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'Atomistic' Mesh Generation for the Simulation of Semiconductor Devices

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Abstract

A methodology for mesh generation with nodes placed on the atomic positions of the structure is presented. The meshing strategy is based on the use of patterns to decompose a unit cell of the target crystal into tetrahedra. The mesh generation procedure has been applied to crystalline Si and SiO_2 (α-quartz) as well as to their interface. The constructed meshes have been consequently randomly populated by dopants using Monte Carlo approach. The dopants are replacing silicon atom in nodes of the crystal. The 'atomistic' mesh populated with random discrete dopants has been used to simulate an ensemble of microscopically different double gate MOSFETs in order to demonstrate the functionality of the meshing methodology.

1 Introduction

High quality mesh generators are required in order to accurately resolve atomic scale effects in the simulation of nanometre scale CMOS devices [1]. At such dimensions the discreteness of atomic positions and charge distribution begins to strongly affects device characteristics [2]. The effects of random dopants on the behaviour of semiconductor devices have been widely studied [2, 3, 4] but, to the best of our knowledge, the exact positions of the dopants in the silicon crystal lattice have not been accurately resolved. While a good-quality mesh can be relatively easily generated for crystalline silicon because its lattice structure has a well-defined symmetry, it remains a challenging to do that for amorphous materials such as silica (a-SiO_2) shown in Fig. 1 (a) [5]. This is especially true for Si/a-SiO_2 interfaces, where an additional element of complexity is introduced by a complex structure of the border layer. In this work we make a considerable step towards solving this general problem by applying the new methodology to an interface of crystalline Si and SiO_2 (α-quartz) shown in Fig. 1 (b). The

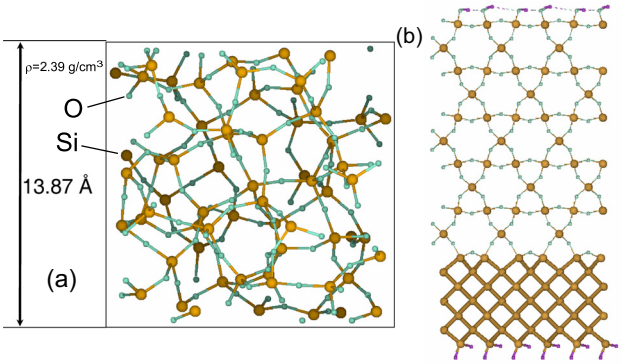

Figure 1: (a) Amorphous SiO_2 structure of 192 atoms obtained using classical molecular dynamics simulations [5]. (b) Atomic structure of crystalline Si/SiO_2 interface passivated by hydrogen atoms [6].

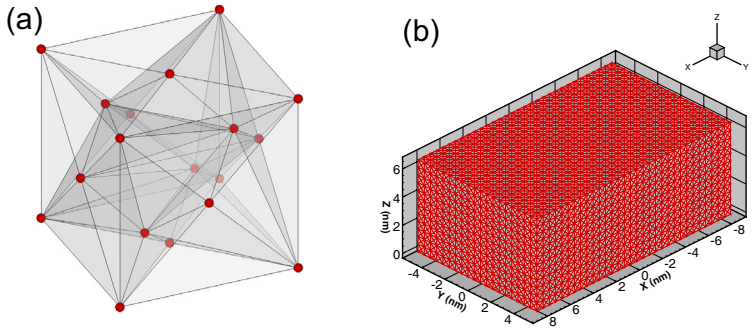

Figure 2: (a) Mesh of the terminal octant obtained using the atoms in the unit cell of Si as nodes. (b) Surface of the mesh generated for approximately 6.5 nm thick Si slab.

mesh generation is tested by simulating the 10 nm double gate (DG) MOSFET with 'atomistic' source–drain (S/D) doping.

2 Atomistic Meshing

We have modified our octree based mesh generator in order to obtain unstructured tetrahedral meshes [7] with nodes compliant with the positions of atoms in the silicon lattice. A new tetrahedra decomposition scheme has had to be implemented for terminal octants based on the silicon unit cell as shown in Fig. 2 (a). An internal symmetry of the unit cell is applied to carry out the decomposition tetrahedralizing a triangular prism and replicating it three times with the corresponding symmetry transformations. An example of the mesh generated for a silicon slab of $31 \times 19 \times 12$ unit cells constructed using the described tetrahedra decomposition scheme is shown in Fig. 2 (b).
Atomistic structure of the Si/SiO_2 interface has been obtained using first principles calculations [6]. The mesh constructed with nodes in the position of the atoms has to be unstructured while keeping the number of nodes reasonably low and allowing

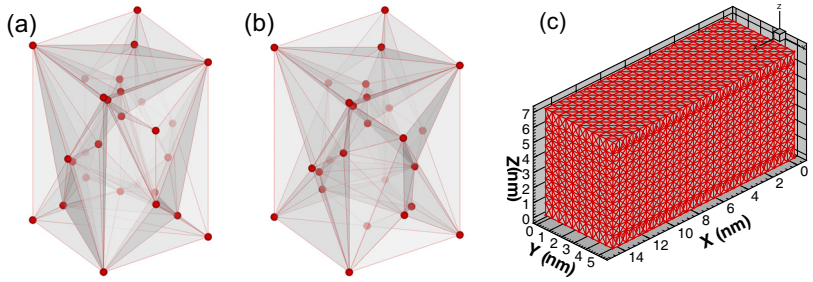

Figure 3: (a) Pattern used to build the mesh of crystalline SiO_2. (b) Pattern used to build the mesh of the interface between crystalline SiO_2 and crystalline Si. (c) Mesh of a DG MOSFET with crystalline SiO_2 as gate dielectric using patterns.

