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Radiation properties in electron waveguides

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We study the radiation properties in electron waveguide structure with multistep discontinuities and soft wall lateral confinement. Radiation mechanism and conditions are examined by numerical simulation of dispersion relations and transport properties. The study of geometry variations shows its significant impact on the radiation intensity and direction. In particular, the periodic corrugation structure exhibits strong directional radiation. This interesting feature may be useful to design a nanoscale transmitter, a communication device for future nanoscale system. © 2007 American Institute of Physics. [DOI: [10.1063/1.2422900](https://doi.org/10.1063/1.2422900)]

I. INTRODUCTION

Recently, there have been a lot of research efforts to investigate nanoscale systems, which have the features of high density, low power consumption, and high computation speed.^{1–16} One of the challenges is the communication between the nanoscale components in the system, such as nanosensors and nanomachines. Conventional communication approaches by optical or electromagnetic propagation are inadequate because of limitations of system size as well as the medium in which the nanoscale components are deployed.² Other schemes are needed to enable the interconnectivity among nanoscale systems and input/output ports with the macro world. Furthermore, suitable nanoscale transmitting and receiving devices are indispensable to the systems. Specifically, radiation properties are of great significance in nanoscale transmitter design. In this article, we propose a nanoscale transmitter device using soft walled electron waveguide structure with multistep discontinuities and explore its radiation performance in terms of radiation intensity and direction.

Electron waveguide is a nanostructure in which the electron wave is locally trapped and is guided along an arbitrary direction. It is well known that the wavelike behavior of electrons in the nanoscale structures is dominant so that the transport of electrons through the heterostructure device is analogous to the propagation of electromagnetic waves in dielectric waveguides.¹⁶ It may be feasible to design an electron antenna in nanoscale similar to electromagnetic wave antenna in macroscale. To date, most of the investigations with simple geometries and hard wall confinement have given many fundamental properties of electron conduction in these systems, but in realistic electron waveguides where the boundaries are defined via electrostatic confinement from metal gates, the geometries and the lateral confinement potential profile are complicated.⁶ Electrons transporting through the structure with finite-height confinement potential (soft wall) have the possibility of escaping from the channel. This escaping (radiation) phenomenon is more observable if the structure has discontinuities along the channel. Disconti-

nity in electron waveguide structure is very important not only for the unavoidable surface roughness problem caused by the manufacture process, but also for some structures in which discontinuity is introduced intentionally. The optimization of the structure is to minimize the electron radiation in the former, whereas to maximize the radiation for specific usages in the latter. As a result, a thorough study of radiation properties is essential in both cases. Although several papers dealing with the discontinuity problem either analytically or numerically have been published,^{11–16} so far there is no systematic study of radiation properties of soft walled electron waveguide structure with multistep discontinuities.

In this article, we make an attempt to study the radiation mechanism, to determine their relation to the geometry of the structure, and to evaluate its potential application as a nanoscale transmitter device. The article is organized as follows. In Sec. II, theoretical equations governing the electron wave in the device are introduced. Mode-matching method based on microwave transmission line theory is used to model step discontinuity in terms of the boundary conditions. A detailed finite element method (FEM) formalism to solve system model numerically is given in the Appendix. In Sec. III, radiation mechanism and conditions are examined by numerical simulation of dispersion relations and transport properties. In Sec. IV, geometry dependent radiation intensity and direction are analyzed for double step discontinuities and periodic corrugation structures. Finally, in Sec. V, we give our conclusions.

II. THEORETICAL MODEL

The electron waveguide as shown in Fig. 1(a) can be decomposed into uniform waveguides and the junctions connecting them. To describe the behavior of electrons in electron waveguides with multistep discontinuities and soft wall lateral confinement, Schrödinger wave equation with finite lateral boundary condition is used for uniform waveguides and rigorous mode-matching method is used for the junctions.

