Fast Monte-Carlo Simulation of Ion Implantation

Binary Collision Approximation
Implementation within ATHENA

MULTI CORE TOKEN WORLD LICENSE

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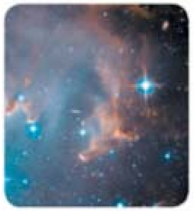

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- Simulation Challenges for Future Technologies
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    - Atomic and nuclear stopping
    - Damage accumulation
    - Defect profile calculation
    - Numerical speedup
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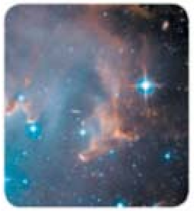
- Non-Silicon substrates calculations
- Conclusion



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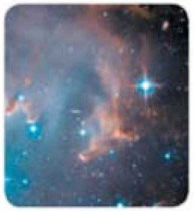
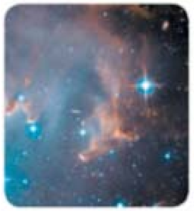


Simulation Challenges for Future (?) Technologies

- 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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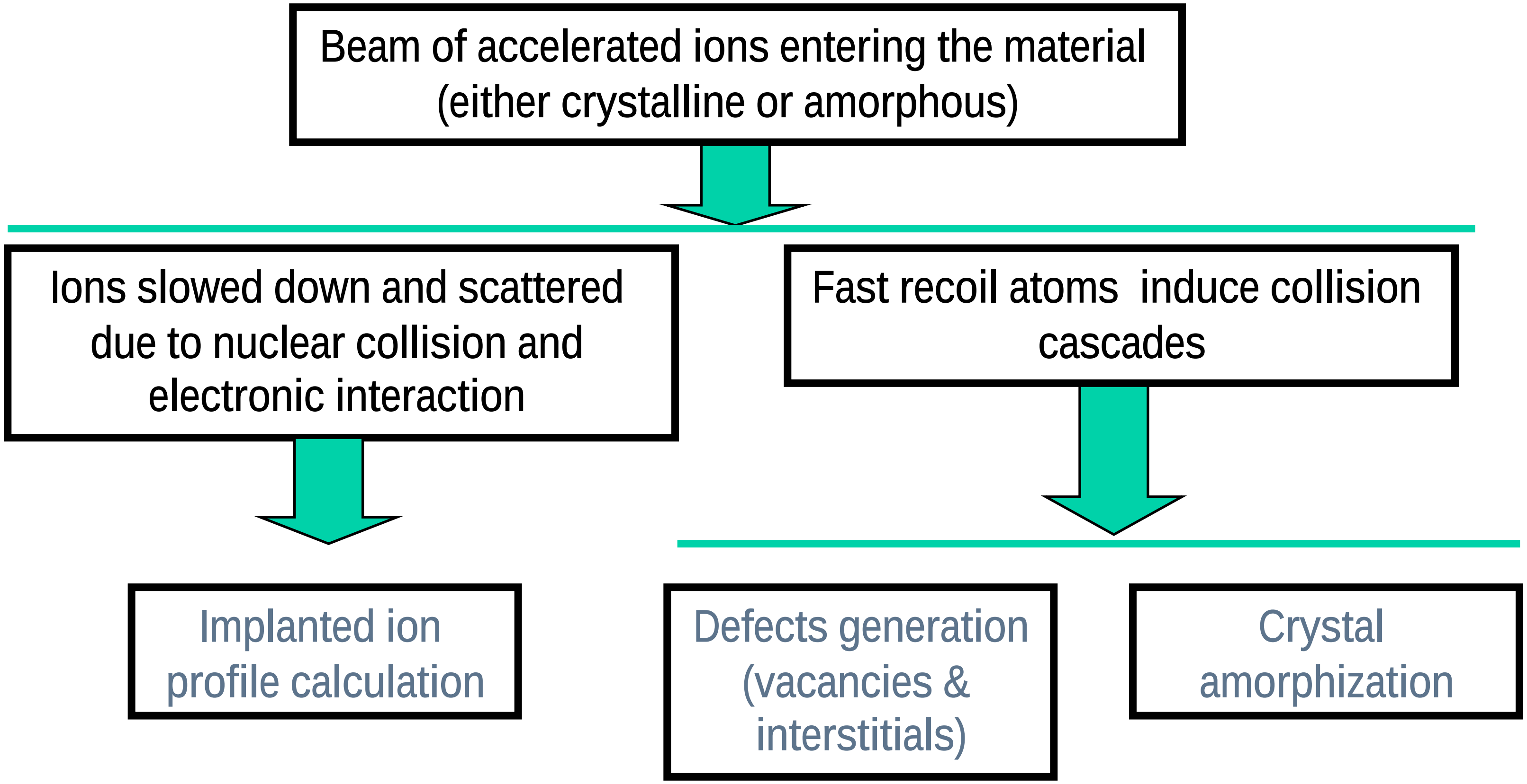
Monte-Carlo Concepts and Models

