

Multiscale Simulations of Plasma Etching in Silicon Carbide Structures

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Abstract. Manufacturing of Silicon Carbide (SiC) based devices will soon require the accuracy and control typical of the advanced Si based nanoelectronics. As a consequence, the processes development will surely benefit of technology computer aided design (TCAD) tools dedicated to the current and future SiC process technologies. Plasma etching is one of the most critical and difficult process for optimization procedures in the micro/nano fabrication area, since the resultant 2D (e.g. in trenches) or 3D (e.g. in holes) profiling is the consequence of the complex interactions between plasma and materials in the device structures. In this contribution we present a simulation tool dedicated to the etching simulation of SiC structures based on the sequential combination of a plasma scale global model and feature scale Kinetic Monte Carlo simulations. As an example of the approach validation procedure the simulations are compared with the characterization analysis of particular real process results.

Introduction

Process Technology Computer Aided Design (TCAD) codes are fundamental tools for speed-up the assessment of the process parameters against the requirements of the next-coming generation of electronics device and they are routinely applied by the R&D teams operating in the field of Si based micro- and nano-electronics. The extraordinary recent development of SiC devices technology has led the specifications for processes' accuracy and control for their manufacturing close to the ones of the advanced Si based nanoelectronics. This progress of SiC based technology will be soon increasingly supported by dedicated TCAD tools with proper model and calibration for this compound wide band gap material. Topography manipulation in 2D (e.g. in trenches profiles) or 3D (e.g. in holes profiles) geometries, obtained with the exposition of a pre-existing structure to etchant plasmas, is the results of the complex kinetics due to the interactions between plasmas and materials, and the development of predictive simulations' methods for this directional etching process is particularly challenging.

A multiscale methodology is necessary for an effective TCAD approach since this chemical-physical simulation should predict the morphology of the etched profile at the device feature scale (i.e. in the 10^{-9} - 10^{-6} m range of dimensions) starting from an input which is a combination of the initial (again at the feature scale) geometry and the process parameters, which generate the plasma conditions at the reactor scale (10^{-1} - 10^0 m range). Therefore, the full predictivity of the plasma processes relies on the suitable combination of two simulating approaches dealing with these to scales: 1) the status of the plasma generated in the reaction chamber and 2) the effect of the exposition of the processed sample to the plasma itself. In this contribution we present a simulation tool dedicated to the plasma simulation in SiC based device technology. Simulation results are compared with real processes microscopic analysis for equivalent macroscopic process parameters in order to demonstrate the reliability of the approach.

Model Description

The simulation method relies on the sequential combination of the following two approaches [Model 1) and Model 2)]. Model 1) operates at the macroscopic scale of the reactor and its scope is predicting as volume averages: the ion and neutral particle distributions, the electron density field, and the electron temperature field as a function of the process parameters (i.e. the chamber pressure, the fluxes in Standard Cubic Centimeters per Minute (SCCM) of the gases at the inlet, the power released by the electrodes in order to activate the chemical and ionization reactions in the plasma see [1]). The output quantities of this plasma model are fundamental for the correct determination of the local fluxes of the active species used as input parameters at the structure feature scale. The Model 2) (feature scale model) simulates (with an in-cell Kinetic Monte Carlo (KMC) simulation technique see Refs. [2]) the evolution of the microstructures (e.g. the evolution of the etching profile) starting from the “as prepared” sample morphology and materials implementing a stochastic approach for the surface reactions between the plasma component and the atoms in the substrates

The developed version overcomes some limitations of a previous tool [2], and specialized to Si substrate in order to allow: a) the application to the phenomenology in a compound semiconductors (i.e. SiC [3,4]) or more in general a two atoms substrate (see fig. 1) instead of a Si substrate and b) a generic input gas composition instead of a fixed “hardcoded” one.

