ViennaTS User Guide

(Working Draft)

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About This Software

ViennaTS

Developer repository for ViennaTS, a C++, OpenMP-parallelized Topography simulator.

ViennaTS is currently in a prototype state.

System Requirements

* C++ compiler

* OpenMP

* Boost C++ Libraries

* HDF5 (optional - required for TDR file support)

Currently Supported Operating Systems

* GNU/Linux

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Founder and initial author was Otmar Ertl; not active anymore.

ViennaTS was developed under the aegis of the 'Institute for Microelectronics' at the 'TU Wien'. To understand more about the software implementation, you are encouraged to read through the dissertation of Otmar Ertl [1].

Getting Started

Building Instructions

To build ViennaTS, clone the repository and issue the following suggested commands:

```
$> cd viennats-dev              # the checked-out GIT folder
$> mkdir build            # the build folder
```

Configure the build, default build type is the 'optimized/release' mode:

```
$> cd build/
$> cmake ..
```

 # Watch for Warning/Error messages during the configuration stage.

Now build the 'viennats' executable

```
$> make
```

CMake Options

CMAKE_BUILD_TYPE = debug, (release) # Turn off/on optimizations (default: release, i.e., optimized mode)

Running the Software

```
./viennats [parameters_file]
```

All simulation and grid parameters are passed through the parameters file, the format of which is described in the next section.

Examples

Several examples are available in the *viennats-dev/examples/* folder. The examples listed there must be executed from the folder containing the parameter file in order to link to the input geometry properly.

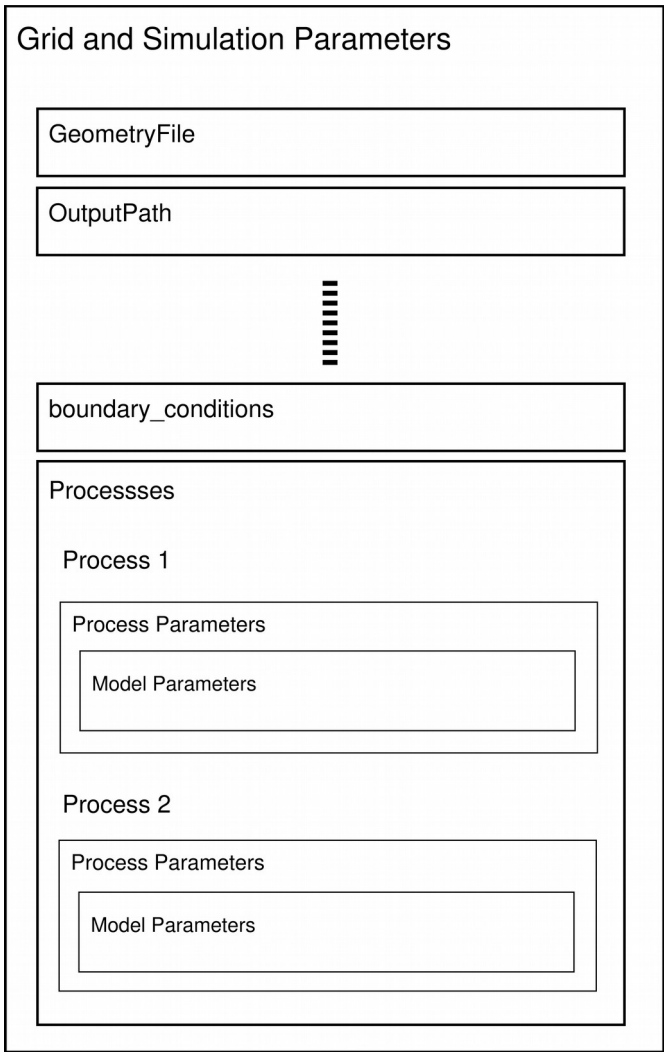
After building the ViennaTS executable (located in the build/ folder), change to an example folder (where the parameter file is located) and call the executable by passing an example parameter file to it.

If you are still in the *build/* folder, do:

```
$> cd ../examples/SiO2_Etching/
$> ../../build/viennats par_2d.txt
```

Populating the Parameters File

The parameters file is build hierarchically. One of the simulation parameters are the processes, which themselves have process-dependent parameters. One of the process parameters are the model-specific parameters.



Grid and Simulation Parameters

The grid and simulation parameters are listed below in two tables. The first table gives the list of available parameters and their types and the second table gives their description and purpose.

