微纳技术著作丛书（影印版）

纳米晶体管：器件物理学，建模和仿真

Nanoscale Transistors: Device Physics, Modeling and Simulation

Mark Lundstrom, Jing Guo

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Nanometer-Scale Transistors:
Device Physics, Modeling and Simulation

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内 容 简 介

近几十年来，晶体管的尺度发展一直是推动电子学的动力，各种分子尺度的器件已经出现，甚至有取代硅晶体管的趋势。本书详细介绍了纳米晶体管的理论、建模与仿真，内容包括弹道纳米晶体管的弹道传输和量子效应，MOSFET 的散射理论等。为了详细说明纳米晶体管，本书还提供了已被详尽数值仿真所证实的物理图片及半解析模型。

本书可供从事纳米电子器件领域的电子工程师、物理学者和化学家参考。

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序

科学出版社准备出版一套《微纳技术著作丛书》，包括原创作品和引进作品（影印或翻译）两种形式，并聘请专家组成编委会。这是一件大事，希望能坚持把它办好。

微纳米技术作为21世纪重要的一项技术，已成为国际科学界和工程技术界研究的热点。近年来，微米纳米技术进展迅速，已经发展成为一个包含机械、材料、电子、光学、化学、生物、基因工程、医学等基础学科的综合领域，而不仅仅属于任何单一的科学和技术门类。就其产品而言，也早已超越了人们广为熟悉的微型加速度传感器和纳米碳管等，呈现出向各个科学和技术领域全面渗透的趋势。

由于微纳米技术使得人们除了可以在同一基片上实现包括机械、流体、化学、生物、光学等器件外，也可以将信号处理和传输系统集成在同一基片上用以处理信息，决定计划，控制周围环境，从而大大提高最终产品的综合性能，实现高度智能化。在未来的航空航天、生物医学、环境监控、无线通信、汽车和交通、石油化工、能源、工农业、国家安全、食品和消费的各个领域都将有广泛应用，对国民经济、科学技术、社会发展与国家安全具有重要意义。今后的几十年里，随着微米纳米技术的迅速发展和向现代科学和技术的各个门类渗透，其对我们现代生活的各个方面带来的影响将是长期和深远的。从某种意义上来说，微米纳米技术的发展，可能改变人类的工作和生活方式，乃至基本概念，其潜在的影响有可能和以计算机技术为代表的微电子工业对世界的影响相提并论。

正是由于其诱人的应用前景和巨大的潜在市场，微米纳米技术目前已成为世界各国大力投资进行研究和发展的热点领域，其研究范围包括了材料、器件和系统，涉及的技术包含机理研究、设计分析、计算仿真、制造工艺、系统集成或组装、测控技术和应用研究等。随着微纳米技术的迅猛发展，近年来国外有大量这方面的专业书籍出版。

《微纳技术著作丛书》涵盖材料开发、系统设计、检测技术、集成技术、通信网络、传感系统、微加工技术等方面，它们都是本领域的研究热点。这套丛书的出版对促进我国微米纳米技术的发展将有很大的推动作用。

这套丛书中，原创作品收录的都是国内从事微纳技术的一线研究人员在本领域的研究成果与心得，具有很强的独立性、创造性和系统性。引进作品都是与国际知名的出版集团合作，经国内专家的甄别，挑选出能反映国外最新研究成果、对国内读者又有借鉴价值的作品，具有权威性、前瞻性和可读性。因为微纳米技

术是一个交叉学科领域，我们有意识的选择了一些由多人合写的专著。通常这类著作都是由相关领域的知名专家，各自在每一章节涵盖一个专题，既有进行综合性的论述，也有个人的具体独创性研究。这样的书籍，通常能帮助读者既获得某一领域的研究概况，又能从一个具体的应用专题中获得收益。

2007 年初推出的第一批影印版图书，我和王万军教授进行了评读，此套丛书很实用，不少作者在该领域有很高的声望。我们建议致力于微米纳米技术的研究人员，包括研究生、技术人员，能够花些时间阅读。

总之，我们对科学出版社组织出版这套丛书的举措很赞赏，也希望他们能将这一工作认真、长期地做下去。同时，我们也希望国内的专家能够积极、踊跃地加盟，为我国微米纳米技术的推进做出贡献。

