SILVACO
INTERNATIONAL

ATHENA

Release Notes

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1:Version 5.16.0.R

1.1: SSUPREM4 Features

1. The Monte Carlo (BCA) implantation module has been multithreaded.

   By default, ATHENA runs on the maximum number of CPUs available online. You can specify the number of CPUs to be used by the parameter "-P <n>" in the athena command line as follows:

   ```
   athena -P 2 input.in
   ```

   When running athena within DECKBUILD, add the "-P 2" option to the "simflags" parameter of the GO statement

   The speedup achieved with the multi-threading of the BCA module is close to linear for simulation of large number of trajectories (N.ION > 50000). This almost optimal behavior is due to the inherent parallel structure of the BCA implantation module.

   There are following limitations for using multi-threading version of MC Implant Module. If you specify the TRAJ.FILE parameter (option to save ion trajectories in a special structure file for subsequent display in TONYPLOT) in the IMPLANT statement, the multi-threading capability will switch off. The FULLROTATION parameter of the IMPLANT statement couldn't be specified simultaneously with multi-threading. Multiple rotation statements should be used instead.
2. Implemented BCA implantation models for {110} and {111} silicon.
3. Added capability to MC Implant Module that allows to simulate damage or preamorphization induced by arbitrary "inert" ion bombardment. You can specify atomic number Z1 and atomic weight M1 in the IMPLANT statement. Only implant damage will be introduced into the structure after the completion of the Z1 ion implant. The level of this damage will affect subsequent "normal" implant profiles.

Note: If M1 is not specified, the atomic weight of the main isotope of element Z1 will be used.

4. Memory management of all modules is substantially improved. As the result, the limits on number of grid points, nodes, and triangles in simulation structure are removed. This allows to perform simulation in large multilayer structures without sacrificing accuracy.
5. Fixed the capability to specify diffusion through "impurity-vacancy pairs" defined by parameters, such as DVX.0, DVX.E.
6. Added positively charged vacancy/impurity pair diffusion parameters to the IMPURITY statement: DVP.0, DVP.E, DVPP.0, and DVPP.E.
7. Added values for diffusion and activation parameters of B, P, As, and SB in Germanium. The experimental data from [1] and [2] were used for parameter estimations.

1.2: Optolith Features

1. Added the multi-image capability to the proximity printing lithography module.
2. Improved MULT.EXPOSE capability. ATHENA now takes into account different values of Dill's C-parameter for each wavelength in case of broadband illumination.

2: Version 5.14.0.R

2.1: SSUPREM4 Features

- Introduced new parameters to control the trajectory visualization capability in Monte Carlo implant: TRAJ.FILE. Specifies the name of the file in which ion trajectories calculated with the Monte Carlo (BCA) method are to be saved and N.TRAJ, which specifies the number of ion trajectories to be saved in the TRAJ.FILE.
- Improved statistics and consequently the effective accuracy of Monte Carlo (BCA) ion implantation simulation in 2D structures. This is achieved by more accurate estimation of number of trajectories near the side edges of the simulation structure.
- Improved stopping power model for 11-20 channel in SiC. This is a rare event channel for standard wavers (0001). But it has some influence in case of angled implants into trenches parallel to the 11-20 plane.
- Added capability to control triangle orientation of initial ATHENA grid. New parameters TRI.LEFT and TRI.RIGHT are added to the LINE statement.
- Added C.VACANCY and C.INTERST to the INITIALIZE statement.
- Added new standard impurity HELIUM. The only practical application available in the moment is Monte Carlo ion implantation of Helium.
- Added capability to oxidize materials other than Si and Poly. New parameter OXIDIZABLE is added to the MATERIAL statement. If OXIDIZABLE is set to TRUE, then all oxidation related parameters for the specified material will be set equal to those for Silicon. You can specify the different values for oxidation parameters in the OXIDE MATERIAL ... statement.
- Improved gridding in oxide that results in smaller number of extremely small triangles are generated in areas of slow oxidation. For example, under the polysilicon gate during reoxidation process.

