An Adaptive Grid Algorithm for Self-Consistent $k \bullet p$ Schrödinger and Poisson Equations in UTB InSb-Based pMOSFETs

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Abstract

Hole mobility in ultra-thin body (UTB) InSb-OI devices is calculated by a microscopic approach. An adaptive grid algorithm is employed to discretize 2-D k space. The accurate valence band structures are obtained via solving the 6-band k • p Schrödinger and Poisson equations self-consistently. Hole mobility is computed using the Kubo-Greenwood formalism accounting for nonpolar acoustic and optical phonons, polar optical phonons, and surface roughness scattering mechanisms.

Introduction

In III-V materials, one of key challenges is to enhance the hole mobility in the pMOSFETs for CMOS application [1]. Recently, $In_xGa_{1-x}Sb$-based p-channel MOSFETs and heterostructure quantum wells have been demonstrated experimentally and exhibited outstanding performance (μ_h > 1230cm^2/V-s) [2-3]. It is of great value to investigate the body thickness on the hole mobility of UTB InSb-based devices.

The accurate valence subband structure can be obtained by solving 6-band $k \cdot p$ Schrödinger and Poisson equation self-consistently. However, this method is time and memory consuming since the 6-band $k \cdot p$ Schrödinger has to be solved for a large number of k points in the $k_{||}$ plane in order to obtain an accurate hole density and the usage of this method is questionable in practice simulation. For this reason, many simplification methods have been carried out [4-8]. In this work, the k space is discretized by an adaptive grid algorithm using a method similar to the one of J. Bude [9]. Adaptive grid algorithm can compute the reasonable number of mesh grids in $k_{||}$ plane adaptively, without special account to the material, body thickness, orientation and strain. Using this approach, dependency of the hole mobility in SG and DG UTB InSb-OI devices with body thickness is investigated by solving the 6-band $k \cdot p$ Schrödinger and Poisson equations self-consistently.

Simulation Method

Fig.1 shows the flowchart of the simulation methodology in pMOSFET. The methodology consists of three parts: (1) the self-adaptive grid algorithm part in order to generate the mesh grids in $k_{||}$ plane, (2) the self-consistent part to certify the tolerable error and (3) the hole mobility calculation considering various scattering mechanisms.

The $k_{||}$ plane is discretized within the irreducible region of the Brillouin zone. The adaptive grid algorithm is to calculate a set of grids which compose triangles. Each edge of a triangle must be fulfill the given error criterion. If not, the longest edge is splitted in the middle by inserting a new grid point. All triangles containing this edge have to be divided. After a splitting process, the error criterion is evaluated for all edges. To avoid triangle with a bad shape before the splitting of an edge, the shape of all triangles containing the edge are checked. The area of the triangle must be at least 0.1/2 times the area of the square with the longest edge length of the triangle. The error criterion relates the real energy solved by 6-band $k \cdot p$ method at the middle of an edge to the energy calculated by linear interpolation between the two endpoints of the edge. For energies below 100meV, the absolute error must be smaller than 1meV. Between 0.1eV and 1.0eV, a relative error of 2% is allowed and above 1.0eV an absolute error of 20meV.

The energy dispersion along the [100] and [110] direction is illustrated in Fig.2. The valence subband structure calculated by the self-adaptive grid number (N_{k_S}) of 22 can completely describe the band structure from uniform mesh of N_k=50. Fig.3 presents the hole density and electrostatic potential for weak and strong inversion in 5nm-thick UTB InSb MOSFETs. The results indicates that the mesh generated by self-adaptive algorithm at zero bias is accuracy enough that futher update during the self-consistent process is not necessary under various biases. It also can be seen that with uniform mesh of N_k=42, the peak of the hole density is lower. It is noted that the computational time mainly depends on the grid number employed in $k_{||}$ plane. The error of hole density and average electric field F_S between the self-adaptive grid number N_{k_S} and the mesh grid number N_k, in which the $k_{||}$ plane is discretized in polar coordinate, are compared in Fig.4. It can be seen that the N_{k_S} for T_B=5nm and 30nm can provide sufficient accuracy without a waste of computational resource. Fig.5 depicts the dependency of grid number N_{k_S} on the materials (InSb, GaSb, Ge and Si), and body thickness.

