List of changes

The following is the list of changes. Mainly the changes are grammatical corrections and elimination of vague sentences. Old sentences or phrases changes to (→) new corrected sentences and phrases.

(In Abstract)

L1 … to the electronic structure calculations for high electron mobility transistor (HEMT).
→ … to electronic structure calculations for high electron mobility transistors (HEMTs).

L2 The layered structure such as field effect transistor (FET), especially HEMT, the current density is mainly dependent on the electron mobility and the electronic field in the vicinity of the gate part, where both of them are recognized as a constant.
→ In layered structures such as field effect transistors (FETs), and especially HEMTs, the current density is mainly dependent on the electron mobility and the electronic field near the gate, where both can be taken to be constant.

L4 … in the vicinity of the gate part, where both of them are recognized as a constant.
→ … near the gate, where both can be taken to be constant.

L5 … and the gate applied voltage can be obtained by one dimensional calculation.
→ … and the applied gate voltage can be obtained by a one-dimensional calculation.

L6 Then, it is easier to evaluate SSPH in the simple quantum device properties. We mainly focus on the I-V characteristics, which is one of the typical device features. The electronic structure was calculated both in SSPH and FD. In the comparison of the characteristics of HEMT, the result of SSPH is in good agreement with that of FD. The accuracy of SSPH is similar to that of FD. In the simple case of SSPH, where three particles in the support region and distributed in the same distance, we shows there is a equivalence to the three point method in FD.
→ Then, it is easy to apply SSPH to evaluate the simple quantum properties of a device. We mainly focus on the I-V characteristics, which are typical device features. The electronic structure of a HEMT was calculated using both SSPH and finite-difference (FD) methods. The results from SSPH calculations are in good agreement with those from the FD method, and the accuracy of SSPH is similar to that of FD. In a simple example, where three particles are employed in the SSPH domain, we show there is an equivalence to the three-point method in FD.

(1. Introduction)

P1L3 … hydrodynamic problems, which deal with …
→ … hydrodynamic problems that deal with …

P1L4 … the SPH based method has been…
→ … SPH-based methods have been…

P1L6 On the other hand, there are few studies for the electronic structure calculation [5, 6].
→ However, there are few studies for electronic structure calculations [5, 6].

P1L8 The SPH based method …
→ An SPH-based method …

P1L9 … that standard SPH method …
→ … that the standard SPH method …

P1L10 In considering the application to practical electronic structure calculation, obtaining the almost equal accuracy to finite-difference method by using meshfree particle method is one of the problems. As one of the improved techniques, Symmetric Smoothed Particle Hydrodynamics (SSPH) [8, 9] have been proposed.

→ In considering applications of mesh-free particle methods to practical electronic structure calculations, obtaining comparable accuracy to the results of finite-difference (FD) methods is one of the problems. Symmetric Smoothed Particle Hydrodynamics (SSPH) [8, 9] have been proposed as one of the improved techniques.

P1L14 …SPH using Taylor series expansion.

→ SPH by using a Taylor-series expansion.

P1L15 We applied this SSPH to the practical electronic device calculation …

→ We applied SSPH to a practical electronic device calculation …

P1L16 As a field-effect transistor (FET) incorporating heterojunctions, HEMT have attracted attention to its features …

→ As field-effect transistors (FETs) incorporating heterojunctions, HEMTs have attracted attention due to features …

P1L18 These features are suitable for the applications in industry such as high-frequency devices and low noise amplifies [10]. In this device, …

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P2L1 … the accumulated electrons, which are known as two-dimensional electron gas (2DEG) [11]. The calculation of the electronic structure can be expressed in one dimensional equation. Thus, it is quite a nice example to check the accuracy of SSPH. When the non-uniform particle distribution of computational points can be treated in the frame work of SSPH, we expect to reduce computational costs significantly. However, our calculation of SSPH was performed in the uniform particle distribution for simplicity.