For this general application and the Models 1) and 2) coupling, a python-based algorithm is designed for the automatic creation and solution of any global plasma models whereas the specific reactions' set is not embedded in the python code but it can be provided by an user defined flexible database. Different chains of surface reactions are activated at the feature scale by the plasma component interacting with the Si and C atom of the substrates (see Fig. 1), they include: neutrals' absorption, ion activated events (etching and sputtering), by-products deposition.

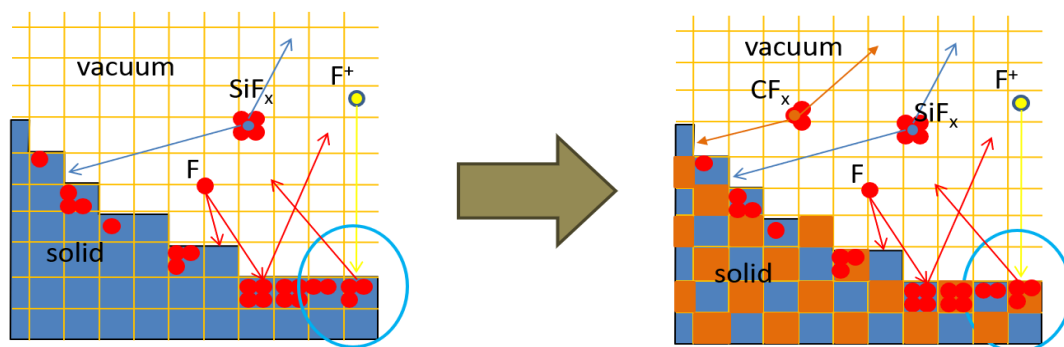


Fig. 1 Upgrade of the plasma etching simulation code scheme from the single atom substrate to a two atoms substrates: left side single element substrate (e.g. Si), right side compound substrate (e.g. SiC). In order to effectively consider separated Si and C reactions' path, the simulation box is divided in a chessboard-like distribution of cubic “cells” with a length $L = 1/\sqrt[3]{2\rho}$ where ρ is the atom density [atoms/cm³] of the SiC material. In the scheme orange cells are occupied by carbon atoms and blue cells by silicon atoms and, as a consequence, due to the associated length, each cell contains the average value of one atom (atomistic resolution). Some possible events for the different reactions chain activated by the events which initiated by the C or Si atoms are indicated.

In the application of the simulation discussed the next section (i.e. a plasma obtained with a in SF₆/O₂/Ar mixture) the model complexity (i.e. the different Monte Carlo particle considered in the Model 2)) comprises:

- 22 cell types (surface coverage types): Si, C, SiF, SiF₂, SiF₃, SiF₄, CF, CF₂, CF₃, CF₄, SiO, SiO₂, CO, CO₂, SiFO, SiF₂O, SiFO₂, SF₂O₂, CFO, CF₂O, CFO₂, CF₂O₂;
- 20 neutrals: SiF, SiF₂, SiF₃, SiF₄, SiF₅, SiF₆, S, F, F₂, O₂, O_{3p}, O_{1d}, SO, SO₂, SOF, SOF₂, SOF₃, SOF₃, SO₂F, SO₂F₂;
- 10 ions: SiF⁺, SiF₂⁺, SiF₃⁺, SiF₄⁺, SiF₅⁺, SiF₆⁺, S⁺, F⁺, O₂⁺, F₂⁺;

- 22 by-products: Si, C, SiF, SiF₂, SiF₃, SiF₄, CF, CF₂, CF₃, CF₄, SiO, SiO₂, CO, CO₂, SiFO, SiFO₂, SiF₂O, SF₂O₂, CFO, CF₂O, CFO₂, CF₂O₂.

