Simulation of Heterojunction Bipolar Transistor with Domain Decomposition Method

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ABSTRACT

Domain decomposition method is used in simulation of the band profile and the majority carrier concentration profile of AlGaN/GaN heterojunction bipolar transistors. The method is very stable and efficient. With this method different device structures are designed and the trade-off is discussed.

Keywords: Domain decomposition method, HBT, GaN, Polarization charge.

1 INTRODUCTION

In simulation of many semiconductor electronic devices, one needs to find first the equilibrium band profile by solving Poisson's equation and the charge distribution equation self-consistently. As the charge density often has an exponential dependence on voltage profile, the convergence process is usually very slow and often unstable. The stability of the solution also depends on the spatial scale; convergence can be achieved readily within a small domain and become quite difficult to achieve as the domain size is increased. The method of domain decomposition [1] divide a large domain into smaller ones, in this way, we can get better stability and rapid convergence. This method is applied to the simulation of AlGaN/GaN heterojunction bipolar transistors (HBT).

2 DOMAIN DECOMPOSITION METHOD

There are a number of variations of domain decomposition method (DDM) [1]. The basic idea is to divide a large domain into smaller sub-domains, where the problems can become more stable and easy to converge; then the boundaries of the sub-domains are treated separately with connection relations. In this way, the grid points in the whole domain are divided into two sets: these inside the sub-domains and those on the boundaries. The method we used for this work eliminated this classification by a dynamic partition scheme.

For heterojunction bipolar transistor (HBT) structures many important properties can be simulated with a one-dimension model. A finite difference method is employed in the simulation. In order to converge quickly the step size is progressively decreased. The simulation starts with an initial guess of the band profile, which is usually far from the correct result. At this stage we set up a loose converge criterion and use a relatively large step size, which is 2 Å. When this criterion is met, we shrink the step size to 1 Å and tighten the converge criterion. In the third stage the step size is reduced to 0.5 Å.

In each stage mentioned above DDM is engaged. In order to avoid the special treatment of the boundary points, we used a dynamic partition scheme. Several successive iterations are grouped into a super cycles; within these super cycles, each iteration chooses a different partition scheme. In the first iteration, a specific partition scheme is used, and the problem is solved in these sub-domains. The pseudo-boundary points of the sub-domains are left there untreated. In the second iteration, a set of new sub-domains is defined. There some of the pseudo-boundary points in the previous iteration fall inside the sub-domains in the present iteration; therefore, they will get updated as well. As different partitions are adopted for the succeeding iterations within the super-cycle, all points in the whole region will be updated.

From certain point of view, DDM is an extension of the self-consistent scheme. For example, at the beginning of a simulation of the HBT problem, both the band profile and the carrier distribution are not available. However, an initial band profile can be proposed; then the charge distribution can be calculated based on the band profile. For a differential equation with Dirichlet boundary condition, if certain points inside the domain are provided with the correct values, they can be used as new boundary conditions. In this way the domain is decomposed into smaller domains. However, there is no way to get those correct data priorly. Parallel to the self-consistent scheme, a set of data points inside the domain is supposed to be correct first and used as temporary boundary conditions, which will be updated in the successive iterations.

Various schemes can be used in selecting the sets of sub-domains, i.e. temporary boundary points. A valid scheme must guarantee that all the pseudo boundary points have a chance to get updated. For simplicity of the algorithm, segments of equal size are used in our partition scheme, and the length in each segment is the product of the step length and a prime number. In our simulation five different prime numbers are used in five succeeding iterations, e.g. p_1, p_2, p_3, p_4, p_5, which form a super cycle. This partition scheme is shown in Fig.1.