周兆英 王万军

2006 年 12 月 7 日

Preface

Silicon technology continues to progress, but device scaling is rapidly taking the metal oxide semiconductor field-effect transistor (MOSFET) to its limit. When MOS technology was developed in the 1960's, channel lengths were about 10 micrometers, but researchers are now building transistors with channel lengths of less than 10 nanometers. New kinds of transistors and other devices are also being explored. Nanoscale MOSFET engineering continues, however, to be dominated by concepts and approaches originally developed to treat microscale devices. To push MOSFETs to their limits and to explore devices that may complement or even supplant them, a clear understanding of device physics at the nano/molecular scale will be essential. Our objective is to provide engineers and scientists with that understanding – not only of nano-devices, but also of the considerations that ultimately determine system performance. It is likely that nanoelectronics will involve much more than making smaller and different transistors, but nanoscale transistors provides a specific, clear context in which to address some broad issues and is, therefore, our focus in this monograph.

This monograph was written for engineers and scientists who are engaged in work on nanoscale electronic devices. Familiarity with basic semiconductor physics and electronics is assumed. Chapter 1 reviews some central concepts, and Chapter 2 summarizes the essentials of traditional semiconductor transistors, digital circuits, and systems. This material provides a baseline against which new devices can be assessed. At the same time, it defines the requirements of a device for it to be useful in a digital electronic system. Chapter 3 presents a nontraditional view of the ballistic MOSFET. By treating a traditional device from a fresh perspective, this chapter introduces electrical engineers to new ways of thinking about small electronic devices. In Chapter 4, we extend the model to discuss the physics of scattering in nanotransistors. Chapter 5 uses the same, general approach to treat semiconductor nanowire and carbon nanotube FETs. Finally, in Chapter 6, we introduce a 'bottom-up' view by discussing electronic conduction in molecules and showing how a simple model for conduction in molecules can also be applied to derive the results of the previous chapters. We also identify the limitations of the approach by discussing a structurally similar, but much different device, the single electron transistor.

We are grateful to numerous colleagues who have been generous in sharing their insights and understanding with us. There are too many to thank individually, but one person stands out - our colleague, Supriyo Datta, whose simple and elegant understanding of nano-devices provided the inspiration for this monograph.

Table of Contents

Chapter 1: Basic Concepts

1.1 Introduction

This chapter is a review of (or introduction to) some key concepts that will be needed as we examine nanotransistors. For the most part, concepts will be stated, not derived. A thorough introduction to these concepts can be found in Datta [1.1]. We also assume that the reader is acquainted with the basics of semiconductor physics (as discussed, for example, in [1.2]). For the quantum mechanical underpinning, see Datta [1.3] and for a more extensive discussion of semiclassical transport theory, see Lundstrom [1.4].

1.2 Distribution Functions

In equilibrium, the probability that a state at energy, E, is occupied is given by the Fermi function as

$$f_0 = \frac{1}{1+e^{(E-E_F)/k_BT_L}}, \tag{1.1}$$

where the subscript, 0, reminds us that the Fermi function is defined in equilibrium, and T_L is the lattice temperature. When states in the conduction band are located well above the Fermi level, the semiconductor is nondegenerate and eqn. (1.1) can be approximated as

$$f_0 \approx e^{(E_F - E)/k_B T_L}. \tag{1.2}$$

By writing the energy as the sum of potential and kinetic energies,

$$E = E_C + \tfrac{1}{2} m^* \upsilon^2, \tag{1.3}$$

where E_C is the bottom of the conduction band, eqn. (1.2) can be written as

$$f_0 \approx e^{(E_F - E_C)/k_B T_L} e^{-m^* \upsilon^2 / 2k_B T_L} = C e^{-m^* \upsilon^2 / 2k_B T_L}, \tag{1.4}$$

where C is a constant. Equation (1.4) states that in a nondegenerate semiconductor, the carrier velocities are distributed in a Gaussian (or Maxwellian) distribution with the spread of the distribution related to the temperature of the carriers. Since $\upsilon^2 = \upsilon_x^2 + \upsilon_y^2 + \upsilon_z^2$, we can also write

$$f_0 \approx C' e^{-m^* \upsilon_x^2 / 2k_B T_L}, \tag{1.5}$$

which shows that the carrier velocities are distributed symmetrically about the x-axis (or for that matter, the y- and z-axes). The average velocity of the entire distribution is zero. Figure 1.1 is a sketch of a Maxwellian velocity distribution.

