Quasi-ballistic electron transport through silicon nanocrystals

Nobuya Mori¹, Hideki Minari¹, Shigeyasu Uno², Hiroshi Mizuta³, and Nobuyuki Koshida⁴
¹Graduate School of Engineering, Osaka University, Suita, Osaka 565-0871, Japan
²Graduate School of Engineering, Nagoya University, Nagoya, Aichi 464-8603, Japan
³School of Electronics and Computer Science, University of Southampton
⁴Graduate School of Engineering, Tokyo University of Agriculture and Technology
Koganei, Tokyo 184-8588, Japan
E-mail: nobuya.mori@eei.eng.osaka-u.ac.jp

Abstract. Monte Carlo simulation of electron transport through a silicon nanocrystal array is performed to clarify the mechanism of high-energy electron emission from a porous silicon diode. The electronic states are calculated within an empirical tight-binding approximation. In the Monte Carlo simulation, optical-phonon emission and elastic tunneling processes are taken into account. It is found that initial electron acceleration, which is enhanced due to the discrete nature of lower energy levels, plays an essential role in generating high-energy electron emission.

1. Introduction
Recently, electron transport properties of nanocrystalline Si (nc-Si) have attracted considerable attention along with the remarkable progress of nc-Si material control technologies [1]. It is widely known that porous Si (PS) comprises tree-like network of many nanometer size nc-Si. When high voltage (∼10 – 20 V) is applied to a PS region, high-energy electrons are emitted from the surface [2] (see Fig. 1). This unique property has been exploited for ballistic electron emitters and various applications. Essential features of the observed emission energy distribution are summarized in Ref. [3]; which include the fact that the energy difference between the Fermi level at the Si substrate and the peak energy of the emitted distribution, \( E_{\text{loss}} \) (see Fig. 2), is nearly independent on the applied voltage \( V_a \). Although high-energy electron emission from a PS diode is clearly observed, the detailed mechanism has not been fully understood and explained.

In the present study, we have performed Monte Carlo simulation of electron transport through Si quantum dots (QDs) to clarify the underlying physics of the high-energy electron emission.

2. Analysis of the emission energy distribution
2.1. Energy levels
We use an sp\(^3\)s\(^*\)d\(^5\) empirical tight-binding method [4] to calculate electron energy levels \( E_i \) \((i = 1, 2, \cdots)\) in a Si QD. Figure 3 shows a level separation, \( \Delta E_i = E_{i+1} - E_i \), as a function of the electron energy for a Si QD with a diameter of \( d = 4.1 \) nm. The quantum confinement makes the level separation larger for lower energy region \( E \lesssim 1.5 \) eV. However, the level separation...
becomes quite small ($\Delta E_i < 10 \text{meV}$) for higher energy region. As will be shown later, this emergence of two regions of low-energy discrete levels and high-energy quasi-continuous levels plays an important role in generating the electron emission from a PS diode.

2.2. Optical-phonon emission rate
Within the Fermi’s golden rule, the optical-phonon emission rate, $W_i$, from an initial energy level $E_i$ can be written as

$$W_i = \frac{2\pi}{\hbar} \sum_j \sum_q |\langle \Psi_j(x)|U(x)|\Psi_i(x)\rangle|^2 \delta(E_i - E_j - \hbar\omega_0),$$

(1)

where $j$ is a final state index, $\Psi_i(x)$ is the wavefunction associated with the $i$-th energy level, $\hbar\omega_0$ is the optical-phonon energy, $U(x)$ is a Fourier component of the electron–optical-phonon interaction potential

$$U(x) = D_{op} \left( \frac{\hbar}{2\rho V \omega_0} \right)^{1/2} e^{i\mathbf{q} \cdot \mathbf{x}},$$

(2)

$D_{op}$ is the optical deformation potential, $\rho$ is the mass density, and $V$ is the sample volume. Note that we set the phonon occupation factor $N_0 = [\exp(\hbar\omega_0/kT) - 1]^{-1}$ ($kT$ is the thermal energy) to 0 and consider the emission process only, which should introduce a negligible error in the final results because we consider high-energy electrons with $E \sim 10 \text{eV}$. From Eqs. (1) and (2), we obtain

$$W_i = \frac{\pi D_{op}^2}{2M\omega_0} g(E_i - \hbar\omega_0),$$

(3)
Figure 3. Level separation as a function of electron energy for a Si quantum dot with a diameter of \( d = 4.1 \) nm (vertical solid line). Box shows an average over a 10 meV interval.