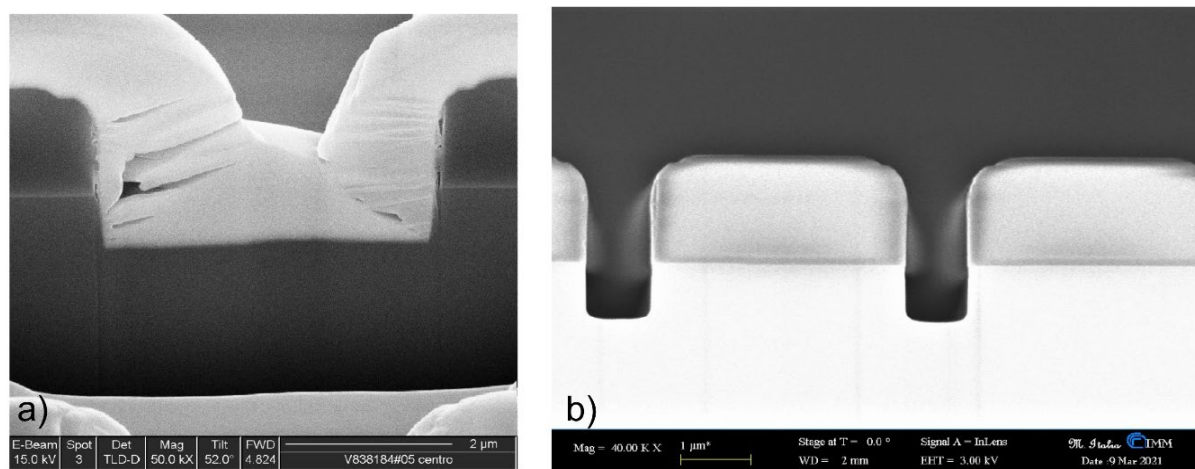


Fig. 2 a) FIB analysis in cross section view of the post-processed sample in the large opened area position; b) SEM analysis in cross section view of the post-processed sample in the trench position.

Impinging of neutrals activate the coverage species formation which detach, as by products, an increased yield with respect to the substrate species (ion-neutral synergism) due to ion-surface interaction events. Subsequence of events is randomly determined by means of the relative particle density estimated by the Model 1) [2].

Results and Discussion

The simulation code has been validated comparing code prediction with experimental characterizations of etching processes where plasma is generated loading the chamber with a SF₆/O₂/Ar mixture. The pre-processing system is composed by a 4H-SiC substrate and a SiO₂ film acting as an Hard-Mask (HM) material. Different geometries have been opened in the HM film in the same wafer in order to study visibility effects on the local etching yield. In fig. 2 we show two images obtained in cross section view with a Focused Ion Beam (FIB, panel a)) and Scanning Electron Microscopy (SEM, panel b)) for a large area and a trench geometry after the same etching process. Microscopy analysis evidences that the average etch rate (ER) is smaller in the trench with respect to the one measured in the open area location evidencing a limited but measurable shadowing effect due to the reduced average visibility solid angle: $ER(\text{trench})/ER(\text{open air}) = 0.94$. Moreover, a double step profile is evidenced at the edge of the mask for both geometries.