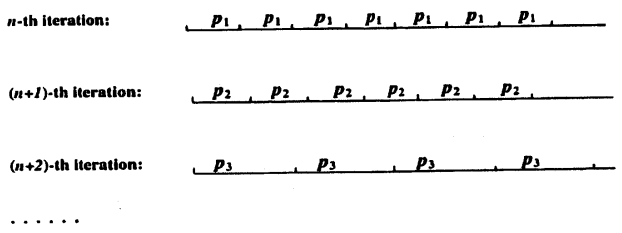

FIG.1 A dynamic partition scheme of domain decomposition method.

As long as their product, $p_1 p_2 p_3 p_4 p_5$, is no less than the total number of grid points in the whole domain, all data points inside the whole domain have a chance to be updated in a super cycle. At the end of the domain there is a remaining section, which is less than the length of the sub-domain in that particular iteration, it can be treated as a special case in the process of numerical simulation.

One of the advantages of this method is its flexibility. For very unstable problems, smaller sub-domains can be used to avoid divergence; while larger sub-domains can be applied to less demanding problems to accelerate convergence.

3 AlGaN/GaN HBT SIMULATION

Armed with this capability, we are able to design and simulate multi-layered GaN-based HBT structures. The goal of this simulation is to find an optimized device structure that has low base resistance, which is likely to be a critical limiting factor for the performance of III-N *n-p-n* bipolar transistors. From the mathematical point of view, the simulation process is self-consistent solution of charge distribution function and the Poisson's equation. In wide-bandgap materials, the majority carrier concentration is much higher than the minority carrier concentration. Therefore, for the simulation of the static band profile, the minority carrier concentration can be ignored. The majority carrier concentration is calculated with an empiric equation of the Fermi-Dirac integral [2], which is correct to better than 3% over the carrier concentration range of interest. Besides the majority carriers and the ionized impurity charges, there are polarization charges in the region where Al-composition changes. Two effects contribute to the polarization charges: spontaneous polarization charges and the piezoelectric charges. They can be calculated by the following equations:

$$\Delta P_{SP} = [P_{SP}(AlN) - P_{SP}(GaN)]x$$

$$\Delta P_{PE} = 2\frac{a - a_0}{a_0}(e_{31} - e_{33}\frac{c_{13}}{c_{33}})$$

where P_{SP} and P_{PE} designate the spontaneous and piezoelectric polarization charges, respectively. The parameters in above equations can be found in reference [3].

3.1 Conventional HBT Structures

There are two conventional HBT structures, abrupt junction HBT and graded HBT. First, an abrupt junction HBT structure is simulated. The emitter material is $Al_{0.1}Ga_{0.9}N$, n-type doped to 10^{18} cm^{-3}, the base consists of a 1000 Å GaN layer, p-type doped to 10^{19} cm^{-3}, and the collector is n-type GaN doped to 10^{17} cm^{-3}. The calculated band profile is shown in Fig. 2 (a).

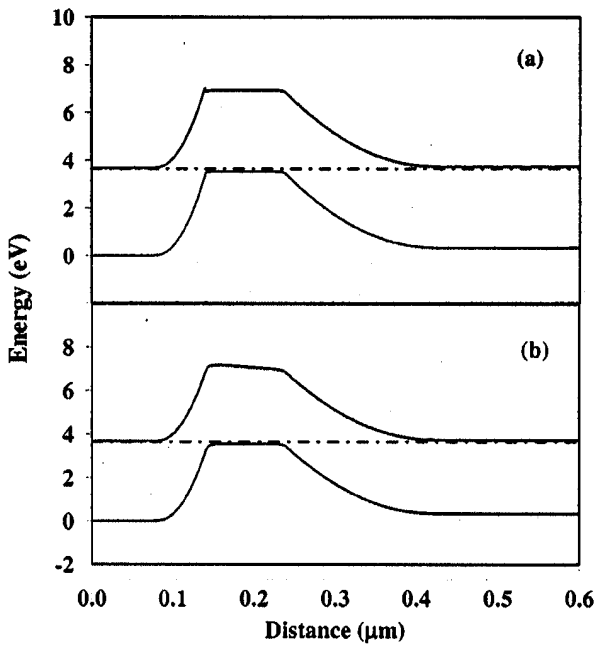

FIG. 2. Calculated band profile of AlGaN/GaN HBT structures: (a) an abrupt junction HBT (b) a linear graded HBT.

