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Approximate H-transformation for numerical stabilization of a deterministic Boltzmann transport equation solver based on a spherical harmonics expansion ☆,☆☆

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ABSTRACT

In this work, we propose a numerical stabilization method for a deterministic Boltzmann transport equation solver based on a spherical harmonics expansion. In the proposed scheme, the approximate H-transformation, a new energy variable approximately follows the total energy. An additional term is generated out of the free-streaming operator and it should be implemented properly. When the kinetic energy is fixed, the distribution function at that energy can be directly accessible at any time instance. The proposed scheme is implemented in our in-house deterministic Boltzmann transport equation solver. The numerical simulation results demonstrate that the proposed stabilization scheme works properly without any numerical difficulties.

1. Introduction

The drift-diffusion model, which has superior numerical stability [1,2], has made great contributions to the theoretical study of semiconductor devices over the past decades and is still the workhorse of today's TCAD (Technology Computer-Aided Design). However, it is also well known that the drift-diffusion model has some limitations when a sharp change in the electric field appears in the device [3,4]. Although the carrier mobility is frequently calibrated to reduce the error due to the model deficiency, its calibration should be performed again when a different device is simulated.

The Boltzmann transport equation is the semi-classical equation to describe the carrier transport in the phase space. By solving the Boltzmann transport equation with an increased computational cost, carrier transport can be described more accurately. Among various ways to solve the Boltzmann transport equation, deterministic Boltzmann transport equation solvers for the three-dimensional electron gas [5–8] have been actively studied. In these studies, the electron distribution function in the three-dimensional momentum space is calculated based on the spherical harmonic expansion. By replacing the dependence on the angle with harmonic coefficients, computational efficiency can be improved.

In the deterministic Boltzmann transport equation, a stabilization method that ensures a positive distribution function is required even under a strong electric field. The H-transformation [5], where the Boltzmann transport equation is written in the total energy space, provides improved numerical stability because the derivative with respect to the energy variable is completely eliminated. In the maximum entropy dissipation scheme [7], an exponential function considering position-dependent total energy is multiplied to improve the numerical stability. For a multi-subband Boltzmann transport equation solver, where the Schrödinger equation is additionally solved to obtain the subband structure, other stabilization schemes can be found. A hybrid method that uses both the phase (inelastic) space and the trajectory (elastic) space according to the scattering mechanism has been proposed [9]. It is noted that numerical simulations directly in the phase space [10] have been also reported.

Recently, the transient simulation results using an implicit time marching technique have been reported in [11]. In [11], the maximum entropy dissipation scheme was adopted. Although the H-transformation is widely adopted in the steady-state simulation, the scheme is not very convenient to be used in the transient simulation, because the distribution functions at previous time instances must be interpolated for the present potential profile. Therefore, the transient simulation capability that is compatible with the H-transformation has not been reported yet.

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In this study, in order to overcome the difficulties originated from the stabilization scheme, an alternative stabilization scheme, the approximate H-transformation, is proposed. The organization of this manuscript is as follows. In Section 2, the proposed simulation methodology is briefly described. In Section 3, numerical results are shown. In Section 4, the research direction to which the proposed methodology can be applied is discussed. Finally, the conclusion is made in Section 5.

2. Approximate H-transformation

It is assumed that the energy variable is uniformly discretized with a spacing, ΔE. For the sake of notational simplicity, the dependence on the position variable is omitted whenever possible. For more complete notations, readers are referred to [12].

Let us consider a case where an implicit time marching scheme is adopted to discretize the time derivative term. At a given kinetic energy, ε, the time derivative of Zf (a product of the density-of-states, Z, and the distribution function, f) at a time instance, t_i, can be written as

$$\left.\frac{\partial[Zf]}{\partial t}\right|_{t=t_i} \approx Z(\varepsilon)\sum_{j=0}^{N-1} a_{i,j} f(\varepsilon, t_{i-j}), \tag{1}$$

where N is the order of the time-marching scheme, $a_{i,j}$ is a coefficient connecting t_i and t_{i-j}. For example, the simplest backward Euler scheme ($N = 2$) has

$$a_{i,0} = -a_{i,1} = \frac{1}{t_i - t_{i-1}}. \tag{2}$$

The free-streaming operator, L, is given by

$$Lf = \frac{1}{\hbar}\mathbf{F}\cdot\nabla_{\mathbf{k}} f + \mathbf{v}\cdot\nabla_{\mathbf{r}} f, \tag{3}$$

where $\hbar$ is the reduced Planck's constant, $\mathbf{F}$ is the force due to the electric field, and $\mathbf{v}$ is the group velocity. Using the electrostatic potential, $\mathbf{F}$ is written as