2.2: ELITE Features

- Added new parameter OUTF.TABLE=<filename> in the RATE.ETCH statement. This can be used for detailed analysis of plasma ions and neutrals distributions. The old parameter OUTFILE in the RATE.ETCH statement has changed to OUTF.ANGLE because it specifies a file with ions vs. angle distribution output.

2.3: OPTOLITH Features

- Reimplemented Proximity Printing Model in OPTOLITH, which simulates imaging without any reduction lens. To use this model, specify the GAP parameter in the IMAGE statement. The model is implemented for Manhattan, Circular, Ring and Multi-Ring masks.
- Added capability to load mask information directly from MASKVIEWS layout file for image calculations in OPTOLITH. This capability has several advantages when comparing with old interface through a special “section” file. The “section” file approximates an arbitrary shaped mask features with only rectangulars. The new interface doesn't do any approximations and internally divides mask polygons into triangles and rectangulars for exact image calculations.
- Considerable speeded up and improved accuracy of image calculations for big area mask layouts when complex geometry light sources are used.
- Added additional standard wavelengths to the ILLUMINATION statement: KRF.LASER (alias is DUV.LINE), ARF.LASER and F2.LASER.
- Added capability to save intensity and mask information separately into the structure file after OPTOLITH image calculations. Now, the MASK parameter in the STRUCTURE statement will save only mask layout information. The INTENSITY parameter now saves only intensity distribution. When you specify both parameters, both mask layout and intensity will be saved.

3: Version 5.10.0.R

3.1: Implantation features

- BCA module has now two different engines for ion trajectory calculations. One of these engines is 2 to 4 times faster than another. In some cases, the faster engine might be slightly less accurate. The new parameter `FAST` for `IMPLANT BCA` statement is introduced. This parameter allows you to specify, which engine to be used during current Monte Carlo simulation. If `FAST=true` (default), the fast engine is used. If `FAST=false`, the slower (potentially more accurate) engine is used.
- Wafer miscut feature is implemented for BCA implant in crystalline materials. Two new parameters are introduced:
- `MISCUT.TH` - Target wafer polar angle miscut measured in the XY plane, Y being the inward direction.
- `MISCUT.PH` - Target wafer azimuth angle miscut measured in the XZ surface plane, Z pointing away from the observer.
- The default version of parameter `DIVERGENCE` (the alias is `BEAMWIDTH`) in the `IMPLANT` statement has changed from 0 to 1°. 0° ion beam divergence is very difficult to achieve. A typical ion beam divergence of industrial implanters is 1 to 1.5°.
- `DAM.FACTOR=0.0` can now be specified in the `IMPLANT` statement. This is used with Advanced Diffusion Module (`DifSim`).
- New parameter `IV.SCALE` is introduced in the `IMPLANT` statement to control estimation of after implant interstitial and vacancy distributions from BCA damage calculations using parameter `DAMAGE`.

3.2: Diffusion/Oxidation Features

- Improved convergency and speed of Advanced Diffusion Models (DifSim) in 2D
- If you specify `METHOD PLS` before the Monte Carlo `IMPLANT` statement, the initial distribution of impurity-defect pairs will now calculate the same way as for analytical implants.
- Improve specification of `POLY.DIFF` model. The model flag used to be set to false unless the statement `METHOD POLY.DIFF` was immediately before `DEPOSIT POLY GR.SIZE=<n>` statement.
- Default value for the `MIN.TEMP` in the `METHOD` statement is returned to original 700°C. The manual had always stated that it is 700°C, though few previous versions get reduced value of 475C. It is more appropriate to set 700°C temperature limit since for most models the default diffusion parameters are not well known at lower temperatures.
- Numerical rounding bug is fixed in geometrical calculation for very flat triangles during oxidation.
- Improved triangulation during oxidation which reduced probability of creating extremely small triangles.