Format of the Parameters File

[parameter] = [parameter_value];

Available Parameters

Parameter	Parameter values	Type
geometry_file geometry_files GometryFile GeometryFiles	“FileName” “FileName1,FileName2,...,FileNameN”	string
output_path OutputPath	“FolderName”	string
surface_geometry	true/false	bool
report_import_errors	true/false	bool
cfl-condition	number	double
input_scale	number	double
grid_delta	number	double
input_transformation	(num1, num2, num3)	vector<int>
input_shift	(num1, num2, num3)	vector<double>
default_disk_orientation default_disc_orientation	(num1, num2, num3)	vector<double>
ignore_materials	(num1, num2, ... numN)	vector<int>
change_input_parity	true/false	bool
random_seed	number	int
num_dimensions	2 or 3	int
omp_threads	number	int
domain_extension	number	double
receptor_radius	number	double

Parameter	Parameter values	Type
further_tracking_distance	number	double
print_vtk	true/false	bool
print_dx	true/false	bool
print_lvst	true/false	bool
bits_per_distance	Number	int
print_velocities	true/false	bool
print_coverages	true/false	bool
print_rates	true/false	bool
print_materials	true/false	bool
print_statistics	true/false	bool
output_volume_extract_single_materials	true/false	bool
max_extended_starting_position	number	int
open_boundary	“[+ | -] [x | y | z]”	char array
remove_bottom	true/false	bool
snap_to_boundary_eps	number	double
process_cycles	number	int
material_mapping	(num1, num2, ... numN)	vector<int>
add_layer	number	int
boundary_conditions	{ {BOUNDARY_x1, BOUNDARY_x2}, {BOUNDARY_y1, BOUNDARY_y2}, {BOUNDARY_z1, BOUNDARY_z2} }	REFLECTIVE, SYMMETRIC, INFINITE, PERIODIC, EXTENDED
processes	{ { PROCESS1 }, { PROCESS2 }, ... { PROCESSn } }	

Description of the Available Parameters

Parameter	Default Value	Description
geometry_file geometry_files GometryFile GeometryFiles	REQUIRED	Location and name of the input geometry; when multiple surfaces are imported, separate with comma; quotation marks are required only at the start and end of the list
output_path OutputPath	REQUIRED	Location and name of the output folder; quotation marks are required; if the path is relative, the path is geometry_file is prepended
surface_geometry	false	True if the input geometry describes a surface (or surfaces). False if it describes a volume
report_import_errors	true	True if you wish to be informed of errors during geometry import; will also interrupt simulation in case an error is found; Recommended
cfl-condition	REQUIRED	Maximum time step for level set method (in grid units); Recommended maximum 0.5 (double)
input_scale	1	Scale the input geometry by the input_scale
grid_delta	REQUIRED	Grid spacing between grid points in each direction
input_transformation	(0, 0, 0)	Transformation for the input geometry for each axial direction
input_shift	(0, 0, 0)	Shift the geometry by the desired values for each axial direction
default_disk_orientation default_disc_orientation	REQUIRED	Default normal orientation
ignore_materials	-empty-	IDs of materials which are to be ignored
change_input_parity	false	Swap order of vertices in an elemnet in case the transformation has changed the triangle/tetrahedron orientation

Parameter	Default Value	Description
random_seed	-empty-	Seed for the random number generator
num_dimensions	REQUIRED	Number of dimensions
omp_threads	0	Number of parallel threads to be used during the simulation
domain_extension	0	Domain extension in case of EXTENDED boundary conditions
receptor_radius	0.8	Radius of the receptor disks
further_tracking_distance	3	Number of grid cubes for a particle to continue to be tracked after surface intersection is recorded
print_vtk	false	Output surfaces in the vtk file format
print_dx	false	Output surfaces in the dx file format
print_lvst	true	Output HRLE levelset structure in binary format
bits_per_distance	8	The number of bits to use per LS value saved in .lvst format in steps of 8 up to 64
print_velocities	false	Include the velocities in the output file
print_coverages	false	Include the coverages in the output file
print_rates	false	Include the surface rates in the output file
print_materials	false	Include the materials numbers in the output file
print_statistics	false	Output a statistics file
output_volume_extract_single_materials	true	Whether each layer should be represented by itself(true) or if it should wrap around layers below it(false)
max_extended_starting_position	1000	Number of grid points by which to extend in case of extended boundaries
open_boundary	REQUIRED	One boundary must be open infinite as it is where the ray tracing particles originate

Parameter	Default Value	Description
remove_bottom	true	True if the location of the bottom of the simulation space can be ignored
snap_to_boundary_eps	1e-6	Small number to ensure the simulation snaps to the full extents of the grid space
process_cycles	1	Number of times to perform the same processing sequence
material_mapping	-empty-	Change how materials are mapped by changing their IDs
add_layer	0	Generate more layers to replicate the top-most surface, required for deposition steps
boundary_conditions	REQUIRED	Define the boundary conditions for the simulation grid; can be REFLECTIVE (SYMMETRIC), INFINITE, PERIODIC, or EXTENDED
Processes	REQUIRED	List of processes to be executed in sequence; the process parameters are described in the section which follows