- Nature of the physical problem



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

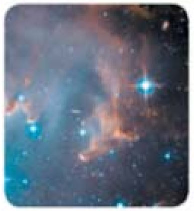
Ions slowed down and scattered due to nuclear collision and electronic interaction

Fast recoil atoms induce collision cascades

Implanted ion profile calculation

Defects generation (vacancies & interstitials)

Crystal amorphization

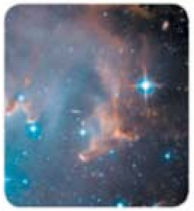


Monte-Carlo Concepts and Models

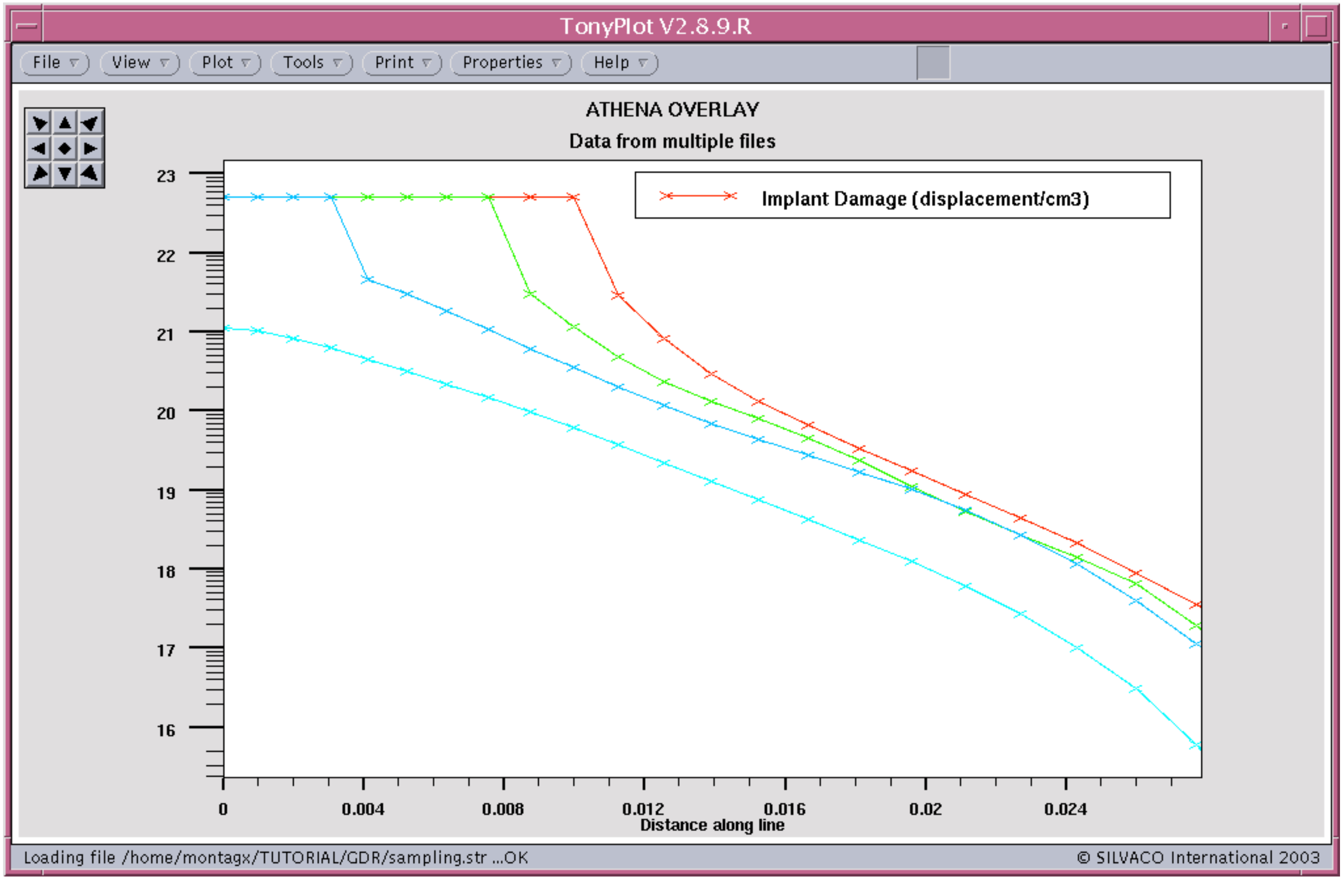
- **Implanted profile calculation**
  - Nuclear Stopping Mechanisms
    - Nuclear Stopping
    - Inter-atomic Potential
  - Electronic Stopping Mechanisms
    - Local inelastic energy losses (Firsov’s semi-classical model)
    - Non-local electronic energy losses (Lindhard & Scharff)