3.3: Etching and Deposition Features

- Improved algorithm of SSUPREM4 deposition. Now, it guarantees that non-uniform spacing specified by DY and YDY parameters is preserved even when number of divisions is changed due to complex grid.
- The SSUPREM4 deposition is improved for the case when number of DIVISIONS is not specified. For thin layers with thickness less than 0.012 microns, an uniform grid with spacing of approximately 0.001 microns will be generated. A non uniform grid with spacing equal to 0.001 microns at the top and bottom of the deposited layer will be generated for thicker layers. The number of divisions is automatically selected dependent on the layer thickness. It is 12 for the layers thinner than 0.02 microns and 18 for layers thicker than 2 microns.
- You can now specify etch rate retardation in the RATE.DOPE statement.
- Fixed a bug for the ETCH START/CONTINUE/DONE sequence when etched window width is zero while using MASKVIEWS.
- Fixed the bug for the case of deposion of ternary materials with variable composition fraction. For example:

```
deposit material=InGaAs thick=0.50 div=20 c.fract=0.1 f.fract=0.5
```

- Fixed a bug in analytical ETCH with the ANGLE parameter. In some cases when the THICKNESS parameter exceeded the total thickness of the structure, a part of the etched layer was not removed.

3.4: Lithography Features

- Added the boolean parameter CENTER to the IMAGE statement. If specified, the layout loaded with .sec file generated in MASKVIEWS will be shifted so its center is in the point (0,0) - the origin of coordinates for computational window. This parameter should be specified when .sec file is generated from the GDS2 file where absolute coordinates of mask features could be arbitrary.
- Removed obsolete parameter NA in the EXPOSE statement. Nonvertical light propagation was not implemented for non-planar structures.

3.5: TMA Compatibility Features

- The following critical changes in ATHENA syntax and functionalities are implemented in order to achieve better compatibility with TSUPREM4 and TSUPREM3
- Added capability to specify that default values of some parameters correspond to those of TSUPREM4. The modified keyfile athenakey.tma with some modified default values is introduced. To run ATHENA with default parameters specified in athenakey.tma file the syntax is:

```
go athena simflags="-tma"
```

  For example, TSUPREM4 defaults for TILT and ROTATION parameters in the IMPLANT statement are 0°, while ATHENA uses 7 and 30° respectively.

- A plus character '+' can be used as a line continuation sign instead of standard backslash '\'.
- Boolean parameters can be set to false by preceding the parameter name with '^' or '!' character.
- The '$' character can be used to specify the comment line. This should only be used at the beginning of the line, because the '$' character can be used for substitution of parameters defined by SET or DEFINE statements of DECKBUILD.
- The maximum length of parameter names has extended from 12 to 16 characters. (some TSUPREM3 names are longer than 12 characters).
- The first character of a parameter name can be a numeral now.
- TSUPREM compatible DEFINE statement and Substitution capability

- IF/ELSEIF/ELSE/IF.END Capability
- LOOP/L.END/ASSIGN/L.MODIFY Capability
- MESH statement and its DX.MAX, DX.MIN, DX.RATIO, DY.ACTIV, DY.BOT, DY.RATIO, DY.SURF, LY.ACTIV, LY.BOT, GRID.FAc, and FAST parameters.
- Automatic grid generation in horizontal direction using MASK statement with IN.FILE and XLINES parameters.
- Capability to use mask information with EXPOSE MASK=<maskname> statement.
- Various aliases for statements with the same functionalities.
- Various aliases for parameters providing the same functionalies in the INITIALIZE, DEPOSIT, IMPLANT, DIFFUSE, ETCH, STRUCTURE, ELECTRODE, METHOD, and MATERIAL statements.
- If you set the E.FIELD parameter to FALSE in the MATERIAL statement, the electrical term will be ignored during diffusion simulation in the specified material.

3.6: Miscellaneous Features

- Supports OMNI Licensing
- Added new standard impurity HYDROGEN. The only practical application available in the moment is Monte Carlo ion implantation of hydrogen.
- Improved triangulation during oxidation which reduced probability of creating extremely small triangles.
- The parameter TWO.DIM in the STRUCTURE statement now always forces 1D to 2D transformation of the current structure. Before it was applied, this happened only when structure was written into the outfile.
- Increased number of material regions up to 1000, which allows you to create a super lattice structures consist of hundreds of layers.