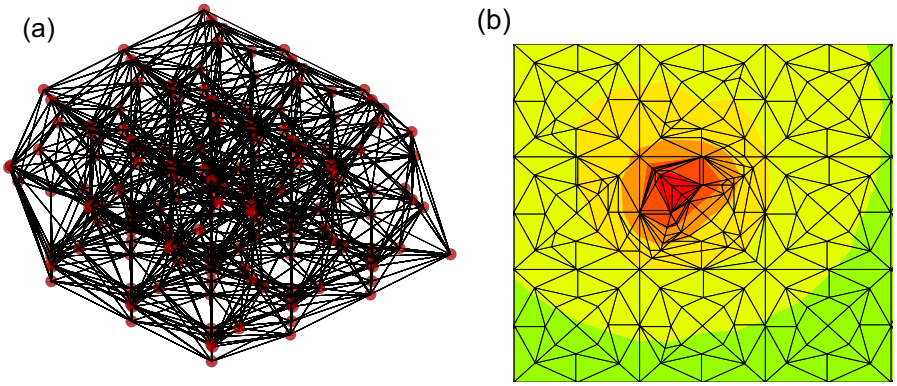

Figure 4: (a) Mesh generated for a 9 Å thick slab of crystalline SiO_2. (b) Detail of the refinement near one impurity atom. Colours correspond to a potential contour.

accurate representation of the atom positions in the gate dielectric. We have extended the mesh generation based on patterns to handle multi-material regions in order to avoid the problems with Delaunay triangulations of quasi-crystalline sets of points. A cell not only for the crystalline material but also for its interface has to be found. Figs. 3 (a), (b) and (c) show an example of the meshing approach for a SiO_2/Si/SiO_2 structure. An example of such mesh created for a crystalline SiO_2 is presented in Fig. 4 (a). These unstructured meshes can be also used to include refinement in specific regions without losing the information on the underlying atomic structure as illustrated in Fig. 4 (b).
This meshing approach has been employed to create an atomistic, high quality mesh for DG thin body transistors. Then, a Monte Carlo approach is used to place a dopant by replacing a silicon atom thus creating a particular distribution of random dopants [2]. Each distribution will produce a unique potential profile as shown in Fig. 5 (a). Fig. 5 (b) shows the $I_D - V_G$ characteristics of the whole ensemble of the 10 nm gate length DG devices at $V_D = 0.05\ V$ obtained from such statistical study. A mean of the characteristics of devices with discrete dopants is compared with the characteristics for the device with continuous S/D doping.

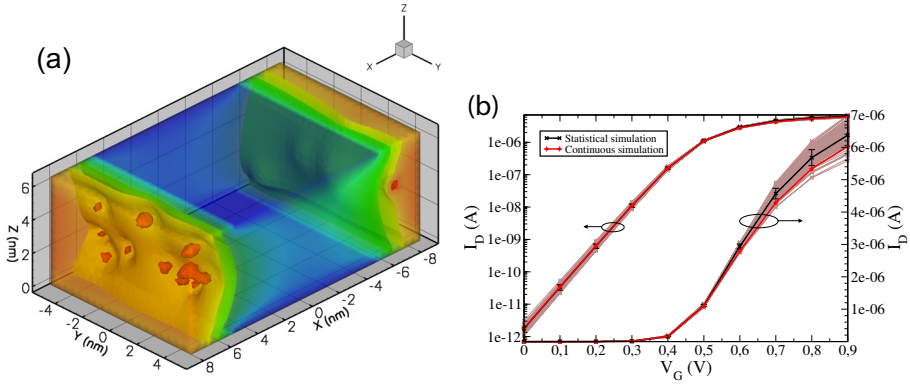

Figure 5: (a) Electrostatic potential at equilibrium for one configuration of the dopants located at atomic positions. (b) $I_D - V_G$ characteristics at $V_D = 0.05$ V for an ensemble of transistors. The result obtained using simulations with continuous doping (red line) and the mean (black line) of the current obtained using random dopants are highlighted.

3 Conclusions

We have presented a strategy to build meshes with nodes in the atomic positions of nanoscaled devices. This meshes become essential when the exact positions of the atoms needs to be resolved in order to obtain a realistic representation of physical quantities as potential, charge and/or wavefunctions. We have demonstrated the applicability of the meshing approach in the simulations of the 10 nm gate length DG MOSFET by studying an ensemble of devices with microscopically different doping characteristics.

Acknowledgments

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