A three-dimensional TCAD system focused on power and nano-scaled devices applications

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***Abstract*— A new 3-D TCAD system has been proposed aiming close coupling of first-principles calculator, process, and device simulators in response to requirements for ultra-small to high-power semiconductor devices. Using the first-principles calculator Schottky-barrier height has been derived. In the process simulator, a robust and high-speed topographical algorithm has been newly proposed and thus easier handling of complicated 3-D structure has been provided. And a 3-D effect due to arsenic deactivation has been demonstrated. In the device simulator, robust calculation for high-voltage breakdown characteristics of wide-gap devices has been demonstrated.**

Keywords—3-D TCAD; first-principles calculator; Schottky-barrier height; process simulator; easier handling; topographical algorithm ; device simulator

I. Introduction

A new 3-D TCAD system has been proposed aiming close coupling of first-principles calculator, process, and device simulators in response to requirements for ultra-small to high-power semiconductor devices of which crystals and materials have been diversified unlimitedly. These three parts are seamlessly operated by integrated control platform with flexible graphical user interface as shown in Fig. 1. Parallel processing using Message Passing Interface (MPI) has been implemented in this system.

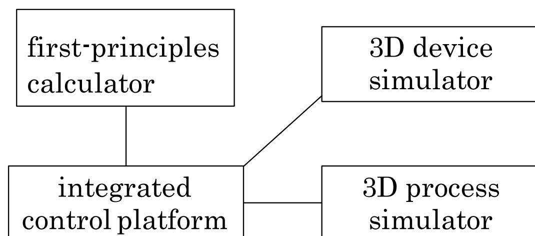

Fig. 1. Advance/TCAD system.

In this paper, topics of each program are demonstrated. The derivation of Schottky-barrier height by first-principles calculator has been demonstrated. In the process simulator, a robust and high-speed topographical algorithm has been newly proposed and a 3-D narrow-channel effect of the threshold voltage of MOSFETs due to arsenic deactivation has been demonstrated. In the device simulator, robust calculation for high-voltage breakdown characteristics of wide-gap devices has been demonstrated.

II. Application of First-Principles Calculator

The Schottky-barrier height (SBH) is an essential parameter for evaluating currents of Schottky-barrier diode (SBD). The SBH of the metal/4H-SiC interface has been calculated by first-principles calculation (Advance/PHASE v3.2) for Si- and C-faced contacts from difference between the Fermi level and the energy of valence band edge as shown in Fig. 2.

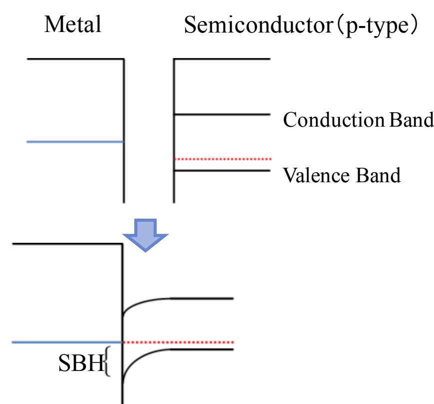

Fig. 2. The introduction of Schottky Barrier Height

Advance/PHASE v3.2 is the first-principles calculation software which facilitates evaluation of electronic states for new crystals and new materials prior to real implementation and thus powerfully supports research and development of nano-technology based on the density functional theory DFT and the plane wave expansion using pseudo potential. GGA-PBE (Generalized Gradient Approximation by Perdew-Burke- Ernzerhof[1]) method has been used for the exchange-correlation energy. As electronic state is calculated on the basis of quantum mechanics, it can obtain the calculation

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result with high precision. This program is available for not only analysis of the existing material but also the design of the new material.

The calculation model in a case of 4H-SiC(0001) -Al (111) is shown in Fig. 3 (a). In Fig. 3 (b) and (c), local densities of states at the interface and bulk are shown. As the interface state was appeared in the vicinity of the Fermi level at the interface in Fig. 3 (b), SBH was derived from difference between the Fermi level and the calculated energy of valence band edge at the bulk in Fig. 3 (c). The calculated p-type SBH of the Si-faced contact was 1.08 eV and C-faced one was 0.32 eV respectively. This dependence of SBH is the same as that for 6H-SiC in which both measurement and calculation were obtained[2].

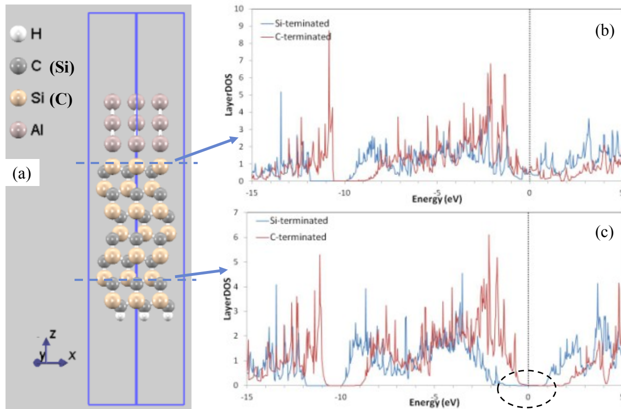

Fig. 3. (a) Calculation model in the case of SiC-Al. LDOS at the interface (b) and bulk (c).