4:Version 5.8.0.R

4.1: Advanced Diffusion Models

A complete set of advanced diffusion models for B, P, and As in silicon based on a special solver module DifSim. The model set includes core diffusion model, defect cluster model, and dopant/defect clusters model. The following elements of the new module are new:

- Simultaneous solving of diffusion and reaction equations
- Proper handling of charge states of defects and pairs
- Dynamic modeling of transient phenomena
- Dynamic dopant activation
- Interstitial clustering based on Oswald Ripening theory
- Various types of defect clusters: small and <311> clusters, perfect and faulted dislocation loops
- Full chain of mixed clusters (e.g. B2I, BI2, B3I, B4I2, ASnV, etc)
- Ability to easily add new reactions and equations
- Thoroughly calibrated unified set of model parameters

Main advantages of the new module are:

- Accurate simulation of Transient Enhanced Diffusion and Activation
- Predictive simulation of RTA and Spike diffusion
- Accurate simulation of low-temperature post-implant diffusion
- Potential to use in defect engineering

4.2: Other Diffusion Simulation Features

- Boron diffusion in SiGe/SiGeC includes two new models which allow to predict suppression of boron trancient diffsuion by carbon incorporation
- C-Interpreter function is now available for Boron diffusion in SiGe/SiGeC
- It is now possible to include non-equilibrium interstitials into epitaxially grown or deposited silicon
- The `TWO.DIM` and `FULL.CPL` models now can be set for all semiconductor materials
- Handling of impurity activation has been improved: the type of activation model is now specified for each impurity/material combination
- `POLYDIFF` model is completely rewritten. It uses experimental data for grain growth rate and other parameters

4.3: Implant Simulation Features

- BCA ion implantation model for Silicon Carbides is implemented
- BCA ion implantation model for superconductor materials Ba2YCu307 and Ba2NdCu307
- The damage accumulation model in BCA simulation is improved. Now it correctly predicts amorphization thickness for B, BF2, P, and As implants in Si
- More accurately calibrated electronic stopping power for higher energies of B and P implants is implemented
- Capability to specify the substrate surface miscut for Si and SiC. This give an opportunity to simulate vertical but off-channel implants into trenchesand other structures where lateral symmetry is important.

4.4: Silicide Simulation Features

- Two or more metal/silicide pairs can be simulated simultaneously
- The volume reduction effect is now specified by two volume ratio parameters ALPHA for metal/silicon and silicide/silicon
- Cobalt and CoSix materials and model parameters for them are added
- User-defined metals and silicides are now recognized as electrodes in the ELECTRODE statement

4.5: Miscellaneous Features

- Support FLEX LM
- Standard material GERMANIUM is added
- New impurities Nitrogen and Oxygen are added to all relevant statements.
- C.FRACTION parameter (composition fraction) could be now specified (INITIALIZE, DEPOSIT statements) not just for standard ATHENA ternary material AlGaAs and InGaAs but also for user-defined materials corresponding to the following standard Silvaco ternary materials: AlInAs, InGaP, GaSbP, GaSbAs GaSbAs InAlAs, InAsP, GaAsP, HgCdTe, InGaN, and AlGaN
- It is now possible to use CLUST.TRANS model when impurities other than B, P, As, and Sb present in the structure. Also, the model can be used in Polysilicon
- It is now possible to simulate deposition or epitaxy of the layers with linearly graded impurity or point defect content. New parameters F.BORON, F.PHOSPHORUS ..F.INTERST, F.VACANCY are added to the DEPOSIT and EPITAXY statements.
- Fixed dopant enhanced etching model in ELITE
- It is now available for or etch types except MC Plasma Etch. Dopant induced etch retardation can be also specified
- Added a NEUTRAL type impurity as an alternative to DONOR/ACCEPTOR in the IMPURITY statement. For example, I.SILICON is considering as DONOR in GaAs but should be NEUTRAL in Si. As the result, Si atoms implanted in order to preamorphized silicon crystal would not affect diffusion of other impurities and will not contribute into the net concentration.
- Time units parameters Seconds, Minutes, and Hours are added to the BAKE statement

Bibliography

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