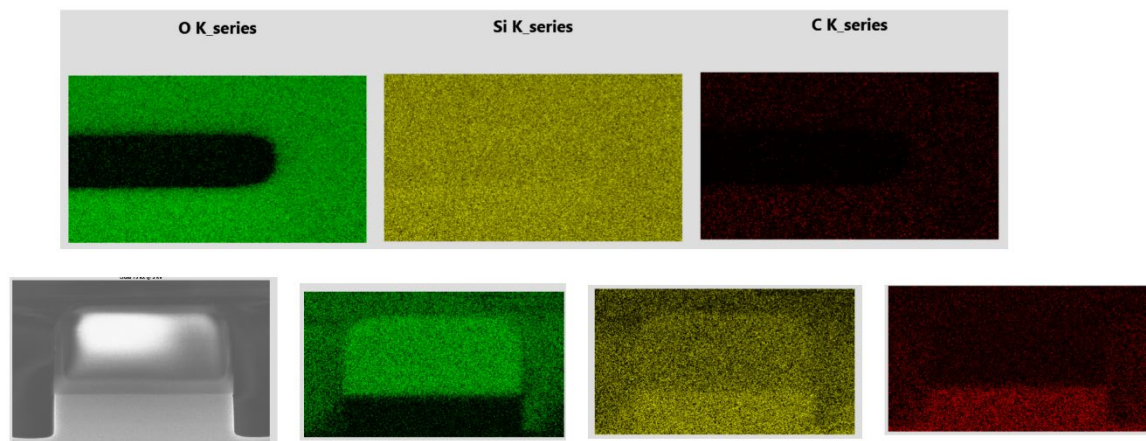


Fig. 3 EDX analysis in plan (top panel) and cross section (bottom panel) view of the post-processed samples in the trench position. Elements' contrast is indicated by the colours: green O, yellow Si, red C.

The hypothesis that the double step feature is due to the presence of an additional film (e.g. a resist residual) in the post-processed sample has been excluded by the Energy Dispersive X-Ray (EDX) analysis (fig. 3) which demonstrates that the mask after the process is made purely by SiO_2 .

A “virtual” process completely equivalent to the one discussed above has been simulated with our tool. The pre-etching structures can be inserted in our code as geometry input using a simplified CAD (see fig. 4) or directly uploading SEMs images with proper pixel contrast. In the present analysis we have used blanked structure to simulate large area case and a simplified rectangular shaped mask (Fig. 4) in order to verify if a pre-existing residual resist layer can explain the SEM and EXD results. The final simulated shape evidences also in the simulation a double step features while the Resist layer is completely removed in agreement with the experimental data. Moreover, also shadowing effect is reproduced by the KMC simulation.

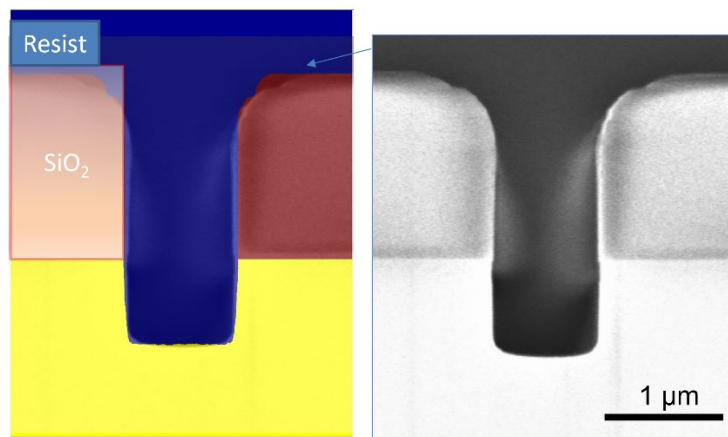


Fig. 4. Simulation results of a plasma etching process of a 4H-SiC trench with a $\text{SiF}_6/\text{O}_2/\text{Ar}$ plasma. The initial system is assumed to be an ideal rectangular SiO_2 hard mask with a residual Resist material on top. Simulation is overlapped with SEM analysis of the same process. Experimental SEM cross section is overlapped in transparency. A limited tapered profile and a reduced vertical etching yield with respect to a planar substrate (shadowing commonly cited as RIE-lag for a 6% reduction) is evidenced by the simulation which consider explicitly the visibility effects.

Summary

We have presented a multiscale methodology for the simulation of plasma etching in SiC structure. Comparisons with experimental analyses of the real process, by varying the initial microstructures geometries and the process parameters have been performed in order to validate the numerical tool. The code can be effectively applied in the process optimization where the vertical etching yield and profile shape (e.g. the angle with respect to the hard mask) are critical features for the devices performance (see Fig. 2). Moreover, the coupling approach can be also extended to the atomistic process simulations [5] for more accurate predictions.

Acknowledgments

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