III. A NEW TOPOGRAPHICAL ALGORITHM

For deposition and etching, a new robust, high-speed topographical algorithm has been proposed based on marching tetrahedral technique[3][4]. The new algorithm describes the boundary as geometric information of angle and curvature using the distance function. The outline of the proposed algorithm is shown in Fig. 4.

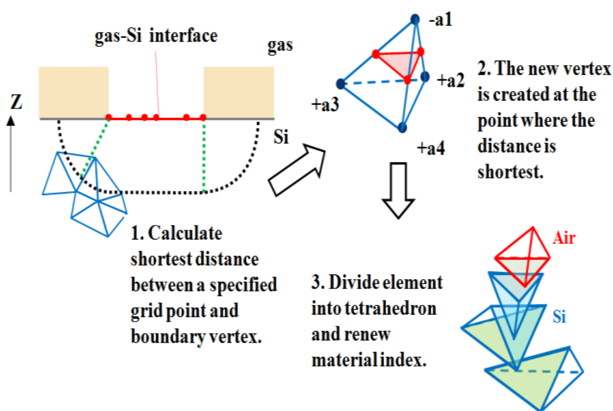

Fig. 4. Proposed 3D form tracing algorithm.

The proposed algorithm of form tracing is very simple. In each element, one kind of material is contained as a material flag, and can be changed by the change of its material flag. 3-dimensional form deformation is described by the distance function which is described as the distance between the edges of elements and material boundaries. As diffusion and ion implantation processes are calculated using 3-dimensional mesh, it is necessary that boundaries in materials are mapped to basic meshes by re-meshing and dividing elements.

Using this algorithm, rich expressions of material interfaces become possible through inserting boundaries in elements. It is possible to move boundaries freely with the moving boundary conditions, independent from the boundaries of the original meshes. However, quality of meshes may decrease with the increase of mesh divisions, thus, there is also a possibility of problem in the processing of ion implantation and impurity diffusion. Therefore it is necessary to adjust with the option which revises the mesh quality. As divided elements are recognized as different elements, they are not merged even after the disappearance of material interfaces through form deformations.

In our system, commands are expressed by six processing models as isotropic deposition, planar deposition, isotropic etching, anisotropic etching, planar etching, and all removal etching.

In this algorithm the division of element is limited only in new boundaries, thus the processing speed is much higher than previous methods which required the entire mesh regeneration. Examples of the final structures are shown in Fig. 5. Complex structure can be created easily by our proposed algorithm.

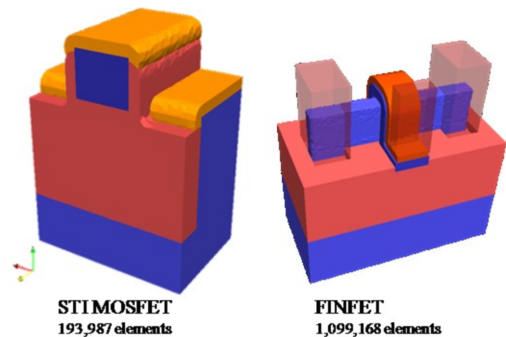

Fig. 5. Examples of the final structures

IV. A NARROW-CHANNEL EFFECT DUE TO THE DEACTIVATION OF ARSENIC

In the developed process simulator, the non-equilibrium diffusion model[5] has been implemented in which the point defect-impurity reactions, the point defect-cluster reactions and the impurity deactivations are considered. Here Monte Carlo method[5] has been implemented for ion implantation process in which crystal structure of Si (cubic) and SiC (hexagonal) can be treated. Binary Collision Approximation (BCA) is employed to calculate ion trajectories in materials including channeling effects. Nuclear scattering in a periodic

crystal structure is included for channeling effect and local and non-local electronic stopping is also included[6][7].

In this diffusion model, the interstitials generated by As-deactivation in highly dosed As enhance boron (B) diffusion. The peak of B distribution shifts toward the peak of As, as shown in Fig. 6. This shift results in the narrow-channel effect of 3D-MOSFET. As shown in Fig. 7, B atoms of halo implantation move towards the peak of As, so B concentration under extension decreases further near the STI (Shallow Trench Isolation) edge due to the 3-D distribution of interstitials, thus induces the narrow-channel effect of the threshold voltage of MOSFETs as shown in Fig. 8. In narrower channel, the threshold voltages decrease due to the decrease of boron concentration near the STI edge.

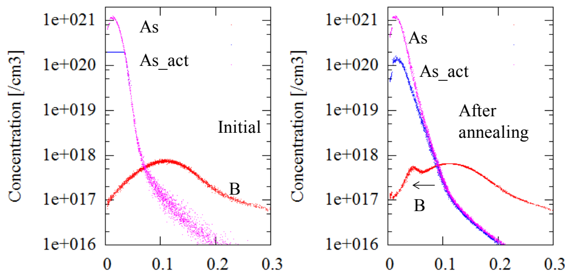

Fig. 6. The distribution of As(total), B(total), As(active) (a) as implantation, (b) after annealing.