- **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



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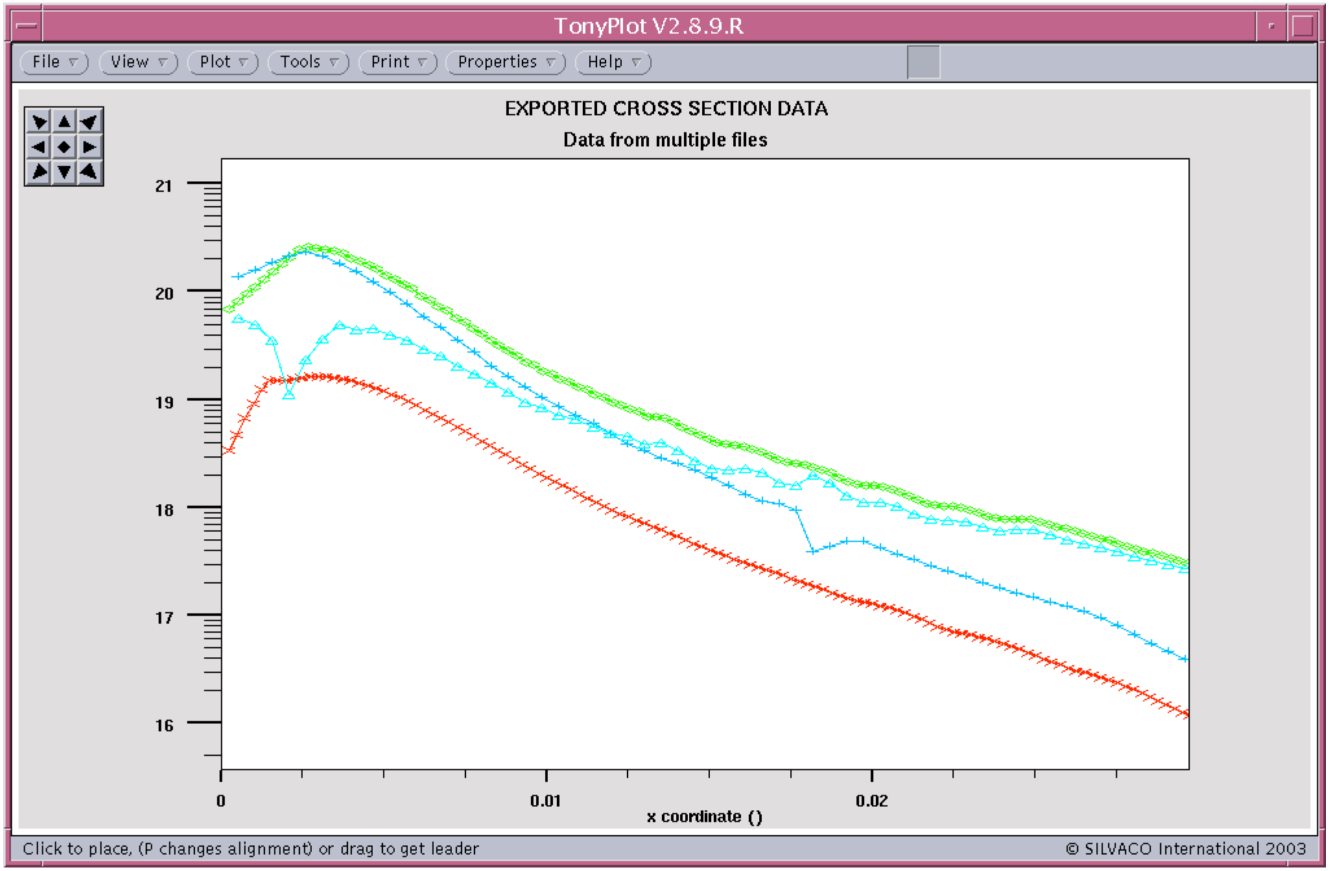
Effect of the implanted dose on the amorphization profile.

Monte-Carlo Concepts and Models



Effect of the implanted dose on the defects profiles.