Assume electron motion in a uniform electron waveguide section is ballistic (without any scattering), the elec-

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FIG. 1. (a) Junction of two uniform electron waveguides. (b) Its equivalent transmission line model.

tron wave is governed by the time-independent Schrödinger equation under the effective mass approximation given as³

$$\nabla \left(\frac{1}{m^*} \nabla \Psi \right) + \frac{2}{\hbar^2} (E - U) \Psi = 0, \quad (1)$$

where Ψ is electron wave function, E is the electron's total energy, U is the potential energy, m^* is the effective mass, and $\hbar$ is the reduced Planck constant.

For simplicity, we assume the wave function Ψ is invariant along the *y* direction ($\partial/\partial y = 0$) and propagating along the *z* direction as shown in Fig. 1(a). Thus, Ψ can be expressed as

$$\Psi(x, z) = \Phi(x) e^{-jk_z z}. \quad (2)$$

The wave function for continuity of probability flow^{3,11} is

$$\psi(x, z) = \frac{\hbar k_z}{m^*(x)} \Phi(x) e^{-jk_z z}, \quad (3)$$

where transverse wave function $\Phi(x)$ satisfies the following one-dimensional (1D) Sturm-Liouville generalized eigenvalue problem:

$$\left\{ \frac{d}{dx} \frac{1}{m^*(x)} \frac{d}{dx} + \frac{2}{\hbar^2} [E - U(x)] \right\} \Phi_m(x) = k_{z(m)}^2 \frac{1}{m^*(x)} \Phi_m(x). \quad (4)$$

An infinite set of eigensolutions of Eq. (4) constitutes wave modes (energy subbands) of the electron waveguide. Eigenvalue $k_{z(m)}$ is the longitudinal propagation constant of the *m*th mode and a corresponding eigenfunction $\Phi_m(x)$ is the *m*th mode transverse wave function. The eigenfunction set Φ_m satisfies the orthonormalization relation as

$$\left\langle \Phi_m \left| \frac{1}{m^*} \right| \Phi_n \right\rangle = \int_0^h \frac{1}{m^*(x)} \Phi_m(x) \Phi_n(x) dx = \delta_{mn}. \quad (5)$$

In order to analyze the discontinuities in electron waveguide, mode-matching method based on transmission line model is adopted as follows:¹¹

$$\Psi(x, z) = \sum_{m=1}^{\infty} V_m(z) \Phi_m(x),$$

$$\psi(x, z) = \sum_{m=1}^{\infty} I_m(z) \frac{\sqrt{E}}{m^*(x)} \Phi_m(x). \quad (6)$$

The total wave function in each uniform waveguide can be expressed in terms of the superposition of a complete set of mode functions as indicated in Fig. 1. In the transmission line model, k_{zm} is the propagation wave number of the *m*th mode; the characteristic impedance of the *m*th mode in the *z* direction is

$$Z_m = \frac{\sqrt{E}}{\hbar k_{zm}}. \quad (7)$$

At the step discontinuity between two waveguides *i* and *i*+1, the two wave functions must be continuous such as

$$\Psi(x, z^{(i,i+1)-}) = \Psi(x, z^{(i,i+1)+}), \quad (8)$$

$$\psi(x, z^{(i,i+1)-}) = \psi(x, z^{(i,i+1)+}). \quad (9)$$

Combining boundary conditions [Eqs. (8) and (9)] with orthonormalization relation [Eq. (5)], we can get¹¹

$$\begin{bmatrix} V^i \\ I^i \end{bmatrix} = M^{(i,i+1)} \begin{bmatrix} V^{i+1} \\ I^{i+1} \end{bmatrix}, \quad (10)$$

$$M^{(i,i+1)} = \begin{bmatrix} P^{(i,i+1)} & 0 \\ 0 & Q^{(i,i+1)} \end{bmatrix}, \quad (11)$$

where

$$P_{mn}^{(i,i+1)} = \left\langle \Phi_m^i \left| \frac{1}{m^*(i)} \right| \Phi_n^{i+1} \right\rangle = \int_0^h \frac{1}{m^*(i)(x)} \Phi_m^i(x) \Phi_n^{i+1}(x) dx, \quad (12)$$

$$Q_{mn}^{(i,i+1)} = \left\langle \Phi_m^i \left| \frac{1}{m^*(i+1)} \right| \Phi_n^{i+1} \right\rangle = \int_0^h \frac{1}{m^*(i+1)(x)} \Phi_m^i(x) \Phi_n^{i+1}(x) dx. \quad (13)$$