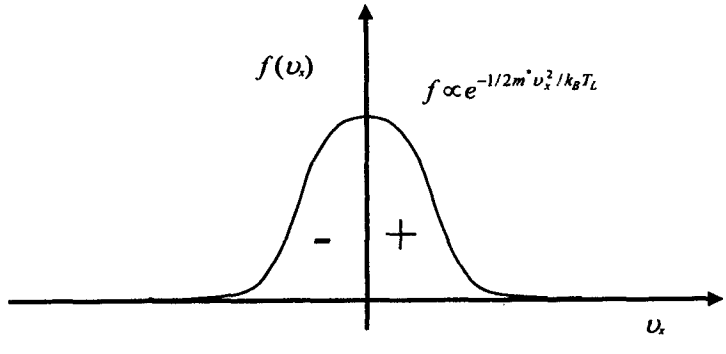

Figure 1.1 Illustration of a Maxwellian velocity distribution. At equilibrium, the distribution is symmetric and centered at $\upsilon_x = 0$, so the average velocity is zero. The spread of the distribution is related to the temperature.

1.3 Three, Two, and One-Dimensional Carriers

Within an effective mass description, the wave function for electrons in a semiconductor is obtained by solving the Schrödinger equation,

$$-\frac{\hbar^2}{2m^*}\nabla^2\psi(\mathbf{r})+U(\mathbf{r})\psi(\mathbf{r})=E\psi(\mathbf{r}). \tag{1.6}$$

If the potential energy, $U(\mathbf{r})$, is constant, the solutions are plane waves

$$\psi(\mathbf{r})=\frac{1}{\sqrt{\Omega}}e^{i\mathbf{k}\bullet\mathbf{r}}, \tag{1.7a}$$

where Ω is a normalization volume.

Consider next electrons in a thin slab as shown in Fig. 1.2. These electrons are confined in the z-direction, but they are free to move in the x-y plane. The wave function of these quasi-two-dimensional electrons is found by solving eqn. (1.6) using separation of variables to find

$$\psi(\mathbf{r})=\phi(z)\,\psi(x,y)=\phi(z)\frac{1}{\sqrt{A}}e^{i(k_x x+k_y y)}=\phi(z)\frac{1}{\sqrt{A}}e^{i\mathbf{k}_{\parallel}\bullet\boldsymbol{\rho}}, \tag{1.7b}$$

where A is a normalization area and $\boldsymbol{\rho}$ is a vector in the x-y plane. If the confining potential is a simple, square well with infinite barriers, then $\phi(z)=\sqrt{2/W}\sin(k_n z)=\sqrt{2/W}\sin(n\pi z/W)$, where $n=1, 2, ...$

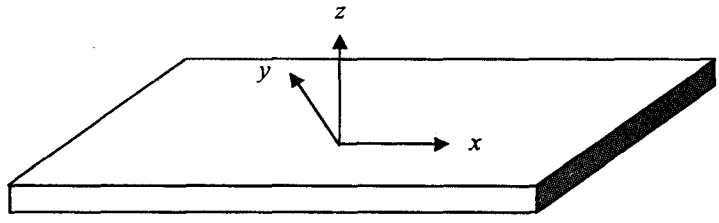

Figure 1.2 Quasi two-dimensional electrons that are confined in the z-direction but free to move in the x-y plane.

Consider next electrons in a thin wire as shown in Figure 1.3. These electrons are confined in the y- and z-directions, but they are free to move in the x direction. The wave function of these quasi-one-dimensional electrons is found solving eqn. (1.6) by separation of variables to find

$$\psi(\mathbf{r}) = \phi(y,z)\,\psi(x) = \phi(y,z)\frac{1}{\sqrt{L}}e^{ikx}. \tag{1.7c}$$

If the confining potential is a simple, square well with infinite barriers, then $\phi(y,z) = (2/W)\sin(m\pi y/W)\sin(n\pi z/W)$, where m, $n = 1, 2, \ldots$

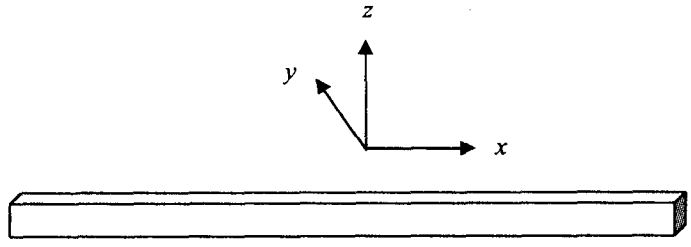

Figure 1.3 Quasi one-dimensional electrons that are confined in the y and z-directions but free to travel in the x-direction.