The hole concentration in the base is integrated along the growth direction, yielding a sheet carrier concentration p_s = 2.45x10^{12} cm^{-2}. For comparison, if the piezoelectric and spontaneous polarization charges are ignored, the integrated hole concentration is 2.22x10^{12} cm^{-2}. Clearly, in

this configuration, the piezoelectric and spontaneous polarization charges are located at the emitter-base interface, serving only to reduce the rather thin depletion layer on the base side of the emitter-base junction. Therefore, the sheet hole concentration in the base is not much affected by the polarization effects.

Next, a graded HBT structure is examined. The emitter material is $Al_{0.1}Ga_{0.9}N$, n-type doped to 10^{18} cm^{-3}. In the base, the AlN mole fraction decreases linearly from 10% to zero over a 1000 Å. This base layer is doped p-type to 10^{19} cm^{-3}. The collector material is GaN, n-type doped to 10^{17} cm^{-3}. Fig. 2 (b) is the calculated band profile; the integrated hole concentration in the base for this structure is $5.14x10^{12}$ cm^{-2}. Although the hole concentration in the base region is twice that of the abrupt junction HBT structure, the value is still quite small.

Hole mobilities in III-Nitride materials are typically found to be quite low. However, calculations have indicated that hole mobilities in lightly doped GaN can be larger than 40 cm^2/Vs [4]. The mobility in AlGaN is likely to be quite sensitive to the uniformity of the material. Fluctuations in alloy composition are likely to result in serious space charge scattering due to the polarization charges that result from local variations in the polarization. However, if the alloy composition is uniform (or slowly varying in the direction perpendicular to the relevant transport as envisioned here) the carrier mobilities in low-doped AlGaN can be fairly high due to the low level of alloy scattering [5]. Assuming a relatively conservative value for the hole mobility of 10 cm^2/Vs [6], the base sheet resistance of the structure shown in Fig. 2(b) is expected to be 122 kΩ/□, which is still too high for most applications.

3.2 Advanced HBT Structures

In order to increase the hole sheet carrier concentration further by means of polarization charges, the AlN content in the base has to be increased [7]. This approach, of course, is limited by the increasing strain, which may lead to the formation of dislocations. In addition, high AlN content may lead to unacceptably high turn-on voltages. Due to the large mismatch of the lattice constants, the thickness of these layers with high Al-concentration must be very small. The material parameters of this HBT structure is shown in the following table.

The sharp change of material parameter and carrier concentration usually is a serious challenge for convergence and stability considerations, but this structure can be modeled successfully with the domain decomposition method. In this simulation, the whole domain contains more than 10,000 grid points, it still converges very well within several hours on a desktop workstation.

E1:	GaN, $N_d = 10^{18}$ cm^{-3}
E2:	$Al_{0.1}Ga_{0.9}N$, $N_d = 10^{18}$ cm^{-3}
E3:	$Al_xGa_{1-x}N$, $x = 0.1 \rightarrow 0.5$, 100 Å, undoped
E4:	$Al_{0.5}Ga_{0.5}N$, 300 Å, $N_d = 10^{18}$ cm^{-3}
D:	$Al_xGa_{1-x}N$, $x = 0.5 \rightarrow 1.0$, 50 Å, $N_d = 6 \times 10^{19}$ cm^{-3}
B1:	AlN, 20 Å, $N_a = 10^{19}$ cm^{-3}
B2:	$Al_xGa_{1-x}N$, $x = 1.0 \rightarrow 0.2$, 50 Å, undoped
B3:	$Al_xGa_{1-x}N$, $x = 0.2 \rightarrow 0$, 900 Å, $N_a = 10^{19}$ cm^{-3}
C1:	GaN, $N_d = 10^{17}$ cm^{-3}
C2:	GaN, $N_d = 5 \times 10^{18}$ cm^{-3}

Fig. 3 (a) shows the calculated band profile without bias. The integrated hole density is $1.88x10^{13}$ cm^{-2}, which is about an order of magnitude higher than that of the conventional structure. The majority carrier distribution is shown in Fig. 4, the thick solid line represent the hole concentration in the base, while the thin solid lines represent the free electron concentrations in the emitter and collector.