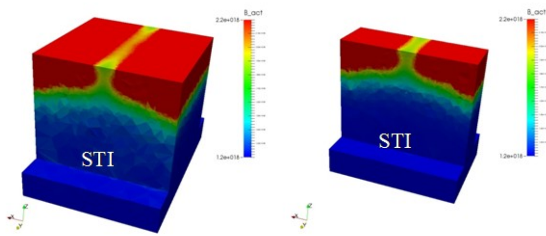

Fig. 7. Change of boron profile by channel width due to the arsenic deactivation (*Wg* = 250 nm (left) / 80 nm (right) and *Lg* = 50 nm)
(STI is not described in the figure).

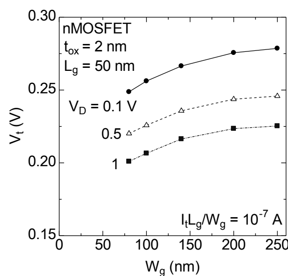

Fig. 8 Appearance of narrow-channel effect due to the change of boron profile by the deactivation of arsenic.

V. DEVICE MODELING FOR POWER DEVICES

By using a user-friendly GUI system, appropriate control volumes have been generated in three dimensions satisfying Delaunay condition for solving partial- differential equations. The ballistic transport mechanism in ultra-short channel devices has been modeled by using generalized mobility as a function of carrier energy [8].

For high-power device applications, material constants of SiC have been preset in the simulator. When a single-level recombination model is assumed, reverse-saturation current on pn junctions in wide-gap semiconductors is extremely low compared to measured one. Therefore, the recombination model assisted with two levels, named 2-level transition model has been developed [9] in addition to the single-level recombination model, so-called Schockley-Read-Hall model [10][11], and this facilitates obtaining solutions under high-voltage operation in SiC diode with a guard ring. The ionizations have been modeled with functions of the electric field following Ref.[12]. SiC diodes and vertical MOSFET have been analyzed, and results are shown in Figs. 9 and 10. High-breakdown voltages over 10 kV for the diode and also over 2 kV for the VMOSFET have successfully been simulated. An on-characteristic of the VMOSFET is illustrated in the insert of Fig. 10.

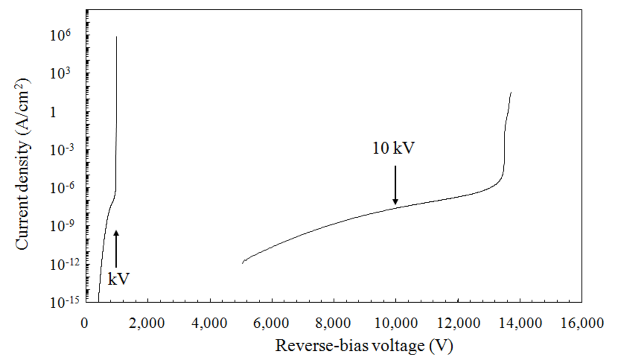

Fig. 9. Current-voltage characteristics of SiC diodes.

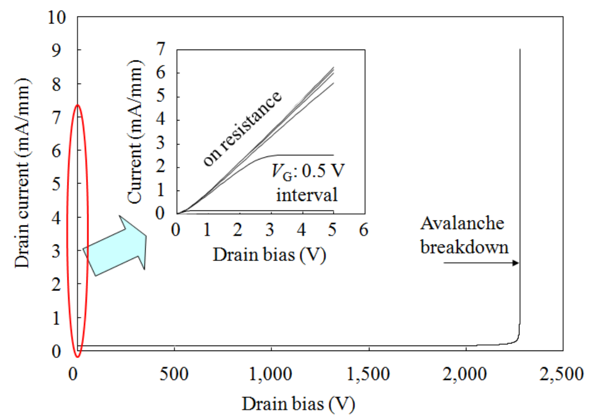

Fig. 10. Current-voltage characteristics of SiC vertical MOSFET.

VI. CONCLUSIONS

A new 3-D TCAD system has been developed featuring close coupling operation among first-principles calculator, process and device simulators. The first-principles calculator facilitates evaluation of electronic states for of new crystals and new materials prior to real implementation, and the derivation of Schottky-barrier height has been demonstrated using the system. In the process simulator, a robust and high-speed topographical algorithm has been newly proposed using the distance function and thus easier handling of complicated 3-D structure has been provided. And a 3-D narrow-channel effect of MOSFET due to arsenic deactivation has been demonstrated. In the device simulator, robust calculation for high-voltage breakdown characteristics of wide-gap devices has been demonstrated based on 2-level transition model. Finally the TCAD platform based on seamless GUI provides easier handling of whole operation.

ACKNOWLEDGMENT

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