Fast Monte-Carlo Simulation of Ion Implantation

Interactive Tools

Binary Collision Approximation Implementation within ATHENA
Contents

- Simulation Challenges for Future Technologies
- Monte-Carlo Concepts and Models
  - Atomic and nuclear stopping
  - Damage accumulation
  - Defect profile calculation
  - Numerical speedup
- Application Examples
- Non-Silicon substrates calculations
- Conclusion
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Simulation Challenges for Future Technologies

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Simulation Challenges for Future (?) Technologies

- Trend: Shrinking down device size
  - Low energy implants
  - High dose concentration
  - Rapid Thermal Annealing (RTA)

- Induced phenomena:
  - Large defect generation
    - Atoms displacement (surface degradation, crystal amorphization)
    - Vacancies and interstitials generation

- Technological concern: Transient Enhanced diffusion (TED)!!
Simulation Challenges for Future (?) Technologies

- Need to accurately model defects generation in order to have their correct profiles for subsequent diffusion steps (RTA, anneals…)
  - Accurate junctions thickness
- What to do when specie not tabulated nor calibrated (ie. low energy/high dose experiments, non silicon substrates) ?
- Implants into multi-layered or non planar structures ?
  - Different materials to go through with different stopping effects
  - Shadowing effect

- Need to use a more robust approach : Monte Carlo implant simulations (Binary Collision Approximation or BCA)
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- Nature of the physical problem

- Beam of accelerated ions entering the material (either crystalline or amorphous)

- Ions slowed down and scattered due to nuclear collision and electronic interaction

- Fast recoil atoms induce collision cascades

- Implanted ion profile calculation

- Defects generation (vacancies & interstitials)

- Crystal amorphization

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Fast Monte-Carlo Simulation of Ion Implantation
Monte-Carlo Concepts and Models

- **Implanted profile calculation**
  - Nuclear Stopping Mechanisms
    - Nuclear Stopping
    - Inter-atomic Potential
  - Electronic Stopping Mechanisms
    - Local inelastic energy losses (Firsov’s semi-classical model)
    - Non-local electronic energy losses (Lindhard & Scharff)

- **Damage accumulation model**
  - Amorphization driven by deposited energy per unit volume

- **Defect accumulation model**
  - Vacancies and interstitials profiles (Kinchin-Pease model)
Monte-Carlo Concepts and Models

Effect of the implanted dose on the amorphization profile.
Effect of the implanted dose on the defects profiles.
Monte-Carlo Concepts and Models

- **Statistic Sampling**
  - An atom impacting the wafer’s surface is more likely to be stopped close to the interface than to channel deeper into the substrate.
  - But probability to have atoms channeling exists: it implies very large number of simulated implanted atoms to fit the profile tail.
  - prohibitive from the simulation point of view (simu. time constraint !)
  - Implementation of a statistical sampling to achieve increased occurrence of these rare events by generating several independent sub-trajectories from less-rare events [1-2]

Monte-Carlo Concepts and Models

Effect of the “sampling” parameter on the simulated profile.
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Advanced Ion Implantation Simulation Solutions (1/2)

- MC Implant gives highly accurate ion distribution profiles in crystalline and multi-layered materials.
- MC Implant predicts ion penetration depths for a wide range of initial energies starting from as low as 200 eV and spanning to the MeV range.
- MC Implant provides a time efficient and cost effective solution of problems encountered in processes using aggressive variance reduction statistical techniques.
Advanced Ion Implantation Simulation Solutions (2/2)

- Comprehensive capabilities of MC Implant enable:
  - accurate simulation of critical process issues such as shallow junction implants
  - multiple implants and pre-amorphization
  - HALO implants and retrograde well formation

- Advanced damage accumulation algorithms allow investigation of novel defect driven diffusion models of implanted species

- Internal object-oriented engine and generic 3D solution of related physics allow MC Implant to account for:
  - complex effects such as reflection and re-implantation
  - deep trenches and voids
  - arbitrary implant direction and wafer rotation
Application Examples

Effect of the oxide thickness on angle randomization
Application Examples

Single point implant illustrating the 3D simulation of all channeling directions.

Manifestation of 3D channeling effects under the gate which is enhanced by the presence of a very thin oxide.

Effect of channeling on lateral distributions.
Application Examples

Angled implantation into a deep trench

Note implanted dose in shadow region resulting from ion reflected from the directly implanted trench wall.
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Non-Silicon Substrates Calculations

- Implantation in any crystal structure for all supported materials in ATHENA
  - **diamond** (Si, Ge, SiGe)
  - **moissanite** (4H-SiC, 6H-SiC)
  - **Zincblende** (GaAs, InP, 3C-SiC)
- **Anysotropic** electronic stopping essential for the proper simulation of ion implantation in the most complex structures such as **4H- and 6H-SiC**
- **Temperature** and **crystal structure** dependent damage model allows “hot” implant simulation
Non-Silicon Substrates Calculations

MC Implant simulated profiles of 60 keV Aluminum in 4H-SiC showing different doses for on-axis direction [3]. The strong dependence of Aluminum distributions on the crystallographic direction of ion implantation is evident.

Non-Silicon Substrates Calculations

Aluminium implants into 6H-SiC at 30, 90, 195, 500 and 1000 keV with doses of $3 \times 10^{13}$, $7.9 \times 10^{13}$, $3.8 \times 10^{14}$, $3 \times 10^{13}$ ions/cm². SIMS data is taken from [4].

Al depth profiles in 6H-SiC after multiple implants: 180keV, 2.7x10^{15}cm^{-2}; 100keV, 1.4x10^{15}cm^{-2}; 50keV, 0.9x10^{15}cm^{-2}. Experimental data are taken from [5].

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Conclusion: MC Implant Features and Models (1/2)

- 3D Binary Collision Approximation Monte-Carlo simulation technology **fully integrated** with the ATHENA process simulation framework
- **Physically based electronic stopping** additionally optimized for most widely used ion/target combinations
- **Precise damage accumulation model**, allows accurate simulation of dose-dependent channeling of implants or pre-amorphization effects
**Conclusion: MC Implant Features and Models (2/2)**

- **Experimentally** verified down to 0.2 keV doping profiles
- Calculation of **de-channeling** effects caused by:
  1. damage buildup and previous implant damage
  2. surface oxides polysilicon and other materials
  3. beamwidth variations
  4. implant **angle** and **energy**
  5. amorphous material in the structure
- 3-D Channeling effects included in the generic solution of ion propagation and stopping