→ … the accumulated electrons, which can be considered as a two-dimensional electron gas (2DEG) [11]. For such a case, calculations of the electronic structure can be expressed using one dimensional equations. This provides quite a nice example to use in checking the accuracy of SSPH calculations. Non-uniform distributions of computational points can be treated in the frame work of SSPH, which we expect to reduce computational costs significantly. However, the SSPH calculation described in this paper was performed for a uniform particle distribution for simplicity.

P2L7 … the simple quantum device of HEMT.

→ the simple quantum device of a HEMT.

(2. Method)

P2L13 The typical simple single heterojunction HEMT is shown in Fig.1. Usually, it is fabricated on the epitaxial mulit-layers. Using the band offset at the heterojunction, the electronic device such as FET, expecially HEMT, works quite efficiently. For a long time, this device have been intensively studied experimentally and theoretically [11, 12]. The electron charge in this system is recognized as a quasi-2D system.

→ A typical, single-heterojunction HEMT is shown in Fig. 1. Usually such a device is fabricated as an epitaxial multi-layer structure. Using the band offset at the heterojunction, electronic devices such as FETs, and especially HEMTs, work quite efficiently. Such devices have been intensively studied both experimentally and theoretically [11,12]. The electronic charge

distribution in this system can be considered as a quasi-2D system.

P2L17 … is controlled the change of the applied voltage to the gate, …
→ … is controlled by changing the voltage applied to the gate, …

P2L19 The current density of the heterosructure FET is decided the ionized impurities, …
→ The current density of the heterostructure FET is determined by the ionized impurities, …

P2L20 The gate electric field is …
→ The electric field is …

P2L21 Also, the electron mobility is recognized as almost constant in the long gate device.
→ Also, the electron mobility can be taken as constant in the long gate device.

P2L23 Thus, in one dimensional analysis according to the depth direction from the surface, which is corresponding to the gate, it is possible to estimate the characteristics, e.g. the relation between the channel current and the applied gate voltage of the practical FET device[10]. The channel is narrow enough to expressed by the quantized states, which are simply described in a one dimensional (1D) equation.
→ Thus, in a one-dimensional analysis, in a direction perpendicular to the surface that corresponds to the gate, it is possible to determine the device characteristics, e.g., the relation between the channel current and the applied gate voltage for a practical FET device [10]. The channel is narrow enough to be expressed in terms of quantized states, which are simply described in a one-dimensional (1D) equation.

P2L29 In the general analysis of the characteristic behavior of the device, we usually solve the effective one-dimensional, one electron Schrödinger equation and the Poisson's equation [15].
→ In our general analysis of the characteristic behavior of the device, we solved the effective one-dimensional, one-electron Schrödinger equation and Poisson's equation [15].

P3L1 … the depth direction beneath the gate, …
→ … the vertical direction beneath the gate, …

P3L4 where E_i is the i-th eigenvalue, …
→ where E_i is the i-th energy eigenvalue, …

P3L6 from the Poisson’s equation.
→ from Poisson’s equation.

P3L7 … a band offset of the both heterointerfaces in the HEMT structure. The potential profile ϕ is determined by the ionized charge ρ_I
→ … the band offset of the two heterojunction interfaces in the HEMT structure. The potential profile ϕ is determined by the ionized charge ρ_I.

P3L10 … which is, mainly in the channel region, calculated by
→ … which exists mainly in the channel region, is given by

P3L11 (the comma at the end of Eq. (4) is replaced by a period)

P3L12 where g_i is a degeneracy of the state, E_F is the Fermi level, T is the temperature, and k is the Boltzmann constant. The electrostatic potential distribution derived from a self-consistent procedure of the Schrödinger and Poisson equations. Usually, these equation in Eqs.(1) and (2) are expressed in the finite difference method (FD), and solved in an appropriate boundary conditions. In addition, the matching conditions at the heterojunction interface should be maintained for the derivatives of wave functions and electrostatic potentials. The solution can be obtained by solving each equation step by step until convergence [13, 14, 15, 16]. From the electronic charge density, V is determined, in which the exchange-correlation potential can be

also involved.