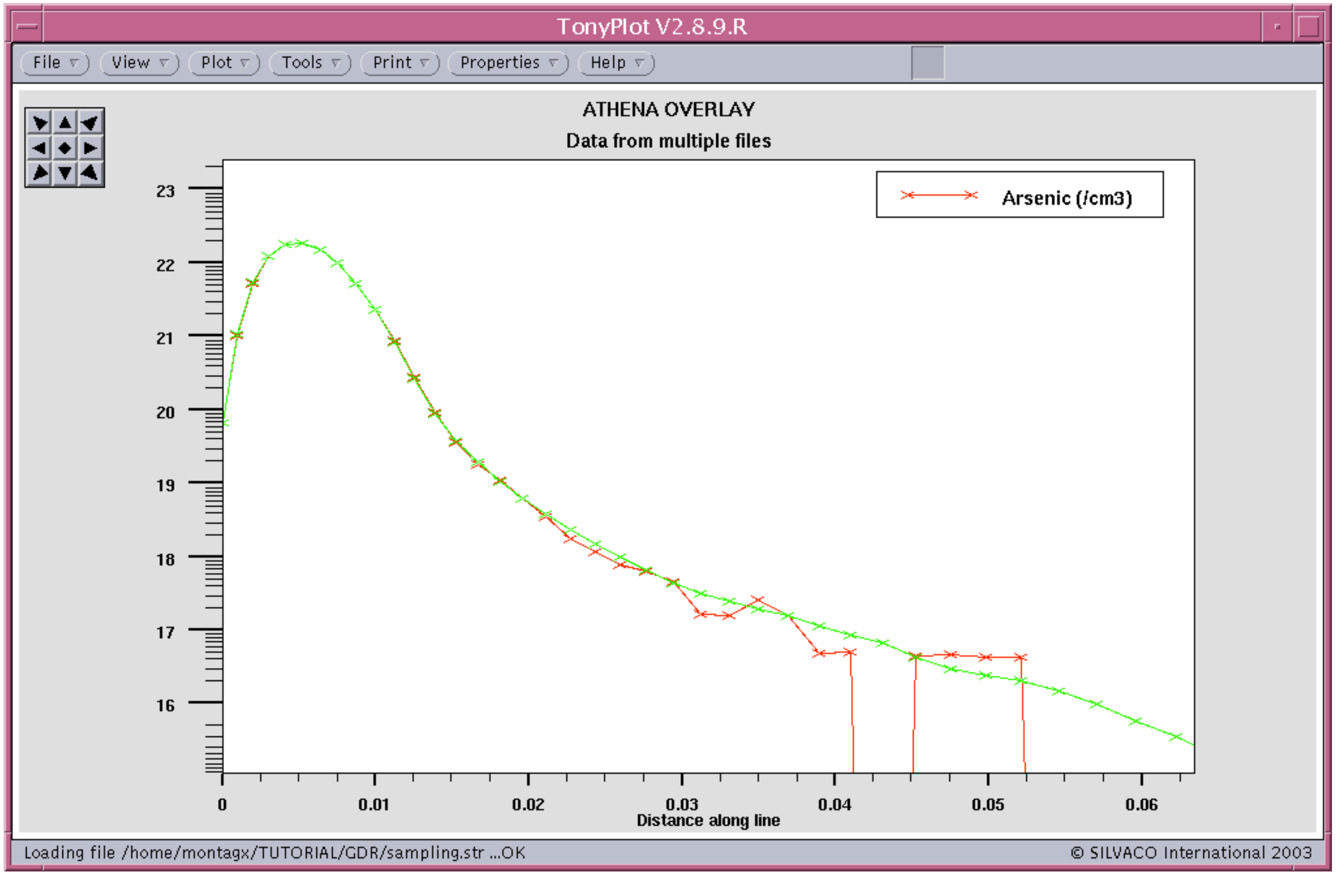
Monte-Carlo Concepts and Models

- **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]

[1] Villién-Altamirano, M. et al., in Proc. 13th Int. Teletraffic Congress, ITC 13, p71, (1991).

[2] Villién-Altamirano, M. et al., in Proc. 14th Int. Teletraffic Congress, ITC 14, p797, (1994).

Monte-Carlo Concepts and Models



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Effect of the "sampling" parameter on the simulated profile.

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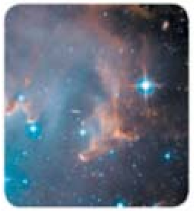

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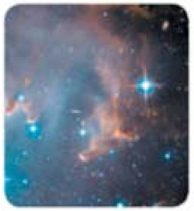
Application Examples