Process Parameters

Format in the Parameters File

```
processes {
{
    [process_parameter] = [process_parameter_value];
}
};
```

Available Process Parameters

Process parameter	Process parameter values	Type
process_time	number	double
smoothing_max_curvature	number	double
smoothing_min_curvature	number	double
smoothing_material_level	number	int
smoothing_max_iterations	number	int
add_layer	number	int
output_times_periodicity	number	int
output_times_period_length	number	double
initial_output	true/false	bool
final_output	true/false	bool
print_velocities	true/false	bool
print_coverages	true/false	bool
print_rates	true/false	bool
print_materials	true/false	bool
max_time_step	number	double
iteration_cycles	number	int
start_iteration_cycles	number	int
model_name	“ModelName”	string
output_times	{time1, time2, … timeN}	vector<double>
output_volume	{time1, time2, … timeN}	vector<double>
finite_difference_scheme	ENGQUIST_OSHER_1ST_ORDER ENGQUIST_OSHER_2ND_ORDER LAX_FRIEDRICHS_1ST_ORDER LAX_FRIEDRICHS_2ND_ORDER	
dissipation_coefficient	number	double
partition_data_structure	NEIGHBOR_LINKS_ARRAYS, FULL_GRID, UP_DOWN_LINKED_TREE	
partition_splitting_strategy	SPATIAL_MEDIAN, OBJECT_MEDIAN, SURFACE_AREA_HEURISTIC	
partition_surface_area_heuristic_lambda	number	double
ald_step	number	int
parameters	{ [parameter1] = [value]; [parameter2] = [value]; ... [parameterN] = [value]; };	model-specific parameters

Description of the Available Process Parameters

Process parameter	Default value	Description
process_time	0	Duration of the current process in seconds
smoothing_max_curvature	max<double>	Maximum parameter for smoothing surface level set every time step
smoothing_min_curvature	min<double>	Minimum parameter for smoothing surface level set every time step
smoothing_material_level	0	ID of material to be smoothed, if smoothing is applied
smoothing_max_iterations	100	Number of smoothing iterations to perform, if smoothing is applied
add_layer	0	Generate more layers to replicate the top-most surface, required for deposition steps
output_times_periodicity	1	Periodicity of output with output_times_period_length
output_times_period_length	0	Periodicity of output with output_times_periodicity
initial_output	false	True if initial output before the process simulation should be performed
final_output	false	True if final output after the process simulation should be performed
print_velocities	false	Include the velocities in the output file
print_coverages	false	Include the coverages in the output file
print_rates	false	Include the surface rates in the output file
print_materials	false	Include the materials numbers in the output file
max_time_step MaxTimeStep	max<double>	Maximum allowed time step

Process parameter	Default value	Description
iteration_cycles IterationCycles	0	The number of iterations (process calculation) before advancing to the next time step
start_iteration_cycles StartIterationCycles	0	The number of iterations at the process simulation start, might be necessary to calculate initial values for coverages
model_name	REQUIRED	The name of the used process model
output_times	-empty-	Vector of times where the output should be printed
output_volume	-empty-	Vector of times when hull mesh should be printed
finite_difference_scheme	ENGQUIST_OSHER_1ST_ORDER	Finite difference scheme to use for the simulation
dissipation_coefficient	-empty-	Dissipation coefficient to use for the Lax Friedrichs scheme
partition_data_structure	NEIGHBOR_LINKS_ARRAYS	Partition data structure to use for the simulation
partition_splitting_strategy	SURFACE_AREA_HEURISTIC	Partition splitting strategy to use for the simulation
partition_surface_area_heuristic_lambda	0.8	Heuristic lambda for the surface area partition
ald_step	-empty-	Only required for models “TiN_ALD” and “TiN_PEALD”. Decides the step in the ALD cycle and can only be ‘1’ or ‘2’
parameters	REQUIRED	Model parameters, which are passsed ot the model given by “ModelName”