We can then obtain the scattering matrix *S* of the step discontinuity by the conversion between transmission (ABCD) matrix *M* and scattering matrix *S*.¹⁹

In our approach, the electron waveguide with multistep discontinuities is first decomposed into uniform waveguides and the junctions connecting them. Eigenvalue and eigenfunction sets found from Eq. (4) of each uniform waveguide are used for mode matching of junctions to get the scattering matrix of each junction. Then, the scattering matrix of the whole structure is obtained by cascading the individual scattering matrix of the uniform parts and junction parts.

FEM is adopted to solve the system models, which is described in detail in the Appendix, because of its versatility in treating arbitrary potential and effective mass profiles.

FIG. 2. Double step continuity structure configurations.

III. RADIATION MECHANISM AND CONDITIONS

Figure 2 gives a three layered electron waveguide with double step discontinuities in two-dimensional (2D) GaAs/Al_rGa_{1-r}As semiconductor heterostructure material configurations. The hard walls with infinite potential are placed far enough away from the film surface as FEM simulation boundaries to satisfy the actual soft wall conditions and to make the continuous spectrum of radiation modes discrete.¹² Electron potential energy U and electron effective mass m^* for Al concentration ratio r are given by¹¹

$$U = 0.7731r \text{ (eV)}, \quad (14)$$

$$m^* = (0.067 + 0.083r)m_0 \text{ (kg)}, \quad (15)$$

where m_0 is the rest mass of an electron and r in three layers is given as $(r_s, r_f, r_c) = (0.2, 0, 0.2)$, which results in a quantum well potential profile with symmetrical finite potential barriers.

With the incidence of the guided mode from the left side of waveguide 1, nonguided modes including the propagating radiation modes are excited at the junctions of the three uniform waveguides because of the discontinuities. On such a discontinuous structure, the fields vary with the successive positions along it. Thus it is necessary to consider rigorously the field continuity conditions on the whole boundary surface of the structure by taking into account the effect not only of the conversion of power among the guided modes and the scattering of power into the radiation modes but also of the coupling of the power of the radiation mode into both guided modes and the other radiation modes. As a result, a complete set of mode analysis is necessary to explain the radiation phenomena.

Dispersion relations (electron energy vs k_z^2) for the first two modes of the uniform waveguides 1 and 2 in Fig. 2 are depicted in Fig. 3, where $W_2 = 2W_1 = 11.3068$ nm. The propagating guided wave modes¹⁵ are determined by wave number (k_s, k_f, k_c) in the three layer regions as

FIG. 3. Dispersion relations (electron energy vs k_z^2) of the first two guide modes in WG1 and WG2.

$$0 \leq k_z^2 \leq k_f^2, \quad k_z^2 > k_s^2 \quad \text{and} \quad k_z^2 > k_c^2, \quad (16)$$

where $k_i^2 = (2m_i^*/\hbar^2)(E - U_i)$, $i = s, f, c$.

As indicated in Fig. 3, two types of cutoff energy can be found from Eq. (16) as low cutoff energy $E_{l(m)}^{(i)}$ and upper cutoff energy $E_{u(m)}^{(i)}$ for the m th mode in waveguide i . As shown in Fig. 3, during the simulated energy range, both waveguides have the dispersion curves of the first two normal modes, whereas only waveguide 1 is a single guided mode structure.

