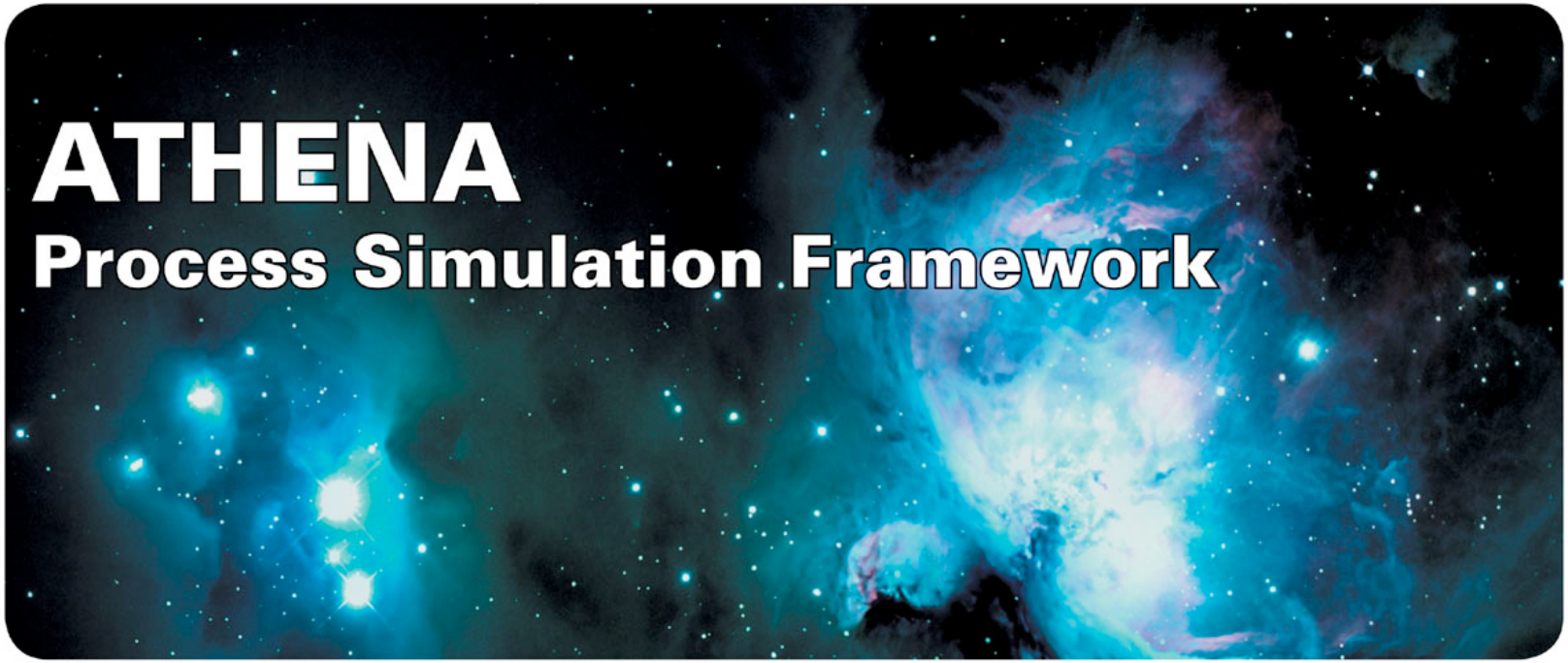
PLS Advanced Diffusion Model



New Advanced Diffusion Model for Dopants in Silicon

MULTI CORE TOKEN WORLD LICENSE

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Advanced Dopant Diffusion Model