Figure 4. Energy distribution of the emitted electrons for applied voltage \( V_a = 18 \) V (□) and 20 V (●) at \( T = 300 \) K. Inset shows applied-voltage dependence of the energy difference between the Fermi level at the Si substrate and the peak energy of the emitted distribution.

where \( M \) is the mass of a silicon atom and the density-of-states \( g(E) \) is given by

\[
g(E) = \frac{2}{N} \sum_j \delta(E - E_j),
\]

with \( N \) being the number of silicon atoms in the QD. Here use has been made of \( F_{ij} = \Omega_D^{-1} \) (\( \Omega_D \) is the QD volume) for

\[
F_{ij} = \int \lvert \Psi_i(x) \rvert^2 \lvert \Psi_j(x) \rvert^2 dx.
\]

The value of the optical deformation potential \( D_{op} \) for high-energy electrons should be different from that for electrons near the conduction band edge. In the present study, we estimated the value from the energy shift caused by the lattice displacement.

We consider acoustic-phonon scattering as a scattering process which causes collisional broadening of the density of states. The level broadening \( \Gamma \) can be calculated in a similar way as in the optical-phonon emission rate and we have

\[
\Gamma = D_{ac} \left( \frac{kT}{\rho s_l^2 \Omega_D} \right)^{1/2},
\]

where \( D_{ac} \) is the acoustic deformation potential and \( s_l \) is the longitudinal sound velocity. The level broadening is introduced by replacing \( \delta(E) \) in Eq. (4) with \( \exp\left[-(E/\Gamma)^2/(\sqrt{\pi}\Gamma)\right] \).

2.3. Monte Carlo simulation

We use a Monte Carlo method to simulate the dynamics of electrons inside a PS diode. An electron in a QD has a probability to emit an optical phonon and a probability to escape from
the QD through elastic tunneling. The optical phonon emission rate is given by Eq. (3). The elastic tunneling time, $\tau_t$, is related to the miniband width $\Delta$ as $\hbar/\tau_t = \Delta/4$. We use a simple one-dimensional Kronig-Penny model [5] to calculate $\Delta$.

Figure 4 shows energy distribution of the emitted electrons for applied voltage $V_a = 18$ V and 20 V. We used the following parameters: the QD diameter $d = 4.1$ nm, the SiO$_2$ thickness $t_{ox} = 1$ nm, the optical phonon energy $\hbar \omega_0 = 60$ meV, the acoustic deformation potential $D_{ac} = 9.5$ eV, and the longitudinal sound velocity $s_l = 9.04 \times 10^5$ cm/s. The data in Fig. 4 is the energy distribution of electrons just before the emission from the PS region and does not include effects of the workfunction of the electrode. We assume that the potential profile from the cathode to the anode electrodes is of the form $V(x) \propto x^{3/2}$ considering the space-charge-limited operation. Coulomb interaction, which will affect the energy level distribution and the potential profile, is to be considered as PS diodes usually operate at room temperature under high applied bias. Figure 4 clearly shows that electrons are quasi-ballistically emitted from a PS diode. There is good agreement between the calculated energy distribution and the experimental results [1]. We find that initial electron acceleration, which is enhanced in QDs due to the discrete nature of lower energy levels [6], plays an essential role in generating high-energy electron emission. Once an electron is accelerated to the higher energy state ($E > \sim 1.5 \text{ eV}$), it can ballistically travel through the quasi-continuous states and is emitted from the anode electrode with high energy. We also find that the simulation results are consistent with the experimental finding that $E_{loss}$ is nearly independent on $V_a$ (see inset of Fig. 4).

3. Summary
We have performed Monte Carlo simulation of electron transport through Si QDs to clarify the underlying physics of high-energy electron emission from a PS diode. We used an empirical tight-binding method to calculate electron energy levels in a Si QD. Using the energy levels, we calculated the optical-phonon emission rate. We then performed Monte Carlo simulation of electron motion through Si QDs. The results clearly show that electrons are quasi-ballistically emitted from a PS diode. We find that initial electron acceleration, which is enhanced in QDs due to the discrete nature of lower energy levels, plays an essential role in generating high-energy electron emission.

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