$$\mathbf{F} = -\nabla_{\mathbf{r}} V \tag{4}$$

where V is the band minimum energy. When the free-streaming operator is projected onto a quantity described by an index of l (for example, a pair of degree and order in the spherical harmonics expansion), the projected operator can be written as

$$Lf \longrightarrow \sum_{l'}\frac{\partial}{\partial\varepsilon}\left[\mathbf{F}\cdot\mathbf{A}_{l,l'} f_{l'}\right] + \nabla_{\mathbf{r}}\cdot\left[\mathbf{A}_{l,l'} f_{l'}\right] - B_{l,l'} f_{l'}, \tag{5}$$

where $\mathbf{A}_{l,l'}$ and $B_{l,l'}$ are coefficients connecting l and l' terms.

The conventional H-transformation uses the total energy, H, which is defined as

$$H = \varepsilon + V = \varepsilon + (-q\phi + E), \tag{6}$$

where q is the absolute elementary charge, ϕ is the electrostatic potential, and E is the energy difference between the band minimum and the local reference energy. Variable transformation from ε to H greatly simplifies the free-streaming operator:

$$Lf \longrightarrow \sum_{l'}\nabla_{\mathbf{r}}\cdot\left[\mathbf{A}_{l,l'} f_{l'}\right] - B_{l,l'} f_{l'}. \tag{7}$$

However, when the transient simulation is involved, the terms related with the time derivation introduce some difficulties. Since $V(t_i) - V(t_{i-j})$ does not vanish in general, $f(\varepsilon = H - V(t_i), t_{i-j})$ is not directly available. An interpolation procedure must be introduced. From the present authors' experience, with a finite resolution of numerical discretization, the interpolation procedure deteriorates the numerical stability.

An alternative approach based on the approximate H-transformation is proposed. Instead of the time-varying band minimum energy, its approximation, $\tilde{V}$, is used to construct a new energy variable, h,

$$h = \varepsilon + \tilde{V}. \tag{8}$$

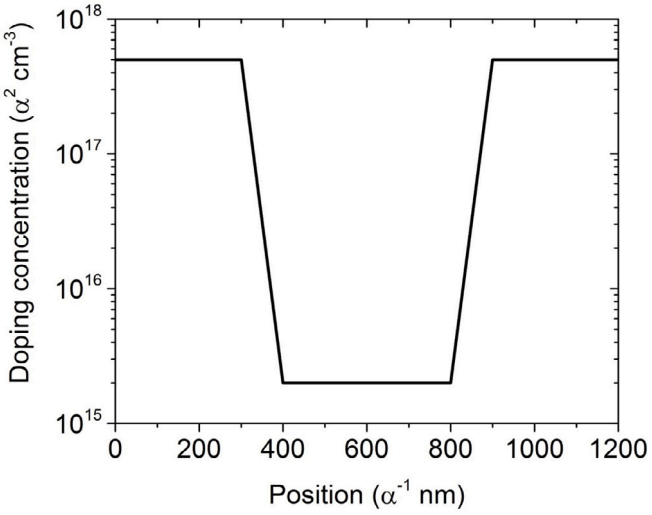

Fig. 1. Doping profile of a N+NN+ resistor simulated in this work. By increasing a scaling factor (α), various structures can be generated. In this work, the scaling factor varies from 1 (1200-nm-long structure) to 10 (120-nm-long structure).

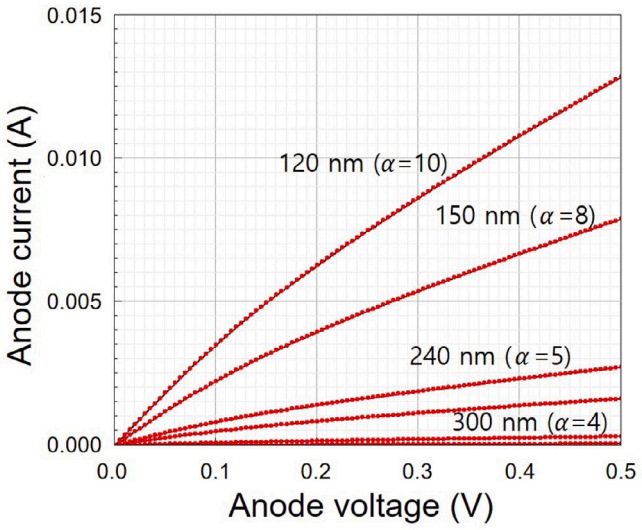

Fig. 2. DC IV characteristics of different structures with various scaling factors. The calculation results with the conventional H-transformation (Black lines) and the approximate H-transformation (Red dots) are almost identical.