Results and Discussion

Hole Mobility is calculated using Kubo-Greenwood formalism accounting for nonpolar acoustic and optical phonons, polar optical phonons (only in III-V materials), and surface roughness scattering mechanisms. Calculated low-field hole mobility for SG and DG SOI MOS structures are shown in Fig.6 and the experiment data in Ref.10 are also plotted in Fig.6. Simulation results are in excellent agreement with the experiment, which verify our simulation method.

The calibration of the model parameters for InSb is performed with experimental data for 5nm-thick compressive strained InSb quantum well from [2] by keeping the phonon scattering parameters (taken from [11]) fixed, while adjusting SR parameters, seen in Fig.7. Fig.8 shows the hole mobility in SG and DG InSb-OI devices as a function of inversion charge density for T_B=3nm and 30nm, and dependency on body thickness is displayed in Fig.9. For thicker body thickness, hole mobility changes slowly with T_B, and μ_h in DG is greatly enhanced in all hole density. While for T_B below 9nm, μ_h decreases steeply with the decrease of T_B and μ_{DG} does not outperform μ_{SG} in a wide range of hole density.

Summary

In this work, the self-consistent 6-band k • p Schrödinger and Poisson equations are solved at the mesh grids generated by an adaptive grid algorithm, which provides sufficient accuracy for hole density without a waste of computational resource. Hole mobility calculated via this method is in excellent agreement with experiments for Si- and InSb-based

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devices. Dependency of μ_h on T_B in SG and DG InSb-OI devices is investigated. It is found that μ_{DG} outperforms μ_{SG} only for thicker T_B, and contrary for T_B below 9nm.

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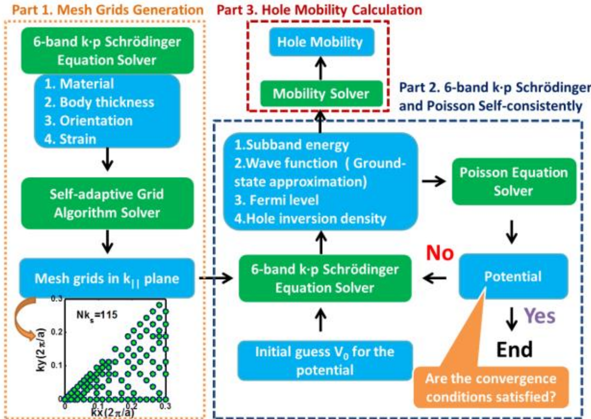

Fig.1 Flowchart of the simulation methodology in pMOSFET. The methodology consists of three parts: (1) mesh grids generation by self-adaptive algorithm, (2) the self-consistent part and (3) hole mobility calculation.

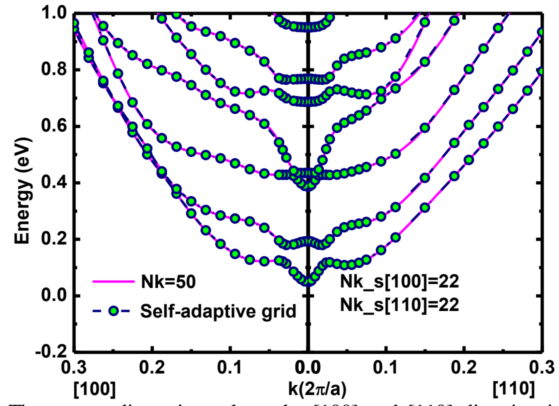

Fig.2. The energy dispersions along the [100] and [110] direction in 5-nm thick InSb are plotted. The solid line corresponds to the uniform **k** points of N_k=50. The line with symbols is derived from self-adaptive grid algorithm which generated 22 grids along [100] and [110] direction, respectively.

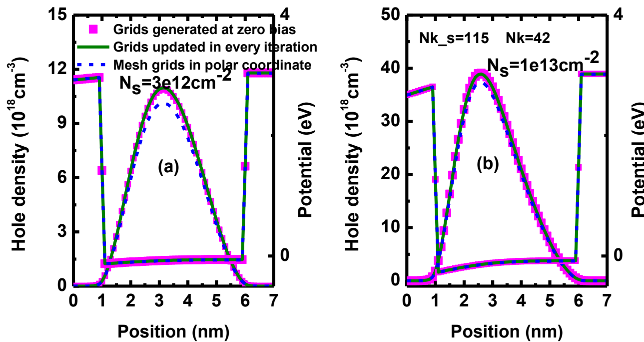

Fig.3 Hole density and electrostatic potential for weak (a) and strong (b) hole inversion in 5nm-thick InSb-OI devices. The solid line is obtained by a set of grids generated at zero bias (N_{k_S}=115), which remains unchanged in the process of self-consistent iteration. The symbol is the results from grids updated in every iteration. While the dashed lines refer to the results from N_k=42.