Quasi one- and two-dimensional electrons are produced by confining them so that they can move in one or two dimensions only. Confinement can be achieved electrostatically by producing a potential well with a gate potential, as for electrons in a bulk MOSFET, or by physically confining them to a thin, silicon film, as in a fully depleted silicon-on-insulator (SOI) MOSFET. Confinement leads to discrete energy levels. Consider the thin silicon slab shown in Fig. 1.2. If the confining potential is large, we may assume an infinite well to obtain

$$\varepsilon_n = \frac{\hbar^2 k_n^2}{2m^*} = \frac{\hbar^2 n^2 \pi^2}{2m^* W^2} \qquad n = 1,2,3\ldots \tag{1.8}$$

If this *quantum well* represents the thin silicon body of a SOI MOSFET, the confining potential lies in the direction normal to the Si/SiO_2 interface and electrons are free to move in the x-y plane, the plane of the interface. Each energy level, therefore, represents a *subband* with many allowed k-states in the plane. The total energy is the sum of the energy due to confinement in the z-direction and the kinetic energy of motion in the x-y plane,

$$E(\mathbf{k}) = \varepsilon_n + \frac{\hbar^2 k_{\|}^2}{2m^*} = \qquad n = 1, 2, 3\ldots \tag{1.9}$$

where $k_{\|}^2 = k_x^2 + k_y^2$. Because each subband has a density of states (Sec. 1.4), and given a Fermi level, we can compute the electron density in each subband (Sec. 1.5). Quantum confinement effectively raises the conduction band by an amount ε_n. In general, the shape of the potential well is more complicated than the simple box shown in Fig. 1.4, and the Schrödinger equation must be solved to determine the energy levels. The essential features remain, however. The subband energies increase and separate as the confinement increases (W decreases), light effective masses give high subband energies, and the carriers behave as quasi-two-dimensional carriers, free to move easily in only two dimensions. (Similarly, in a quantum wire, electrons are confined in two dimensions and behave as quasi-one-dimensional electrons.)

Figure 1.4b shows the constant energy surfaces for electrons in silicon, which are ellipsoids along the <100> directions. The ellipsoids are characterized by two effective masses, so the question of which effective mass to use in eqns. (1.8) and (1.9) arises. The subband energies are determined by the effective mass in the direction of the confining potential. Electrons in the two ellipsoids along the z-axis have a large effective mass (the longitudinal effective mass, $m_\ell = 0.98\, m_0$) and give rise to the unprimed series of subbands in Fig. 1.4a. On the other hand, electrons in the four other subbands have a light effective mass in the confinement direction (the transverse effective mass, $m_t = 0.19 m_0$) and produce the separate, primed series of subbands in Fig. 1.4c. So in eqn. (1.8), we use m_ℓ^* for the energy levels of the unprimed series and m_t^* for the primed series.

The heaviest effective mass gives the lowest subband energy, so the first level of the unprimed series is the lowest subband. For this level, the transverse effective mass in the plane, where electrons are free to move, is the light effective mass, m_t. This is the effective mass to use in eqn. (1.9). For the primed subbands, electrons have different effective masses when moving in the x- and y-directions, so an average effective mass must be used. When we evaluate the density-of-states, similar questions will arise. For electrons in silicon, it is often a good approximation to assume that all electrons occupy the lowest subband, especially when the confining potential is strong. Because it makes the bookkeeping easy, we will assume that only the lowest subband is occupied (see [1.5] for a more general treatment). For

the first subband, the confinement energy is determined by the longitudinal effective mass and motion in the x-y plane by the transverse effective mass.