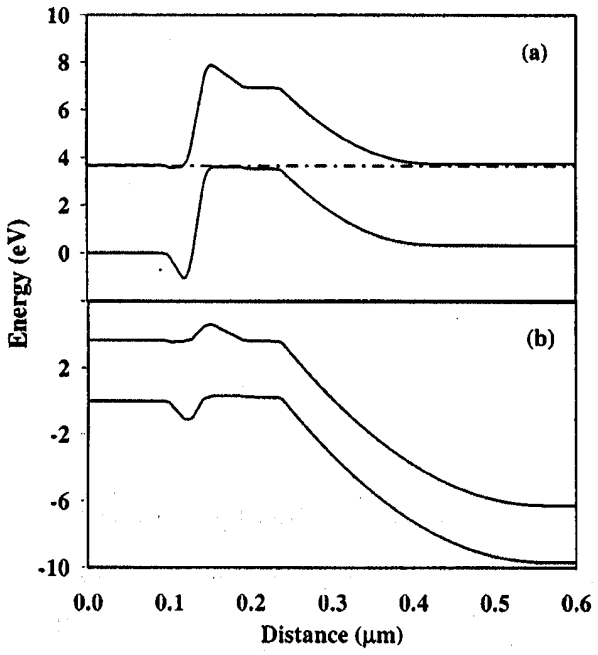

FIG. 3 Calculated band profile of an advanced HBT structure. (a) in equilibrium and (b) with forward bias.

Fig. 3 (b) is the band profile in the biased situation; the base-emitter bias taken to be 3.3 V and collector-emitter bias is 10 V. The peak in the conduction band is 0.99 eV above the quasi Fermi level in the emitter, while and the dip in the valence band is 1.47 eV below the quasi Fermi level in the base. This 0.48 eV difference of the barrier heights, together with the large effective mass of holes, can effectively prevent holes from being injected into the emitter. In addition, a large accelerating field of about 250 kV/cm is acting on injected electrons. This field

can effectively suppress lateral transport of electrons in the base region and reduce their base transit time.

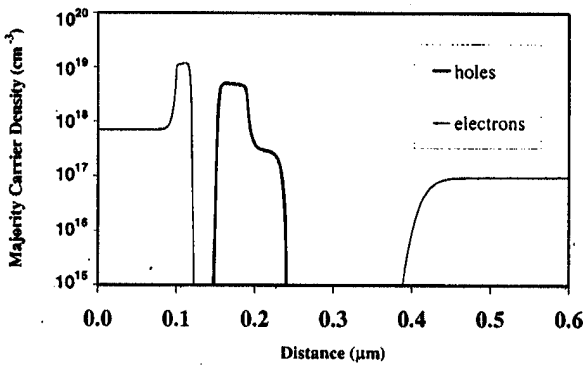

FIG. 4 Calculated majority carrier distribution structure shown in Fig. 3(a). The thick line represents the hole concentration in the base and thin lines represent the electron concentration in the emitter and collector, respectively.

4 CONCLUSION

With domain decomposition method we simulated several conceivable AlGaN/GaN HBT structures, where the polarization charges are utilized to increase the hole concentration in the base while possibly maintaining an acceptably high hole mobility. Through a careful choice of design trade-offs, the thicknesses of the strained layers are kept small, an electron-accelerating field is built into the base, and hole injection into the emitter is suppressed. These HBT structures have much smaller base resistances and shorter base transit times than could be achieved in a conventional structure.

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