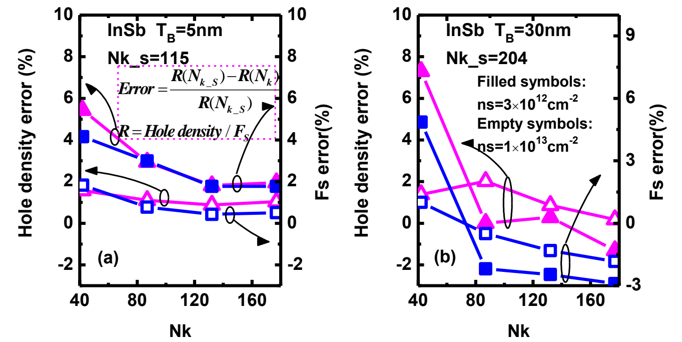

Fig.4 Error of hole density and average electric field Fs versus the mesh grid number N_k, in which the $k_{||}$ plane is discretized in polar coordinate. The error is related to the results obtained from self-adaptive grid algorithm. The errors are plotted for (a) T_B=5nm and (b) 30nm InSb-OI devices with different inversion densities, respectively.

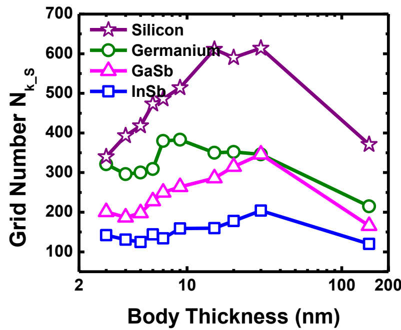

Fig.5 Grid number N_k_s generated by self-adaptive grid algorithm as a function of the body thickness for InSb, GaSb, Ge and Si.

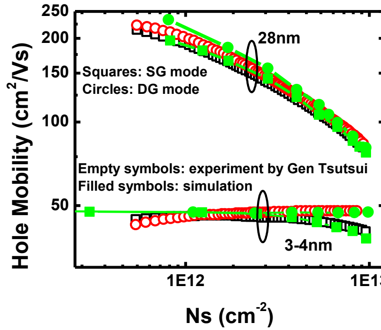

Fig.6 Calculated low-field hole mobility for SG and DG SOI MOS structures and measurements.

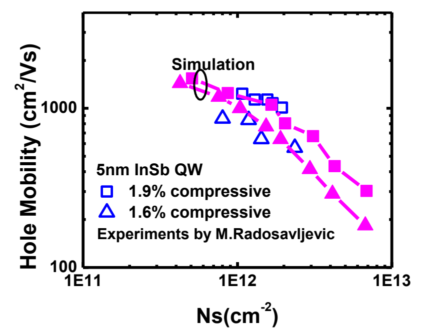

Fig.7 Comparison between simulated and experimental [2] data for hole mobility in InSb-on-insulator MOSFET with T_B of 5nm are presented.

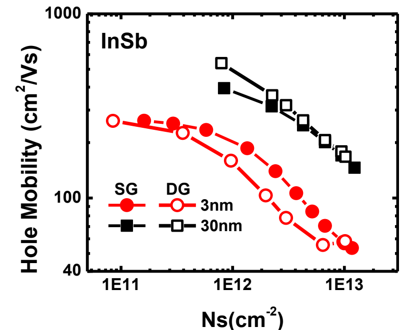

Fig.8 Hole mobility in SG and DG InSb-OI devices as a function of inversion charge density for T_B =3nm and 30nm, respectively.

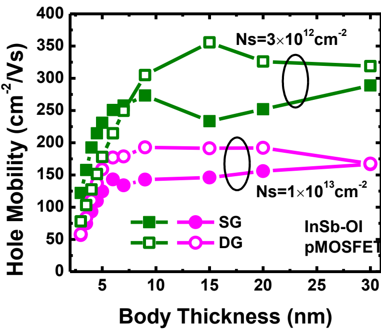

Fig.9 Dependency of hole mobility in SG and DG InSb-OI devices on body thickness for different inversion densities.

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