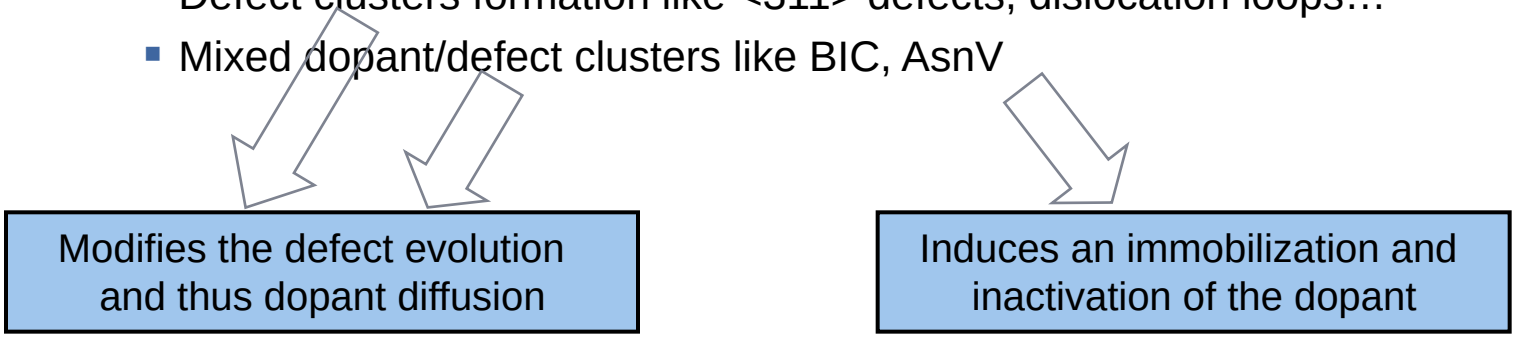
- Introduction
- Why a new dopant diffusion model?
- PLS model
  - Core diffusion model
  - Interstitial clusters model
  - Mixed Dopant/Defect Clusters model
- Results in 1D
- Results in 2D
- Conclusion and ongoing works

Introduction

- PLS model was developed in close collaboration with CNRS-Phase, CEA-Leti and Silvaco France
- The idea was to have:
  - A unique model for simulation of dopant diffusion and activation for advanced technologies
  - A physical model
  - One set of model parameters
  - Accurate simulation of TED
  - Easy to use, modular and flexible model

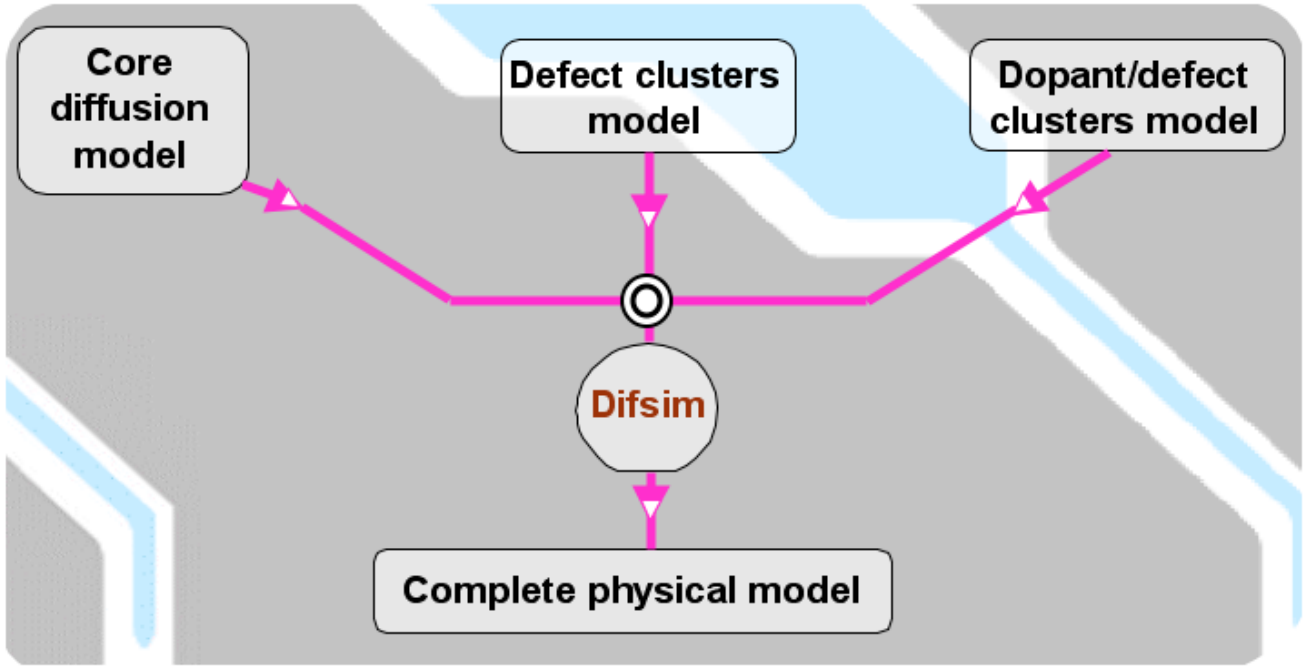
Why a New Diffusion Model ?