Under this new transformation, an additional term appears out of the free-streaming operator.

$$\begin{aligned} Lf \longrightarrow & \sum_{l'}\left(\mathbf{F} + \nabla_{\mathbf{r}}\tilde{V}\right)\cdot\frac{\partial}{\partial h}\left[\mathbf{A}_{l,l'} f_{l'}\right] \\ & + \nabla_{\mathbf{r}}\cdot\left[\mathbf{A}_{l,l'} f_{l'}\right] - B_{l,l'} f_{l'}. \end{aligned} \tag{9}$$

Fortunately, since the additional term is proportional to $V - \tilde{V}$, which is small for a reasonable $\tilde{V}$, a suitable discretization technique can be developed.

The major progress made in this work is to propose a condition for $\tilde{V}$, with which the interpolation procedure in the time derivation can be completely eliminated. We propose a condition of

$$\tilde{V}(t_i) = k(t_i)\Delta E, \tag{10}$$

where $k(t_i)$ is an integer function and ΔE is a constant energy spacing. Moreover, $k(t_i)$ is unambiguously determined to minimize the absolute

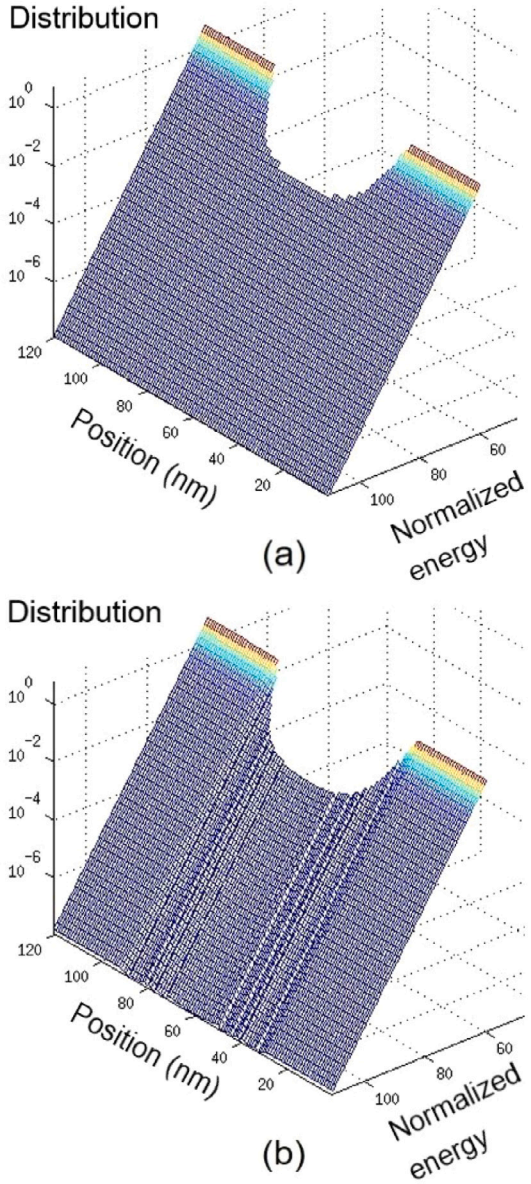

Fig. 3. Distribution function at equilibrium calculated with (a) the conventional H-transformation or (b) the approximate H-transformation. The total length is 120 nm. At a given position variable, each distribution function decays exponentially as the energy variable increases. The additional term out of the free-streaming operator plays an important role in the approximate H-transformation. The energy variable is normalized with the energy spacing of 10 meV.