Process Models

Available Process Model	Model Name
Anisotropic wet etching	“WetEtching”
BCl_3 plasma etching	“BCl3PlasmaEtching”
Boolean operation	“BooleanOperation”
CFx Deposition	“CFx_Deposition”
Chemical mechanical planarization	“Planarization”
Constant rates	“ConstantRates”
Flux calculation	“CalculateFlux”
Focused ion beam	“FIB”
HfO2 deposition	"HfO2_Deposition"
Mask addition	“Mask”
Non-linear deposition	“NonlinearDeposition”
Palsma etching HBr/O_2	“HBr_O2PlasmaEtching”
Plasma etching Cl_2/CH_4	“Cl2_CH4PlasmaEtching”
Etching Cl_2/N_2	"Cl2_N2Etching"
Plasma etching HBr/O_2	"HBr_O2PlasmaEtching"
Plasma etching SF_6/CH_2F_2	"SF6_CH2F2PlasmaEtching"
Plasma etching SF_6/O_2	“SF6_O2PlasmaEtching”
Plasma etching SiO_2	“SiO2_PlasmaEtching”
Simple deposition	“SimpleDeposition”
TiN atomic layer deposition	"TiN_ALD"
TiN plasma enhanced atomic layer deposition	"TiN_PEALD"
TiO_2 atomic layer deposition	"TiO2_ALD"

Model Parameters

The model parameters are implemented as one section of the process parameters.

Format in the Parameters File

```
processes {
{
	[process_parameter1] = [process_parameter1_value];
	[process_parameter2] = [process_parameter2_value];
		...
	[process_parameterN] = [process_parameterN_value];
	parameters = {
		[model_parameter] = [model_parameter_value];
	};
}
};
```

Boolean Operation

This model is used to perform boolean operations between two surfaces. From [1]:
If one considers the sets M_A, M_B, and M_C and the corresponding boundaries $S_A = \partial M_A$, SB = ∂M_B, and $S_C = \partial M_C$, which are represented by the LS functions Φ_A, Φ_B, and Φ_C, the LS counterparts of Boolean operations are listed in the following.

$$\text{Union:} \quad M_A = M_B \cup M_C \Leftrightarrow \Phi_A = \min(\Phi_B, \Phi_C)$$

$$\text{Intersection:} \quad M_A = M_B \cap M_C \Leftrightarrow \Phi_A = \max(\Phi_B, \Phi_C)$$

$$\text{Complement:} \quad M_A = R^D \setminus M_B \Leftrightarrow \Phi_A = -\Phi_B$$

$$\text{Relative complement:} \quad M_A = M_B \setminus M_C \Leftrightarrow \Phi_A = \max(\Phi_B, -\Phi_C)$$

Model name = “BooleanOperation”

Process parameter	**Process parameter values**	**Type**
geometry_file	“FileName”	string
level	number	int
invert	true/false	bool
surface_geometry	true/false	bool
levelset	number	int
remove_bottom	true/false	bool
wrap_surface	true/false	bool

Process parameter	**Default value**	**Description**
geometry_file	REQUIRED or levelset	Name of file with which to perform the boolean operation
level	0	positive – union negative – intersection The number of Levelsets this is applied to from topmost to lowest.
invert	false	Invert geometry before performing boolean operation
surface_geometry	false	True if the input geometry describes a surface (or surfaces). False if it describes a volume
levelset	REQUIRED or geometry_file	The internal levelset to use for boolean operation.
remove_bottom	true	True if the location of the bottom of the simulation space can be ignored.
wrap_surface	false	Whether top levelset should wrap around all lower ones.

Mask Addition

A mask is introduced with a pattern transfer using boolean operations.

Model name = “Mask”

Process parameter	Process parameter values	Type
mask_file	“FileName”	string
surface_geometry	true/false	bool
remove_bottom	true/false	bool
ignore_other_materials	true/false	bool

Process parameter	Default value	Description
mask_file	REQUIRED	Name of geometry file to be used as a mask layer
surface_geometry	false	True if the input geometry describes a surface (or surfaces). False if it describes a volume
remove_bottom	true	True if the location of the bottom of the simulation space can be ignored
ignore_other_materials	false	True if the mask should be placed, regardless of any other material already being there. False when mask should only be placed in space not occupied by any other material.

Chemical Mechanical Planarization

Chemical mechanical planarization (CMP) assumes that everything above a certain height is removed.

Model name = “Planarization”

Process parameter	Process parameter values	Type
coordinate	number	double
fill_up	true/false	bool

Process parameter	Default value	Description
coordinate	REQUIRED	Value which determines the level at which the surface should be flattened
fill_up	false	False when no new material is introduced during planarization

Constant Rates

The constant rates model prescribes a given velocity to the level set geometries.

