS OF DISTILLATION COLUMN



MAGNIFIED VIEW OF ONE SECTION OF STRUCTURED PACKING

The Components of the Distillation Column are designed to maximize mass transfer in a small space.

cant temperature difference in the reboiler. The two-phase flow then enters a separator, where the vapor is vented, and the liquid is sent to the distributor. Once operation has reached a steady state, mass transfer between the down-flowing liquid and the up-flowing vapor