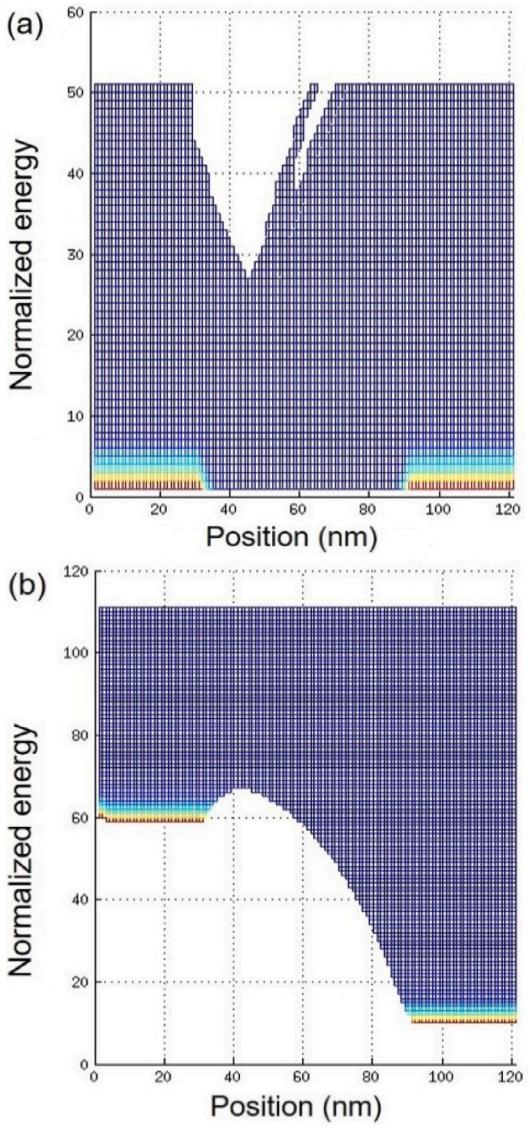

Fig. 4. Color map of the distribution function calculated with (a) the maximum entropy dissipation scheme or (b) the approximated H-transformation. The total length is 120 nm and the applied anode voltage is 0.5 V. Negative distribution functions are clearly observed in (a). Of course, an integral of the distribution function along the energy axis is positive and areas with negative distribution functions can be reduced by adopting a finer grid. On the other hand, in the case of the proposed method, the distribution function is non-negative everywhere, even with the same grid. The energy variable is normalized with the energy spacing of 10 meV.

value of $V - \tilde{V}$. With the above condition, we readily have

$$\tilde{V}(t_i) - \tilde{V}(t_{i-j}) = [k(t_i) - k(t_{i-j})]\Delta E. \tag{11}$$

Again, the time derivation requires $f(h - \tilde{V}(t_i), t_{i-j})$. Since the energy shift is just an integer-multiple of ΔE, the required distribution function can be readily accessible without any interpolation procedure. Therefore, with the approximate H-transformation, the transient simulation becomes possible while enjoying the superior numerical properties of the conventional H-transformation.

3. Numerical results

The proposed method has been implemented into our in-house deterministic Boltzmann transport equation solver. The physical models are the same with those in [11]. Three different stabilization schemes (the maximum entropy dissipation scheme, the conventional H-transformation, and the approximate H-transformation) are available.

Fig. 1 shows the structure under simulation. Starting from a 1200-nm-long N^+NN^+ resistor, a scaled structure can be generated by increasing a scaling factor, α. As shown in Fig. 2, the DC IV characteristics of all simulated structures show excellent agreement between two methods (the conventional H-transformation and the approximate H-transformation). It is much expected because the approximate H-transformation is a modified version of the conventional H-transformation.

The distribution function at equilibrium is drawn in Fig. 3. Two stabilization schemes (the conventional H-transformation and the approximate H-transformation) are compared. As expected, the conventional H-transformation follows the Boltzmann distribution, which is

not dependent on the position variable. On the other hand, with the approximate H-transformation, the distribution function varies over the position variable, because the energy variable slightly differs from the total energy.

When a high DC voltage is applied to the anode terminal, the stabilization scheme based on the kinetic energy suffers from negative distribution functions. In Fig. 4, the color map of the distribution is shown. Empty areas at high energies represent discretized points with negative distribution functions. Of course, an integral of the distribution function along the energy axis is positive and areas with negative distribution functions can be reduced by adopting a finer grid. For the same case, as shown in Fig. 4(b), the distribution function calculated with the approximate H-transformation is non-negative everywhere. Again, it is the property inherited from the conventional H-transformation.

The simulation results have been calculated with the energy spacing of 10 meV. The energy spacing is chosen not to exceed the minimum phonon energy (12.1 meV). For such a relatively large energy spacing, the simulation can be performed without any problem. It is because the effective force term is always kept small in the proposed stabilization scheme. Of course, in order to avoid the artificial diffusion [9,10], a small energy spacing is desirable.

4. Outlook

The approximate H-transformation employs a special $\tilde{V}$. $\tilde{V}$ is close to the band minimum energy and proportional to an integer-multiple of the discrete energy spacing. The approximate H-transformation is a suitable method for transient simulations because it is not affected by the time-varying potential energy. This method may be applied to the two-dimensional/one-dimensional electron gas (multi-subband Boltzmann transport equation) as well as the three-dimensional electron gas. However, when the potential energy is time-varying, the wavefunction of each subband may change. It seems that such an effect cannot be captured in the present scheme. Addressing this issue would be an interesting topic for future exploration.

5. Conclusion

In conclusion, a novel stabilization scheme has been successfully implemented into the deterministic Boltzmann transport equation solver. For the three-dimensional electron gas, the distribution functions at past time instances can be directly accessible without any interpolation procedure and the stability of the conventional H-transformation can be shared. The proposed method can be readily applied to the transient simulation.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

Data will be available on reasonable request.

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