- A high concentration of point defect created by the implantation step induces a fast acceleration of the diffusion (TED)
  - What older model can simulate:
    - Defect/dopant coupling diffusion
    - Frenckel pair annihilation
    - Recombination at the surface or in the bulk
- What older model cannot simulate:
    - Defect clusters formation like <311> defects, dislocation loops…
    - Mixed dopant/defect clusters like BIC, AsnV



PLS Model

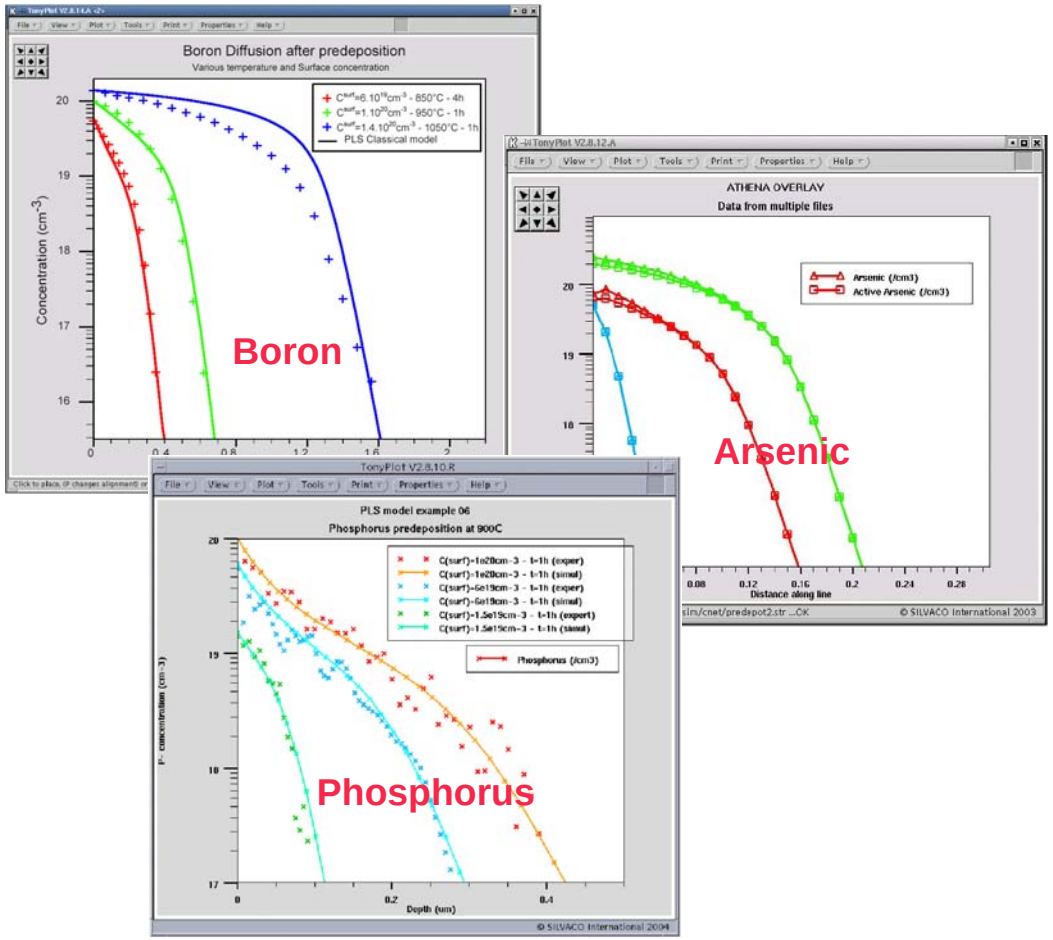
- One phenomena: one model
- PLS model = Three coupled models