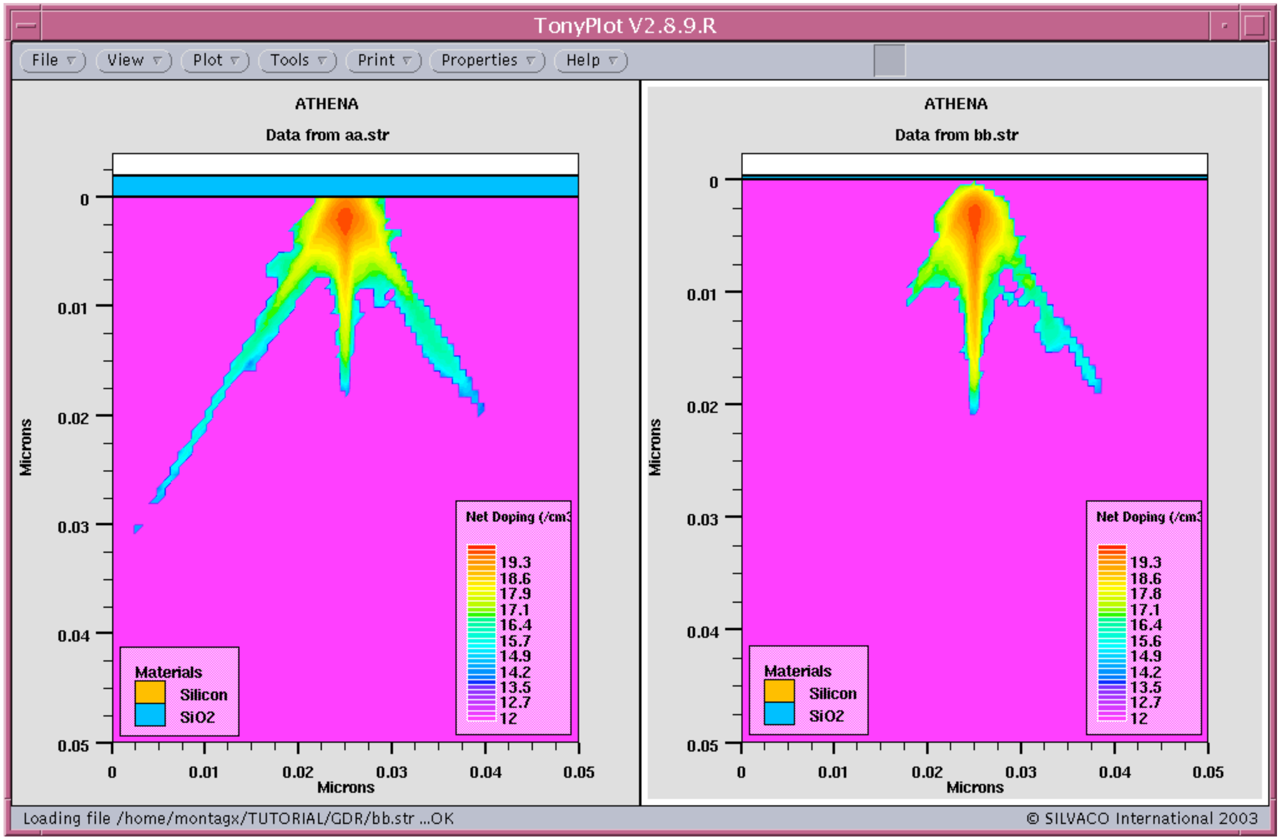
- **Advanced Ion Implantation Simulation Solutions (1/2)**
  - MC Implant gives highly accurate ion distribution profiles in **crystalline** and **multi-layered** materials
  - MC Implant predicts ion penetration depths for a wide range of initial energies starting from as low as **200 eV** and spanning 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



Application Examples

- **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



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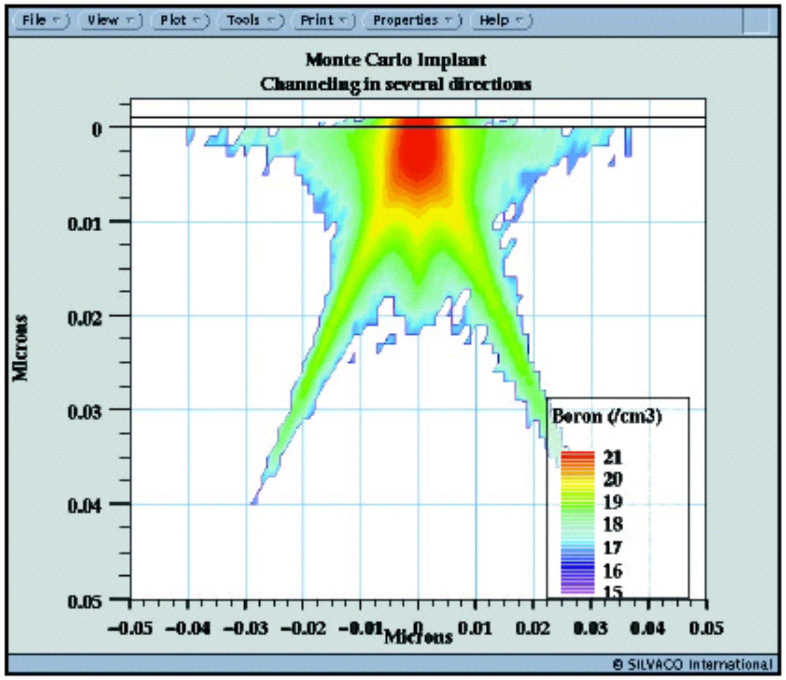
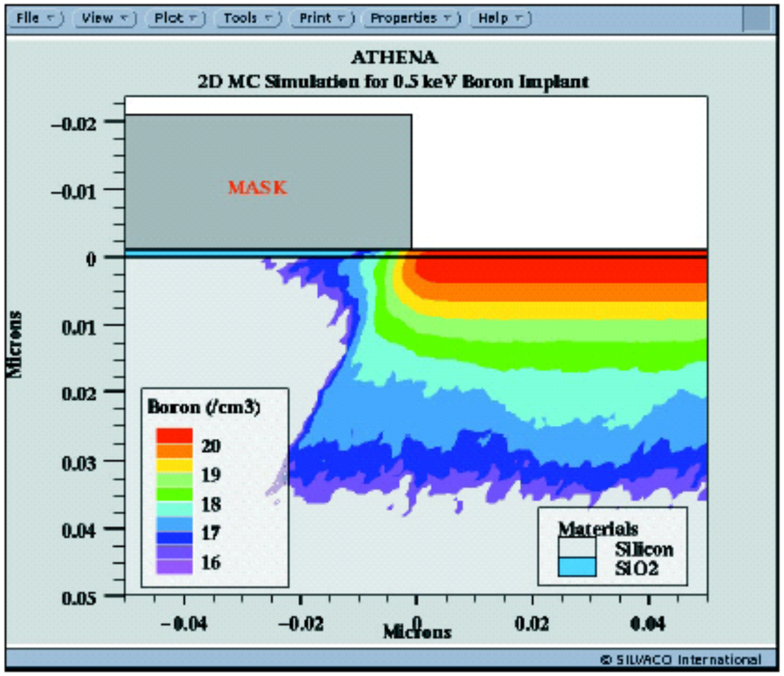
Effect of the oxide thickness on angle randomization