When the guided mode is incident from the left side of waveguide 1, the transport properties are given in Fig. 4(a) as a function of electron energy, where $L = W_2$. Transport properties can be classified according to three energy range cases: (1) When $E < E_{l(1)}^{(1)}$, as shown in Fig. 3, no propagating guided mode exits in three waveguides and no transmission occurs; (2) when $E_{l(1)}^{(1)} \leq E \leq E_{s(c)}$, as indicated in Fig. 3, guided modes exit in three waveguides, but no radiation mode is propagating. So the addition of guided mode reflection and transmission is equal to 1; (3) when $E > E_{s(c)}$, as found in Fig. 3, propagating radiation modes begin to appear. As a result, the addition of guided mode reflection and transmission is smaller than 1.

Radiation probabilities as shown in Fig. 4(b), coinciding with the result of transport properties, are greater than zero at electron energy range $E > E_{s(c)}$. Forward radiation probability is larger than the backward one. During the simulated energy range, radiations tend to increase with the increasing energy in large energy range, but oscillate in short energy range.

Radiation mechanism can be further explained by the probability distribution of electron along the x direction derived from the transverse wave mode function as shown in Fig. 5. As can be seen from Fig. 5(a), for the fundamental mode, electron wave propagates mainly in the film region and the electron wave penetrates into substrate and cover regions near the upper cutoff energy. Figure 5(b) plots the case for the first high order mode in waveguide 1. We can find that propagating mode occurs when electron energy is

FIG. 4. (a) Guided mode transport properties as a function of electron energy of the structure in Fig. 2. (b) Guided mode radiation characteristics as a function of electron energy of the structure in Fig. 2.

greater than $E_{s(c)}$. Since waveguide 1 is a single guided mode structure, such propagating mode is due to the radiation of electron wave into the substrate and cover regions. It will result in the escaping of electrons for soft walled waveguide structure in practice.

IV. GEOMETRY DEPENDENT RADIATION INTENSITY AND DIRECTION

As we can expect, if there are no discontinuities along the film layer, there will be no radiation mode excited. Geometry should have a strong impact on the radiation properties, which are further investigated for specific energy as shown in Fig. 6 in terms of the degree of step discontinuity and the width of middle waveguide for double step discontinuity structure.

As indicated in Fig. 6(a), guided mode transports through the structure without radiation for small step discontinuity. With increasing step discontinuity, guided mode radiates more until it reaches the maximum radiation point at a specific step discontinuity. After that point, radiations decrease with increasing step discontinuity. As shown in Fig. 6(b), radiation characteristics are simulated as a function of

FIG. 5. (a) k_z^2 and E dependences of the transverse wave function for the fundamental mode in WG1. (b) k_z^2 and E dependences of the transverse wave function for the first high order mode in WG1.

the width of waveguide 2 for $E=0.2$ eV. Guided mode will transmit without radiation at very small width as can be expected. With increasing width, radiations tend to oscillate. This phenomenon can be explained by the phase shift of the electron wave propagating in the middle waveguide. The oscillation period can be estimated by the half guide wavelength of the major guided mode in WG2. From Fig. 3, k_z^2 of the major guided mode in WG2 is 0.4 nm^{-2} , which is equal to the half guide wavelength of $0.45W_2$. The deviation of the period is caused by the existence of high order guided mode in WG2.

In addition to the magnitude, the space radiation direction properties are of great significance. It is possible to control the radiation direction and intensity by adjusting the geometry. Radiation pattern is investigated with respect to W_1/W_2 and L/W_2 , as shown in Fig. 7. The results show that for the double step discontinuity structure, the radiation direction is not quite selective although the radiation direction and intensity are still a strong function of the geometry.