Model name = “ConstantRates”

Process parameter	Process parameter values	Type
direction	{num1, num2, num3}	double[3]
constant_rates	{num1, num2, … numN)	vector<double>
Isotropic_rates	{num1, num2, … numN)	vector<double>
directional_rates	{num1, num2, … numN)	vector<double>
vector_rates	{num1, num2, … numN)	vector<double>

Process parameter	Default value	Description
direction	-empty-	Direction in which the “directional_rates” should proceed
constant_rates	-empty-	Anisotropic velocity of the surface, defined for each material
Isotropic_rates	-empty-	Isotropic velocity of the surface, defined for each material
directional_rates	-empty-	Directional velocity of the surface, defined for each material; combined with the “direction” parameter
vector_rates	-empty-	Vector velocity of the surface, defined for each material

Anisotropic Wet Etching

The implemented model for the anisotropic wet etching of silicon is described in [2].

Model name = “WetEtching”

Process parameter	Process parameter values	Type
direction100	{num1, num2, num3}	vector<double>
direction010	{num1, num2, num3}	vector<double>
r100	number	double
r110	number	double
r111	number	double
r311	number	double
has_mask	true/false	bool

Process parameter	Default value	Description
direction100	REQUIRED	Normal vector for the crystallographic direction [100]
direction010	REQUIRED	Normal vector for the crystallographic direction [010]
r100	REQUIRED	Etch rate in the [100] crystallographic direction
r110	REQUIRED	Etch rate in the [110] crystallographic direction
r111	REQUIRED	Etch rate in the [111] crystallographic direction
r311	REQUIRED	Etch rate in the [311] crystallographic direction
has_mask	false	True if the etch should be performed around a mask

Simple Deposition

The simple deposition model is used when a single neutral depositing species is required for the process. Details of the implementation can be found in [1] and [3].

Model name = “SimpleDeposition”

Process parameter	Process parameter values	Type
direction	{num1, num2, num3}	double[3]
flux	number	double
sticking_probability	number	double
star_angle_distribution	number	double
reemitted_angle_distribution	number	double
stop_criterion	number	double
yield	number	double
statistical_accuracy	number	double

Process parameter	Default value	Description
direction	REQUIRED	Average direction of the incoming particles
flux	REQUIRED	Flux of the depositing species
sticking_probability	REQUIRED	Sticking probability of the depositing species on the surface
start_angle_distribution	1	Angular distribution of the incoming particles
reemitted_angle_distribution	1	Angular distribution of the particles which are reflected from the surface
stop_criterion	REQUIRED	Particle tracking continues until its probability reaches the stop_criterion
yield	REQUIRED	Relates the surface rates to the final velocity
statistical_accuracy	REQUIRED	Number of particles to use for each time step

Non-Linear Deposition

The implemented non-linear deposition model is described in more details in [4].

Model name = “NonlinearDeposition”

Process parameter	Process parameter values	Type
direction	{num1, num2, num3}	double[3]
deposition_rate	number	double
sticking_probability	number	double
reaction_order	number	double
stop_criterion	number	double
statistical_accuracy	number	double

Process parameter	Default value	Description
direction	REQUIRED	Average direction of the incoming particles
deposition_rate	REQUIRED	Average rate for the deposition
sticking_probability	REQUIRED	Sticking probability of the depositing species on the surface
reaction_order	REQUIRED	Order of the surface reaction; used to combine the effects of the depositing species coverage with the reflection coefficient and rate
stop_criterion	REQUIRED	Particle tracking continues until its probability reaches the stop_criterion
statistical_accuracy	REQUIRED	Number of particles to use for each time step

Flux Calculation

The flux calculation model is used to calculate the flux on a given geometry for various reflection models. The model will output two CSV files: rates.csv and rates_griddelta.csv.

rates.csv	–	Output file of the surface rates for all active grid points in grid spacing units defined by the grid_delta parameter
rates_griddelta.csv	–	Output file of the surface rates for all active grid points in global units (nm, µm, cm, m, ...)

Model name = “CalculateFlux”

Process parameter	**Process parameter values**	**Type**
direction	{num1, num2, num3}	double[3]
reflection_model	NONE DIFFUSIVE_SINGLE DIFFUSIVE_MULTIPLE SPECULAR DIFFUSIVE_COMBINED	-
reflection_diffusive_upperbound	number	int
flux	number	double
sticking_probability	number	double
star_angle_distribution	number	double
reemitted_angle_distribution	number	double
stop_criterion	number	double
yield	number	double
statistical_accuracy	number	double

Process parameter	**Default value**	**Description**
direction	REQUIRED	Average direction of the incoming particles
reflection_model	DIFFUSIVE_SINGLE	Applies the desired particle reflection model
reflection_diffusive_upperbound	4	Maximum number of new particles to generate when DIFFUSIVE_MULTIPLE reflection is selected
flux	REQUIRED	Flux of the depositing species

Process parameter	Default value	Description
sticking_probability	REQUIRED	Sticking probability of the depositing species on the surface
start_angle_distribution	1	Angular distribution of the incoming particles
reemitted_angle_distribution	1	Angular distribution of the particles which are reflected from the surface
stop_criterion	REQUIRED	Particle tracking continues until its probability reaches the stop_criterion
yield	REQUIRED	Relates the surface rates to the final velocity
statistical_accuracy	REQUIRED	Number of particles to use for each time step

Focused Ion Beam

The level set model for 2D FIB simulations is given in [5], while the 3D extension is described in further details in [1].