Application Examples



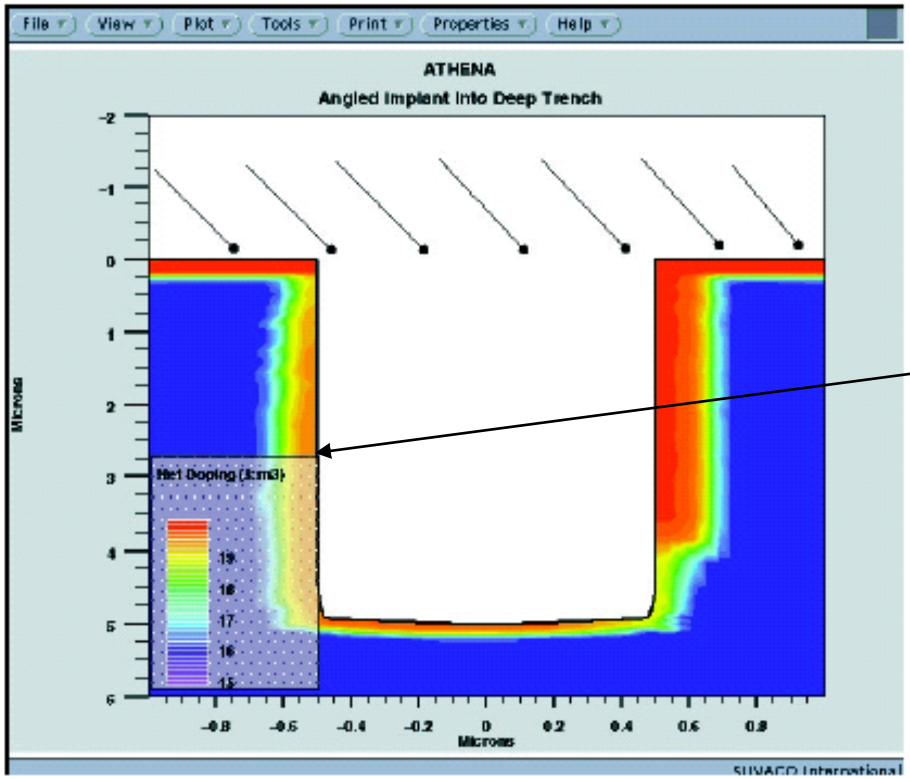
Single point implant illustrating the 3D simulation of all channeling directions.



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

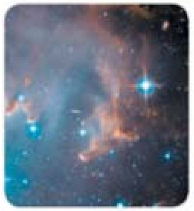
Effect of channeling on lateral distributions

Application Examples



Note implanted dose in shadow region resulting from ion reflected from the directly implanted trench wall.