In order to take advantage of the possible high radiation direction selectivity, let us next consider the periodic corrugations of finite length¹⁸ as shown in the inset of Fig. 8(a). This structure is given by the cascade connection of a finite number of networks given by Fig. 2. By applying our approach, described in Sec. II, we can obtain the numerical results shown in Fig. 8. These examples are obtained for a structure with the dimensions indicated in the inset and for a

FIG. 6. (a) Guided mode radiation characteristics as a function of W_2/W_1 at $E=0.2$ eV. (b) Guided mode radiation characteristics as a function of WG_2 width L at $E=0.2$ eV.

different number N_c of corrugations. In order to explain the results physically, the parameters of the structure are chosen so that only the major guiding mode propagates in each uniform waveguide section and we consider that this mode incident from the left-hand side excites the structure. Figure 8(a) shows the reflected probability of the major guiding mode where $N_c=10$ and 20 corrugations, as a function of the normalized period $2L/\lambda_f$. λ_f is the wavelength of the electron wave in the film layer. Figure 8(b) shows the forward and backward radiation probabilities. If the structure under consideration is infinite in length, the center of the Bragg reflection can be calculated by $2(k_{z1}L_1 + k_{z2}L_2) = 2n\pi$. From the structure dimensions, we can derive that the center of the first Bragg reflection is at $2L/\lambda_f = 0.55$, while the second Bragg reflection is at $2L/\lambda_f = 1.10$. As seen from Fig. 8(a), it is found that strong reflection indeed appears at around $2L/\lambda_f = 0.55$, corresponding to the center of the first Bragg reflection region, and also that significant radiation occurs between the first Bragg reflection and the second Bragg reflection region. However, there are many subsidiary reflection peaks even outside the first Bragg reflection region, and

FIG. 7. Radiation patterns for the double step discontinuity structure (a) vs W_2/W_1 with $L=W_2$ and $E=0.2$ eV: (left) forward and (right) backward; (b) vs L/W_2 with $W_2=2W_1$ and $E=0.2$ eV: (left) forward and (right) backward.

the radiation still occurs in the first Bragg reflection region with a complicated feature arising from the finite length of the periodic structure.

The backward radiation patterns of the periodic structure are simulated as shown in Fig. 9 for structures with $2L/\lambda_f = 0.7, 0.8$, and 0.9 in the case where $N_c=10$ and 20. The peak value is normalized to unity for each radiation pattern, and the axes along $\theta=0^\circ$ and 90° coincide with the x and the negative z directions, respectively. The effect of the finite length is indeed clearly seen in the narrowing main lobe as the number of corrugations increases, but more significantly, such an effect results in complicated spurious lobes. However, the direction of each maximum lobe is in good agreement with each other [$\theta=41^\circ$ for Fig. 9(a), $\theta=60^\circ$ for Fig. 9(b), and $\theta=73^\circ$ for Fig. 9(c)]. If the structure under consideration is infinite in length, the radiation direction can be calculated by $\theta = \cos^{-1} | [k_{z(1)}^{(1)} k_{z(1)}^{(2)} - (\pi/L)] / k_{s(c)} |$ [$\theta=41.36^\circ$ for Fig. 9(a), $\theta=60.54^\circ$ for Fig. 9(b), and $\theta=73.11^\circ$ for Fig. 9(c)]. The numerical simulation matches the theoretical analysis very well.

V. CONCLUSION

Radiation mechanism and geometry dependent properties are studied for electron waveguides with multistep discontinuities and soft wall lateral confinement based on the finite element method (FEM) and rigorous mode-matching method. The simulation results show that electron waveguide exhibits a very similar physical behavior with electromagnetic waveguide although it has its own features. Electron waveguide radiation patterns give a detailed picture of how electron wave radiate in soft walled structures. The periodic corrugation structure exhibits strong directional radiation.

FIG. 8. The periodic structure with a finite number N_c of corrugations: (a) reflected probability of the incident major guided mode and (b) radiation probabilities vs the normalized period $2L/\lambda_f$.

This interesting feature may be useful to design a nanoscale transmitter, a communication device for future nanoscale system.