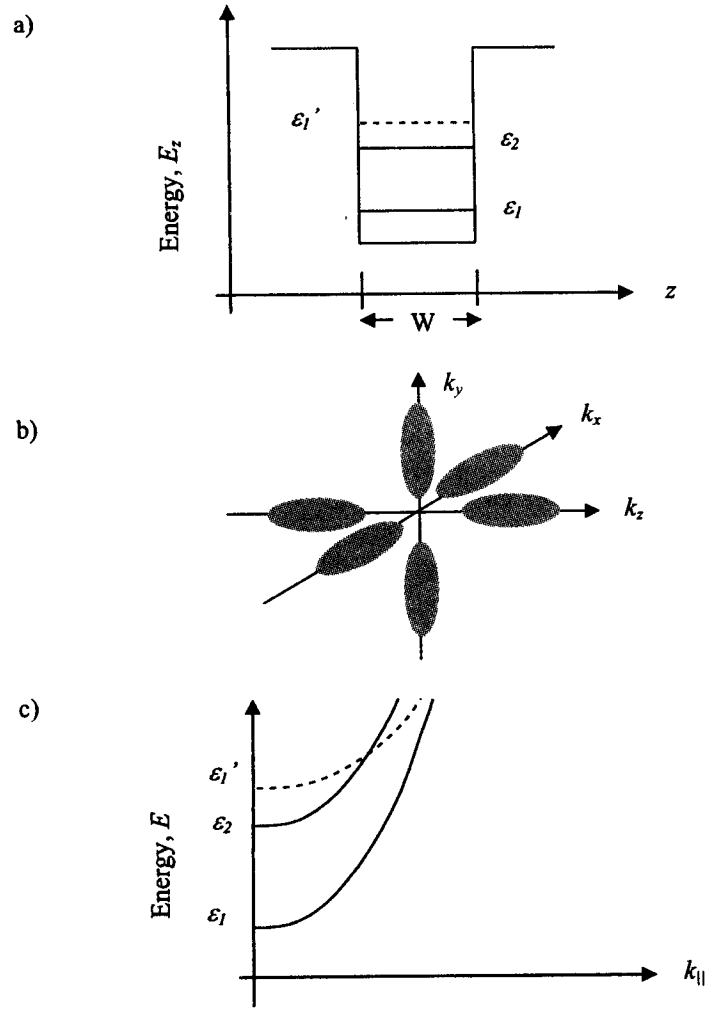

Figure 1.4 Quantum confinement in a well of width, W, with electrons free to move in the x-y plane. (a) Energy levels for a Si quantum well. (b) Constant energy surfaces for electrons in bulk Si, and (c) The $E(k)$ relation for electrons in the plane of the quantum well.

1.4 Density of States

For a bulk semiconductor with a volume, Ω, applying periodic boundary conditions to the wave function, eqn. (1.7a), leads to a discrete set of allowed k-states. The density of states in k-space is a constant,

$$N_{3D}(k)d^3k = 2\times\frac{\Omega}{8\pi^3}, \tag{1.10}$$

where Ωis a normalization volume, and the factor of 2 arises from spin degeneracy. We can use this result and the dispersion relation, $E(k)$, to derive the density of states in energy,

$$N_{3D}(E)dE = N_{3D}(k)d^3k. \tag{1.11}$$

For three-dimensional carriers, we find

$$D_{3D}(E) = \frac{N_{3D}(E)}{\Omega} = \frac{(2m^*)^{3/2}}{2\pi^2\hbar^3}\sqrt{E-E_C}. \tag{1.12}$$

Similar arguments can be used to derive the density of states for two-dimensional carriers. In k-space,

$$N_{2D}(k)d^2k = 2\times\frac{A}{4\pi^2}d^2k, \tag{1.13}$$

where A is a normalization area in the two-dimensional plane. The two-dimensional density of states per unit energy and area is

$$D_{2D}(E) = \frac{m^*}{\pi\hbar^2}. \tag{1.14}$$

Finally, for one-dimensional carriers,

$$N_{1D}(k)dk = 2\times\frac{L}{2\pi}dk, \tag{1.15}$$

where L is a normalization length for the wire. The one-dimensional density of states per unit energy and length is

$$D_{1D}(E) = \frac{\sqrt{2m^*}}{\pi\hbar}\frac{1}{\sqrt{E-E_C}}. \tag{1.16}$$