→ Here g_i is the degeneracy of the state, E_F is the Fermi level, T is the temperature, and k is Boltzmann's constant. The electrostatic potential distribution is obtained from a self-consistent solution of the Schrödinger and Poisson equations. Usually, Eqs. (1) and (2) are expressed in finite-difference (FD) form, and are solved subject to appropriate boundary conditions. In addition, matching conditions at the heterojunction interfaces are required for the derivatives of wave functions and electrostatic potentials. The solution can be obtained by solving each equation step-by-step until convergence is achieved [13, 14, 15, 16]. The electronic charge density determines the potential V, which can also include the exchange-correlation potential.

P3L26 where h is the smoothing length, that defines the support region Ω. As the kernel function, we adopt the Wendland function in one dimensional system [17]. It is finite, and convenient for numerical calculations.

→ where h is the smoothing length that defines the domain Ω. We adopt the Wendland function as the kernel function in the one-dimensional system we consider [17]. It is finite and is convenient for numerical calculations:

P3L31 SSPH corrects the approximation of SPH using the Talor series expansion of $\psi(\mathbf{r})$. The right-hand side of Eq.(5) and its moment can be rewritten as follows;

→ SSPH corrects the approximation of SPH using a Taylor-series expansion of $\psi(\mathbf{r})$. The right-hand side of Eq. (5) can then be rewritten as follows:

P4L1 where $k = 0, 1, \ldots, m$. In the expression of SSPH, there is no derivative of the kernel function, which sometimes causes errors in SPH calculations. The accuracy of SSPH is mainly depend on the order of Taylor series expansion[5]. Equation (7) have a form of simultaneous linear equation $P = KD$ as shown below, where P is the moment of the identity, D is the series of derivatives, and K is a symmetric matrix, whose element consists of the moment of the kernel. This integral equation is approximated by the summation of the particles in the support region Ω corresponding to the smoothing length h.

→ where $k = 0, 1, \ldots, m$. The integral equation is thus approximated by the summation over the particles in the domain Ω corresponding to the smoothing length h. In this version of SSPH, there is no derivative of the kernel function, which sometimes causes errors in SPH calculations. The accuracy of SSPH mainly depends on the order of the Taylor-series expansion [5]. Equation (7) has the form of simultaneous linear equation, $P = KD$, as given below:

P4L11 Naturally, Schrödinger equation in Eq.(1) is expressed in a generalized eigenvalue problem. The small volume of the j-th particles around the particle i is expressed ΔV_j, which is calculated the number density $n(z_j)$

→ Naturally, the Schrödinger equation in Eq. (1) is a generalized eigenvalue problem. The small volumes occupied by the j-th particles surrounding particle i are defined as ΔV_j, which is calculated the number density $n(z_j)$:

P4L15 Taking account of $D_0 = \psi|_{z_i}$, $D_1 = \frac{\partial \psi}{\partial z}|_{z_i}$, and $D_2 = \frac{1}{2}\frac{\partial^2 \psi}{\partial z^2}|_{z_i}$, the Schrödinger and Poisson equations Eqs.(1) and (2) at the position of the i-th particle can be rewritten in the expression of the SSPH discretization. For example, in the simplest case of a constant effective mass, Schrödinger equation Eq.(1) of the i-th particle in SSPH can be described as

→ Defining $D_0 = \psi|_{z_i}$, $D_1 = \frac{\partial \psi}{\partial z}|_{z_i}$, and $D_2 = \frac{1}{2}\frac{\partial^2 \psi}{\partial z^2}|_{z_i}$, we can write the Schrödinger and Poisson equations Eqs. (1) and (2) at the position of the i-th particle in the form of the SSPH discretization. For example, in the simplest case of a constant effective mass, the Schrödinger equation, Eq. (1), for the i-th particle in SSPH can be written as

P4L20 Poisson equation in Eq.(2) with constant permittivity is also simply described, similar to the derivation of Eq.(10).
→ Poisson's equation in Eq. (2), with constant permittivity, also can be simply described in a manner similar to the derivation of Eq. (10).