Angled implantation into a deep trench



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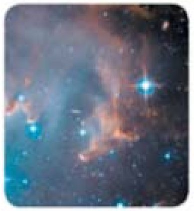
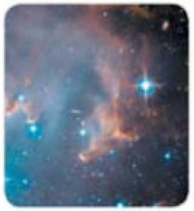


Non-Silicon Substrates Calculations

- 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



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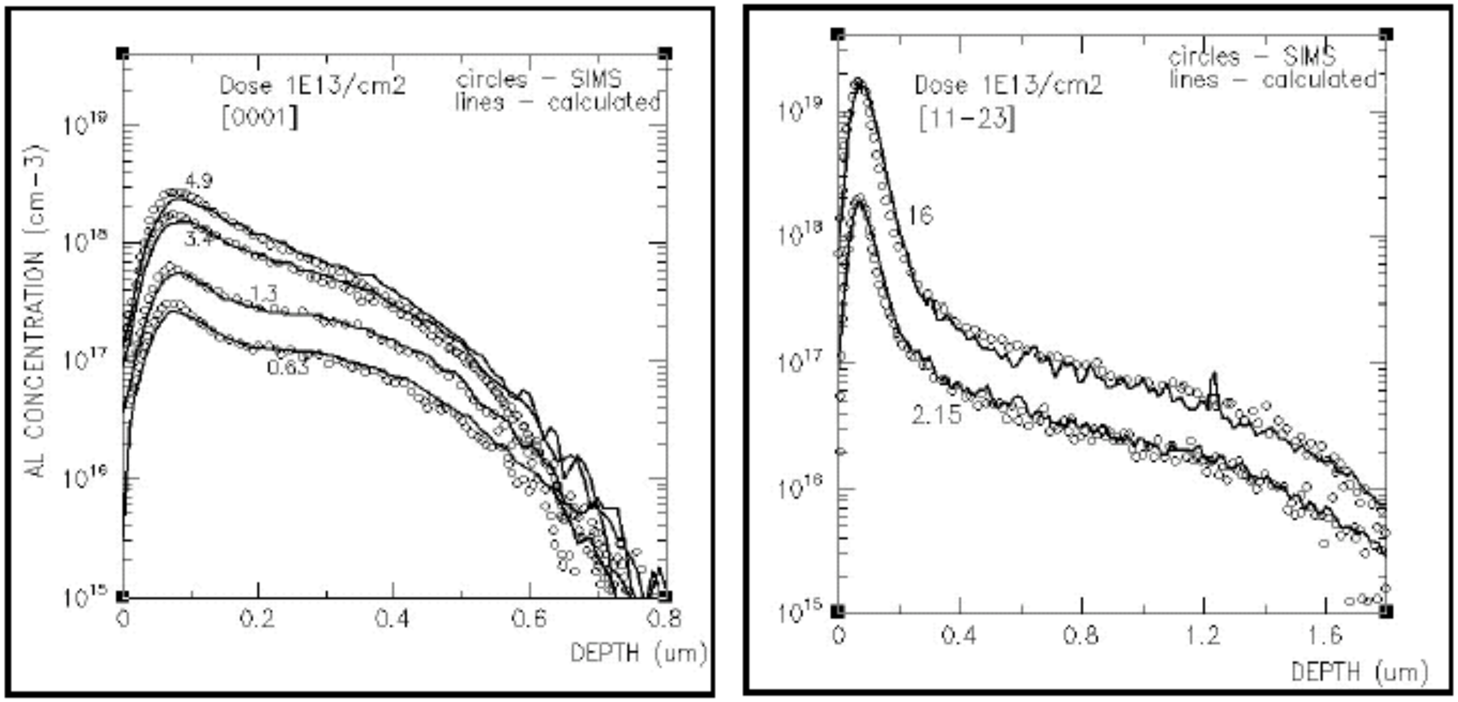
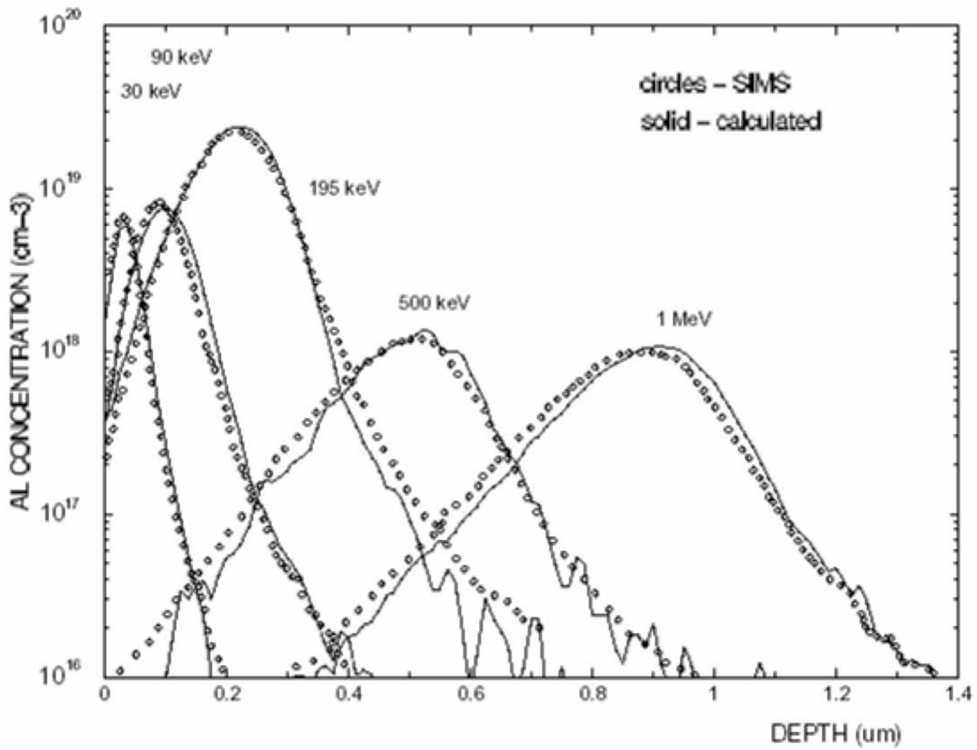