Model name = “FIB”

Process parameter	**Process parameter values**	**Type**
position	{num1, num2, num3}	double[3]
direction	{num1, num2, num3}	double[3]
FWHM	number	double
yield_0	number	double
yield_max	number	double
angle_max	number	double
current	number	double
num_reemited_particles	number	int
target_density	number	double
stop_criterion	number	double
sticking_probability	number	double
sputter_yield_file	“FileName”	string
num_simulated_particles	number	int

Process parameter	**Default value**	**Description**
position	REQUIRED	Location of the source of the incoming particles
direction	REQUIRED	Average direction of the incoming particles
FWHM	REQUIRED	Full width at half maximum for the incoming particle beam
yield_0	-empty-	Required Yamamura model parameter
yield_max	-empty-	Required Yamamura model parameter
angle_max	-empty-	Required Yamamura model parameter
current	REQUIRED	Flux of the incoming particles

Process parameter	Default value	Description
num_reemited_particles	1	Number of particles to be re-emitted after surface reflection
target_density	REQUIRED	Density of the targeted material
stop_criterion	0	Particle tracking continues until its probability reaches the stop_criterion
sticking_probability	0	Sticking probability of the depositing species on the surface
sputter_yield_file	-empty-	If a file should be used instead of the Yamamura model, then a file should be given
num_simulated_particles	REQUIRED	Number of particles to use for each time step

Plasma Etching – HBr/O_2

The model implemented within the level set framework is explained in more details in [6], while the parameters used in the model are given in [7].

Model name = “HBr_O2PlasmaEtching”

Process parameter	**Process parameter values**	**Type**
direction	{num1, num2, num3}	double[3]
flux_ion	number (/cm^3)	double
flux_oxygen	number (/cm^3)	double
flux_bromine	number (/cm^3)	double
a_oxygen	number	double
statistical_accuracy	number	int
min_ion_energy	number	double
delta_ion_energy	number	double

Process parameter	**Default value**	**Description**
direction	REQUIRED	Average direction of the incoming particles
flux_ion	REQUIRED	Incoming ion flux
flux_oxygen	REQUIRED	Oxygen flux at the feature surface
flux_bromine	REQUIRED	Bromine flux at the feature surface
a_oxygen	REQUIRED	Model parameter related to the oxygen yield
statistical_accuracy	REQUIRED	Number of particles to use for each time step
min_ion_energy	REQUIRED	Minimum energy of the incoming ions
delta_ion_energy	REQUIRED	Delta energy of the incoming ions, used to generate an ion particle energy distribution

Plasma Etching – SF_6/O_2

The model implemented within the level set framework is explained in more details in [1], while the parameters used in the model are given in [8].

Model name = “SF6_O2PlasmaEtching”

Process parameter	**Process parameter values**	**Type**
direction	{num1, num2, num3}	double[3]
flux_ion	number (/cm^3)	double
flux_oxygen	number (/cm^3)	double
flux_fluorine	number (/cm^3)	double
a_oxygen	number	double
statistical_accuracy	number	int
min_ion_energy	number	double
delta_ion_energy	number	double

Process parameter	**Default value**	**Description**
direction	REQUIRED	Average direction of the incoming particles
flux_ion	REQUIRED	Incoming ion flux
flux_oxygen	REQUIRED	Oxygen flux at the feature surface
flux_fluorine	REQUIRED	Fluorine flux at the feature surface
a_oxygen	REQUIRED	Model parameter related to the oxygen yield
statistical_accuracy	REQUIRED	Number of particles to use for each time step
min_ion_energy	REQUIRED	Minimum energy of the incoming ions
delta_ion_energy	REQUIRED	Delta energy of the incoming ions, used to generate an ion particle energy distribution

Plasma etching - SiO_2

The model implemented within the level set framework is explained in more details in [6], while the parameters used in the model are given in [9].