P4L21 … and exchange-correlation potentials are also determined as well.
→ and the exchange-correlation potentials are also determined.

P4L23 … so as to obtain a certain level of accuracy.
→ … so as to obtain a specific level of accuracy.

P3L23 This is an particular feature of this method, and we can expect to reduce the computational cost significantly.
→ This is a particular feature of this method, which we expect to reduce the computational cost significantly.

(3. Results and discussion)

P4L27 We have calculated the device characteristics both in SSPH and FD, and compared both of the results. In the calculation of SSPH, we adopted the smoothing length $h = 0.2$ Å and the constant particle distributions in the distance $\Delta x = 0.2$ Å. The mesh size of FD were used as the same value $\Delta x = 0.2$ Å as the particle distribution of SSPH. Figure 2 shows that the band structure and the charge profile of the results of SSPH and those of Finite difference (FD) are plotted along the depth direction. Both of the results of SSPH are in good agreement with those of FD.
→ We have calculated device characteristics both in SSPH and FD, and have compared the results. In the SSPH calculation, we adopted the smoothing length $h = 0.2$ Å and assumed constant particle distributions over the distance $\Delta x = 0.2$ Å. For the FD mesh size, we used the same value $\Delta x = 0.2$ Å as for the particle distribution in SSPH. Figure 2 shows that band structure and the charge profile of the results from both the SSPH and FD calculations, plotted in the vertical direction. Both results from SSPH are in good agreement with those from the FD calculation.

P4L34 … is estimated from …
→ … is determined by …

P4L35 … as a function of the gate voltage V_g.
→ … as functions of the gate voltage V_g.

P4L35 These are indicated …
→ These provide …

P5L1 Changing the applied gate voltage is corresponding to calculating the characteristics in the different boundary condition at the surface $z = 0$. We have calculated the charge profile to the different gate voltage by the step of $\Delta V_g = 0.005$. The sheet carrier density N_s is integrated over the the whole region and plotted in Fig.3.
→ Changing the applied gate voltage corresponds to calculating the characteristics using different boundary conditions at the surface $z = 0$. We have calculated the charge profile for different gate voltages in the steps of $\Delta V_g = 0.005$. The sheet carrier density N_s integrated over the whole region and is plotted in Fig. 3.

P5L5 … in a difference scheme, which is also plotted in Fig. 3.

→ … in a difference scheme; this is also plotted in Fig. 3.

P5L7 The accuracy is quite enough for the practical device simulation. In the calculation of SSPH, we have also tried the different smooth length $h = 0.3$ Å, which includes five particles in the support region. The results of the calculation were the same as the calculation with the smooth length $h = 0.2$ Å.

→ The accuracy is sufficient for practical device simulations. In the SSPH calculation, we have also tried the different smoothing length $h = 0.3$ Å, which includes five particles in the calculation domain, rather than three. The results were the same as for the calculation performed with the smoothing length $h = 0.2$ Å.

P5L11 There is a quite difference in the expression between SSPH and FD. The former one is based on integral equations, and the other is on the differential equation, respectively. On the other hand, there is an equivalence in the simplest cases, which means that SSPH uses three particles in the support region, and FD uses the three points method. The reason of the equivalence is because there is no difference between SSPH and FD from the discretization point of view. Let us think this typical case as practically shown in Fig.4. Three particles are distributed in a constant spacing Δ in the support region defined by the smoothing length h The matrix size of K reduces the size of 3×3.