APPENDIX: FEM FORMALISM

In FEM,²⁰ the wave function can be approximated by the node value in each element as

$$\Phi(x) = \sum_{e=1}^{N_e} \sum_{i=1}^2 \Phi_i^e N_i^e(x), \quad (\text{A1})$$

where 1D linear interpolation functions are given by

$$N_1^e(x) = \begin{cases} \frac{x_2^e - x}{x_2^e - x_1^e}, & x_1^e < x < x_2^e \\ 0 & \text{otherwise,} \end{cases} \quad (\text{A2})$$

$$N_2^e(x) = \begin{cases} \frac{x - x_1^e}{x_2^e - x_1^e}, & x_1^e < x < x_2^e \\ 0 & \text{otherwise.} \end{cases} \quad (\text{A3})$$

Using Galerkin's method²⁰ with weighting function $W_m(x) = N_j^e(x)$, we obtain

FIG. 9. Radiation patterns for the periodic structure with a finite number N_c of corrugations: (a) normalized period $2L/\lambda_f=0.7$, (b) normalized period $2L/\lambda_f=0.8$, and (c) normalized period $2L/\lambda_f=0.9$. (Left) $N_c=10$ and (right) $N_c=20$.

$$\begin{aligned} \sum_{i=1}^2 \Phi_i^e \left\{ \int_{x_1^e}^{x_2^e} \left[-\frac{1}{m^*(x)} \frac{dN_i^e(x)}{dx} \frac{dN_j^e(x)}{dx} + \frac{2}{\hbar^2} (E - U(x)) \right. \right. \\ \left. \left. - \frac{1}{m^*(x)} k_z^2 N_i^e(x) N_j^e(x) \right] dx \right\} + \left[\frac{1}{m^*(x)} \frac{d\Phi}{dx} \right]_{x=h} \\ - \left[\frac{1}{m^*(x)} \frac{d\Phi}{dx} \right]_{x=0} = 0. \end{aligned} \quad (\text{A4})$$

We can change it to elemental matrix form

$$[A_{ij}^e] \{\Phi_j^e\} + [\text{end}] = k_z^2 [D_{ij}^e] \{\Phi_j^e\}, \quad (\text{A5})$$

where

$$A_{ij}^e = \int_{x_1^e}^{x_2^e} \left[-\frac{1}{m^*(x)} \frac{dN_i^e(x)}{dx} \frac{dN_j^e(x)}{dx} + \frac{2}{\hbar^2} (E - U(x)) \right] dx, \quad (\text{A6})$$

$$D_{ij}^e = \int_{x_1^e}^{x_2^e} \frac{1}{m^*(x)} N_i^e(x) N_j^e(x) dx, \quad (\text{A7})$$

[end]

$$= \begin{cases} -\frac{1}{m^*(x)} \frac{d\Phi}{dx} \Big|_{x=0} & \text{at boundary node } x = x_1^1 = 0 \\ \frac{1}{m^*(x)} \frac{d\Phi}{dx} \Big|_{x=h} & \text{at boundary node } x = x_2^{N_e} = h \\ 0 & \text{otherwise.} \end{cases} \quad (\text{A8})$$

Each wave function mode is normalized as

$$\overline{\Phi_m} = \Phi_m / \sqrt{A_m}, \quad (\text{A9})$$

where

$$A_m = \int_0^h \frac{1}{m^*(x)} \Phi_m(x) \Phi_m(x) dx = \sum_{e=1}^{N_e} \frac{1}{m^*(x_1^e)} [\Phi_{m1}^e \Phi_{m2}^e] \\ \times \begin{bmatrix} \int_{x_1^e}^{x_2^e} N_1^e(x) N_1^e(x) dx & \int_{x_1^e}^{x_2^e} N_1^e(x) N_2^e(x) dx \\ \int_{x_1^e}^{x_2^e} N_1^e(x) N_2^e(x) dx & \int_{x_1^e}^{x_2^e} N_2^e(x) N_2^e(x) dx \end{bmatrix} \begin{bmatrix} \Phi_{m1}^e \\ \Phi_{m2}^e \end{bmatrix}. \quad (\text{A10})$$

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