Core Diffusion Model

- Key Features:
  - Physical Model based on Fick law and various reactions occurring during annealing
  - Dopant migrates with the help of point defects
  - Charge states for point defects and pairs dopant/defects are taken into account
  - Recombination and exodiffusion at the surface
  - Dynamic model for transient phenomena (ICs, BiC, AsnV ..)
  - Dynamic simulation of dopant activation (solid solubility)

Core Diffusion Model Results

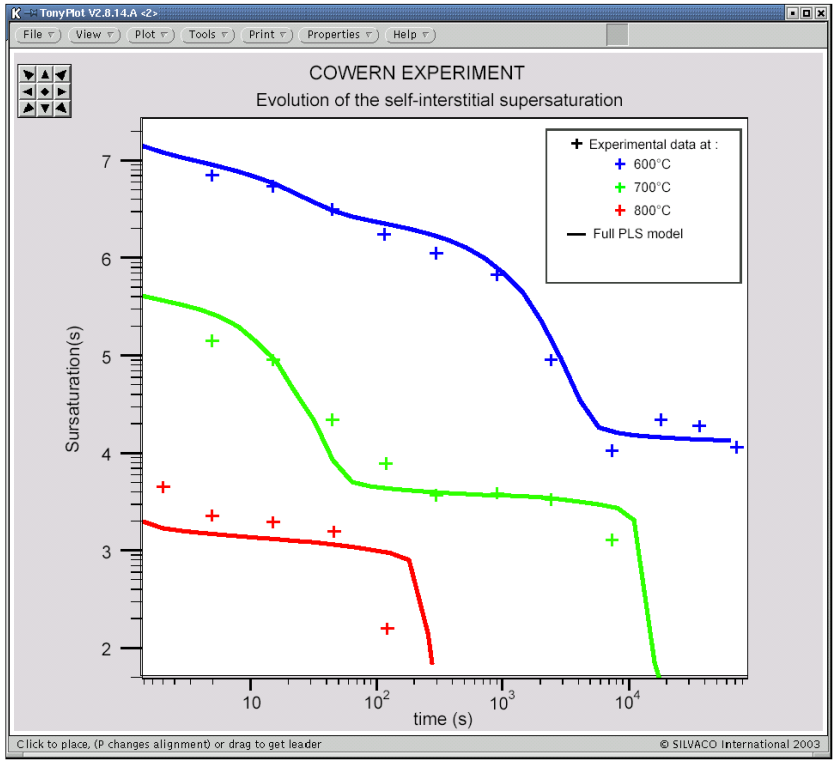


- **PLS model** simulation of a pre-deposition which represents a meaningful test for advanced diffusion models
- **PLS model** is able to reproduce the characteristic profiles of each dopants

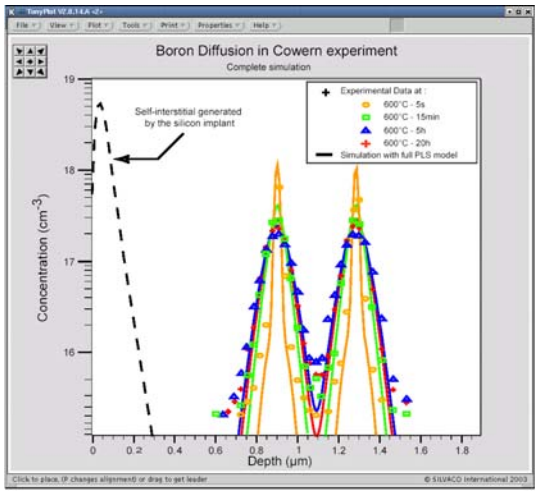
Interstitial Cluster Model

- Key Features:
  - Physical Model based on recent works done in the literature on Ostwald Ripening theory
  - Various type of extended defects are taken into account:
    - Small clusters
    - <311> defects
    - Perfect and faulted dislocation loops
  - Ability to predict accurately the diffusion acceleration