MC Implant simulated profiles of 60 keV Aluminum in 4H-SiC showing different doses for on-axis direction [3]. The strong dependence of Aluminum distributions on the crystallographic direction of ion implantation is evident.

[3] Experimental is taken from “Woug-Leung et al, Journal of Applied Physics, vol. 93, pp 8914-8916, 2003”.

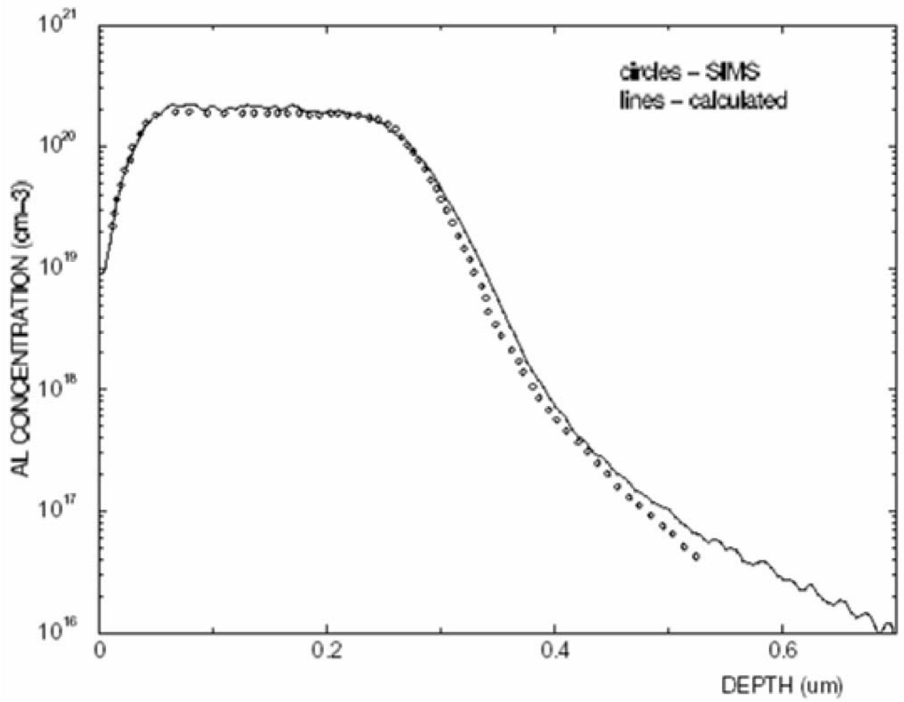
Non-Silicon Substrates Calculations



Aluminium implants into **6H-SiC** at **30**, **90**, **195**, **500** and **1000 keV** with doses of **3_10^{13}**, **7.9_10^{13}**, **3.8_10^{14}**, **3_10^{13}** ions/cm^{2}. SIMS data is taken from [4].

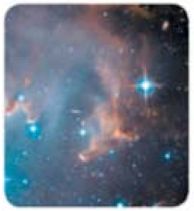
[4] J. M. Hernandez-Mangas, J. Arias, M. Bailon, and J. Barbolla, “Improved binary collision approximation ion implant simulators,” Journal of Applied Physics 91, pp. 658–667, 2002.

Non-Silicon Substrates Calculations



Al depth profiles **in 6H-SiC** after multiple implants: **180keV, 2.7×10^{15}cm^{-2}**; **100keV**, **1.4×10^{15}cm^{-2}**; **50keV**, **0.9×10^{15}cm^{-2}**. Experimental data are taken from [5].

[5] T. Kimoto, A. Itoh, H. Matsunami, T. Nakata, and M. Watanabe, “Aluminum and boron ion implantations into 6H-SiC epilayers,” Journal of Electronic Materials 25, pp. 879–884, 1996.



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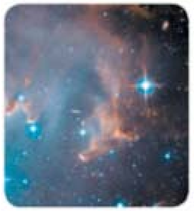
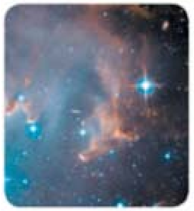


Conclusion: MC Implant Features and Models (1/2)

- 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