→ There is a significant difference in the form of the SSPH and FD equations. The former is based on integral equations, and the latter on differential equations. However, there is an equivalence in the simplest case, in which SSPH uses three particles in the computational domain, and FD uses a three-point method. The reason is that, from the discretization point of view, there is no difference between SSPH and FD in this case. Let us consider a typical case, as shown in Fig. 4. Three particles are distributed over a constant spacing Δ in the computational domain defined by the smoothing length h. In this case, the matrix size of K reduces to 3×3.

P5L18 The inverse matrix K^{-1} can be manually calculated, and the equation $D = K^{-1}P$ is expressed as …

→ The inverse matrix K^{-1} can be calculated manually, and the equation $D = K^{-1}P$ can then be expressed as …

P6L3 We can immediately see the equivalence, substituting each element such as $D_0 = \psi_i$, $D_1 = (-\psi_{i-1} + \psi_{i+1})/(2\Delta)$, and $D_2 = (\psi_{i-1} - 2\psi_i + \psi_{i+1})/(2\Delta^2)$ into Eq.(10). The practical formula of three point FD can be reproduced through the SSPH procedure.

→ We can immediately see the equivalence by substituting each element – that is, $D_0 = \psi_i$, $D_1 = (-\psi_{i-1} + \psi_{i+1})/(2\Delta)$, *and* $D_2 = (\psi_{i-1} - 2\psi_i + \psi_{i+1})/(2\Delta^2)$ – into Eq. (10). The practical formula obtained from three-point FD can thus be reproduced through the SSPH procedure.

(4. Summary)

P6L7 We introduced SSPH as one of the discretization techniques in the device simulation. SSPH was applied to the electronic structure calculations for HEMT. In the comparison of the characteristics of HEMT calculated in SSPH and FD, the result of SSPH is in good agreement with that of FD.

→ We introduced SSPH as a discretization technique for device simulations. SSPH was applied to an electronic structure calculations for a HEMT. In comparing the characteristics of HEMTs calculated using SSPH and FD, we find that the results from SSPH are in good agreement with those obtained using FD.

P6L11 From the technical point of view, it increases as the order of Taylor series expansion becomes higher. However, the equivalent to FD were also shown in the simple case, where the three particles in the support region of SSPH and the three point method in FD. If the number of the particles of SSPH is enough to describe the steep change of the one dimensional Schrödinger equation, the fairly accuracy will be provided. Our results indicate that SSPH can be applicable to the other electronic structure calculations that require high accuracy.

→ From the technical point of view, the computational effort increases as the order of the Taylor-series expansion becomes higher. However, SSPH and FD were also shown to be equivalent in a simple case corresponding to the three particles in the SSPH computational domain and to a three-point FD method. If the number of SSPH particles is large enough to describe steep changes in the one-dimensional Schrödinger equation, reasonable accuracy can be obtained. Our results indicate that SSPH can be applied to other electronic-structure calculations that require high accuracy.

(Figure 1. Caption)

P2 The structure of HEMT.

→ The structure of a HEMT.

(Figure 2. Caption)

P5 Conduction band level and charge profile of HEMT, calculated by SSPH (dashed line) and FD (solid line)

→ Conduction band structure and charge profile, calculated using SSPH (dashed line) and FD (solid line).

(Figure 3. Caption)

P5 Characteristic properties of HEMT. The sheet carrieer density N_s and dN_s/dV_g, calculated by SSPH (dashed line) and FD(solid line).

→ Characteristic properties and sheet carrier density N_s and dN_s/dV_g, calculated using SSPH (dashed line) and FD(solid line).

(Figure 4. Caption)

P5 Example of the kernel function W in the case of constant distribution Δ of the three particles in the smoothing length, and the value of each point is $W(z_i) = e_H$, $W(z_{i-1}) = W(z_{i+1}) = e$, respectively.

→ Example of the kernel function W in the case of a constant distribution Δ of three particles over the smoothing length. The values at each point are $W(z_i) = e_H$, and $W(z_{i-1}) = W(z_{i+1}) = e$, respectively.