Model name = “SiO2_PlasmaEtching”

Process parameter	**Process parameter values**	**Type**
direction	{num1, num2, num3}	double[3]
flux_ion	number (/cm^3)	double
flux_polymer	number (/cm^3)	double
flux_etchant	number (/cm^3)	double
statistical_accuracy	number	int
min_ion_energy	number	double
delta_ion_energy	number	double
temperature	number	double

Process parameter	**Default value**	**Description**
direction	REQUIRED	Average direction of the incoming particles
flux_ion	REQUIRED	Incoming ion flux
flux_polymer	REQUIRED	Flux of the polymer which is simultaneously deposited along the profile during the etching step
flux_etchant	REQUIRED	Flux of the etchant used to chemically etch the oxide layer
statistical_accuracy	REQUIRED	Number of particles to use for each time step
min_ion_energy	REQUIRED	Minimum energy of the incoming ions
delta_ion_energy	REQUIRED	Delta energy of the incoming ions, used to generate an ion particle energy distribution
temperature	REQUIRED	Temperature of the simulation; The effective etchant flux has an Arrhenius relationship to the incoming flux

Plasma Etching - BCl_3

The model implemented within the level set framework is explained in more details in [6], while the parameters used in the model are given in [9].

Model name = “BCl3PlasmaEtching”

Process parameter	**Process parameter values**	**Type**
direction	{num1, num2, num3}	double[3]
flux_ion	number (/cm^3)	double
flux_BCl3	number (/cm^3)	double
statistical_accuracy	number	int
min_ion_energy	number	double
delta_ion_energy	number	double

Process parameter	**Default value**	**Description**
direction	REQUIRED	Average direction of the incoming particles
flux_ion	REQUIRED	Incoming ion flux
flux_BCl3	REQUIRED	Flux of the BCl3 gas
statistical_accuracy	REQUIRED	Number of particles to use for each time step
min_ion_energy	REQUIRED	Minimum energy of the incoming ions
delta_ion_energy	REQUIRED	Delta energy of the incoming ions, used to generate an ion particle energy distribution

CF_x Deposition

The model implemented within the level set framework is explained in more details in [6], while the parameters used in the model are given in [9].

Model name = “CFx_Deposition”

Process parameter	**Process parameter values**	**Type**
direction	{num1, num2, num3}	double[3]
end_probability	number	double
IonFlux	number (/cm^3)	double
CFxFlux	number (/cm^3)	double
statistical_accuracy	number	double

Process parameter	**Default value**	**Description**
direction	REQUIRED	Average direction of the incoming particles
end_probability	REQUIRED	Particle tracking continues until the particles scattering probability reaches this value
IonFlux	REQUIRED	Incoming ion flux
CFxFlux	REQUIRED	Flux of the CF_x gas
statistical_accuracy	REQUIRED	Number of particles to use for each time step

Plasma Etching - Cl_2/CH_4

The model implemented within the level set framework is explained in more details in [6], while the parameters used in the model are given in [9].

Model name = “Cl2_CH4PlasmaEtching”

Process parameter	**Process parameter values**	**Type**
direction	{num1, num2, num3}	double[3]
flux_ion	number (/cm^3)	double
flux_CH4	number (/cm^3)	double
flux_chlorine	number (/cm^3)	double
statistical_accuracy	number	int
min_ion_energy	number	double
delta_ion_energy	number	double

Process parameter	**Default value**	**Description**
direction	REQUIRED	Average direction of the incoming particles
flux_ion	REQUIRED	Incoming ion flux
flux_CH4	REQUIRED	Flux of the polymer which is simultaneously deposited along the profile during the etching step
flux_chlorine	REQUIRED	Flux of chlorine used to chemically etch the substrate
statistical_accuracy	REQUIRED	Number of particles to use for each time step
min_ion_energy	REQUIRED	Minimum energy of the incoming ions
delta_ion_energy	REQUIRED	Delta energy of the incoming ions, used to generate an ion particle energy distribution

Etching - Cl_2/N_2

Model name = “Cl2_N2PlasmaEtching”

Process parameter	Process parameter values	Type
direction	{num1, num2, num3}	double[3]
flux	number (/cm^3)	double
pressure	number (Pa)	double
temperature	number	double

Process parameter	Default value	Description
direction	REQUIRED	Average direction of the incoming particles
flux	REQUIRED	Incoming Cl_2/N_2 flux
pressure	REQUIRED	Gas pressure in the reactor
temperature	REQUIRED	Temperature in the reactor

Plasma Etching – SF_6/CH_2F_2

The model implemented within the level set framework is explained in more details in [6], while the parameters used in the model are given in [9].

Model name = “SF6_CH2F2PlasmaEtching”

Process parameter	**Process parameter values**	**Type**
direction	{num1, num2, num3}	double[3]
flux_ion	number (/cm^3)	double
flux_polymer	number (/cm^3)	double
flux_etchant	number (/cm^3)	double
statistical_accuracy	number	int
min_ion_energy	number	double
delta_ion_energy	number	double

Process parameter	**Default value**	**Description**
direction	REQUIRED	Average direction of the incoming particles
flux_ion	REQUIRED	Incoming ion flux
flux_polymer	REQUIRED	Flux of the CH_2F_2polymer which is deposited along the profile
flux_etchant	REQUIRED	Flux of SF_6 used to chemically etch the substrate
statistical_accuracy	REQUIRED	Number of particles to use for each time step
min_ion_energy	REQUIRED	Minimum energy of the incoming ions
delta_ion_energy	REQUIRED	Delta energy of the incoming ions, used to generate an ion particle energy distribution

HfO_2 deposition

Model name = “HfO2_Deposition”

Process parameter	Process parameter values	Type
direction	{num1, num2, num3}	double[3]
pressure	number (Pa)	double
temperature	number (K)	double
stop_criterion	number	double
statistical_accuracy	number	int

Process parameter	Default value	Description
direction	REQUIRED	Average direction of the incoming particles
pressure	REQUIRED	Gas pressure inside reactor.
temperature	REQUIRED	Temperature inside reactor.
stop_criterion	REQUIRED	Particle tracking continues until the particles scattering probability reaches this value
statistical_accuracy	REQUIRED	Number of particles to use for each time step

TiN Atomic Layer Deposition

Model name = “TiN_ALD”

Process parameter	Process parameter values	Type
direction	{num1, num2, num3}	double[3]
step_size	number	double
molecular_thickness	number	double
m_NH3	number	double
m_TDMAT	number	double
reaction_order	number	double
stop_criterion	number	double
sticking_probability	number	double
statistical_accuracy	number	int

Process parameter	Default value	Description
direction	REQUIRED	Average direction of the incoming particles
step_size	1e-4	Time discretization factor for solving the coverages equation
molecular_thickness	0.433 Å	Thickness of a single atomic layer of the deposited film
m_NH3	4	Volume ratio NH_3 molecule compared to an atomic unit of TiN
m_TDMAT	1	Volume ratio TDMAT molecule compared to an atomic unit of TiN
reaction_order	REQUIRED	Order of surface reaction
stop_criterion	REQUIRED	Particle tracking continues until the particles scattering probability reaches this value
sticking_probability	REQUIRED	Probability of particle sticking on the surface after impact
statistical_accuracy	REQUIRED	Number of particles to use for each time step

TiN Plasma Enhanced Atomic Layer Deposition

Model name = “TiN_PEALD”

Process parameter	Process parameter values	Type
direction	{num1, num2, num3}	double[3]
step_size	number	double
molecular_thickness	number	double
stop_criterion	number	double
sticking_probability	number	double
statistical_accuracy	number	int

Process parameter	Default value	Description
direction	REQUIRED	Average direction of the incoming particles
step_size	1e-4	Time discretization factor for solving the coverages equation
molecular_thickness	0.433 Å	Thickness of one layer
stop_criterion	REQUIRED	Particle tracking continues until the particles scattering probability reaches this value
sticking_probability	REQUIRED	Probability of particle sticking on the surface after impact
statistical_accuracy	REQUIRED	Number of particles to use for each time step

TiO_2 Atomic Layer Deposition

Model name = “TiO2_ALD”

Process parameter	**Process parameter values**	**Type**
direction	{num1, num2, num3}	double[3]
TTIP_Flux	number	double
H2O_Flux	Number	double
molecular_thickness	number	double
sticking_TTIP	number	double
sticking_H2O	number	double
end_probability	number	double
statistical_accuracy	number	int

Process parameter	**Default value**	**Description**
direction	REQUIRED	Average direction of the incoming particles
TTIP_Flux	REQUIRED	Flux of TTIP
H2O_Flux	REQUIRED	Flux of H_2O
molecular_thickness	0.5e-8 cm	Thickness of one layer
sticking_TTIP	REQUIRED	Sticking probability of TTIP
sticking_H2O	REQUIRED	Sticking probability of H_2O
end_probability	REQUIRED	Particle tracking continues until the particles scattering probability reaches this value
statistical_accuracy	REQUIRED	Number of particles to use for each time step

Application Programming Interface

In the */src/viennats.cpp* file, the *main* directory is found. The only argument which needs to be passed during execution is the parameters file.

Please look at the */docs/ViennaTS_documentation.html* for a more detailed documentation of the ViennaTS code.

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