Interstitial Clusters Model Results



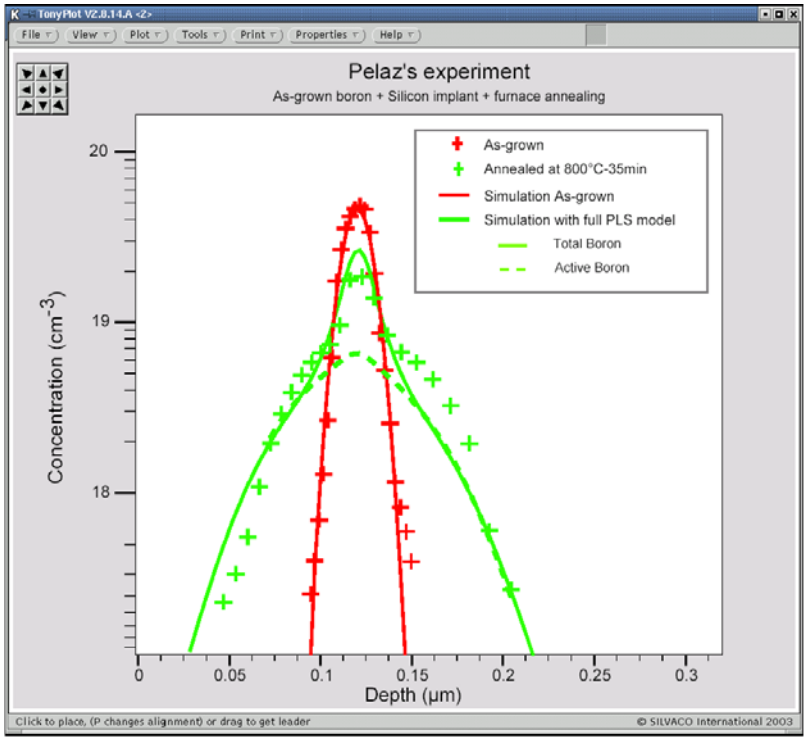
- **PLS model** simulation of Cowern experiment allows to predict accurately the evolution of silicon self-interstitial. This evolution controls the acceleration of the dopant diffusion (TED).



Mixed Dopant/Defect Clusters Model

- Key Features:
  - Physical Model based on recent ab-initio calculations
  - For Boron, various type of BICs are possible:
    - B2I and BI2 are precursors
    - B3I and B4I2 are estimated to be more stable
  - Arsenic Vacancy clusters AsnV
  - Ability to easily add some new reactions in order to improve simulations

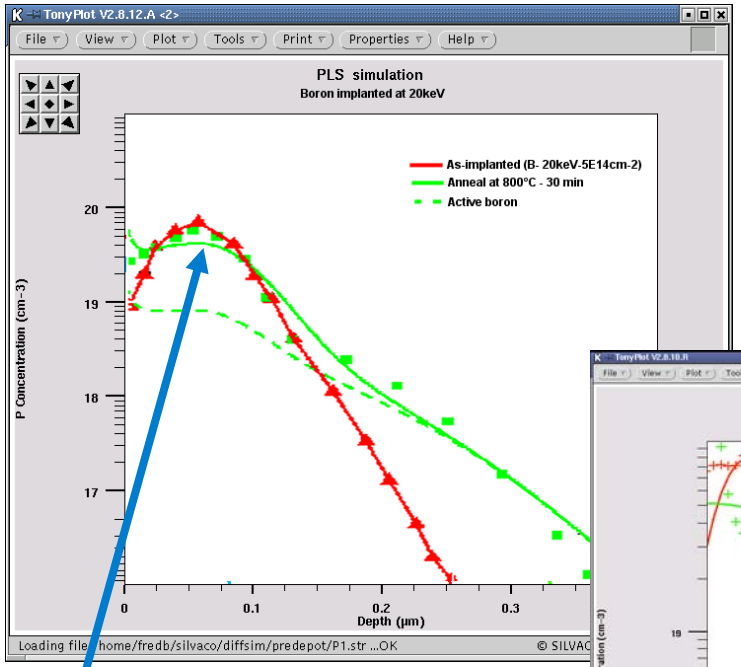
Mixed Dopant/Defect Clusters Model



- PLS model simulation of Pelaz experiment allows to predict accurately the immobilization and the inactivation of boron. This is mainly due to the formation of mixed dopant/defect clusters (BIC)

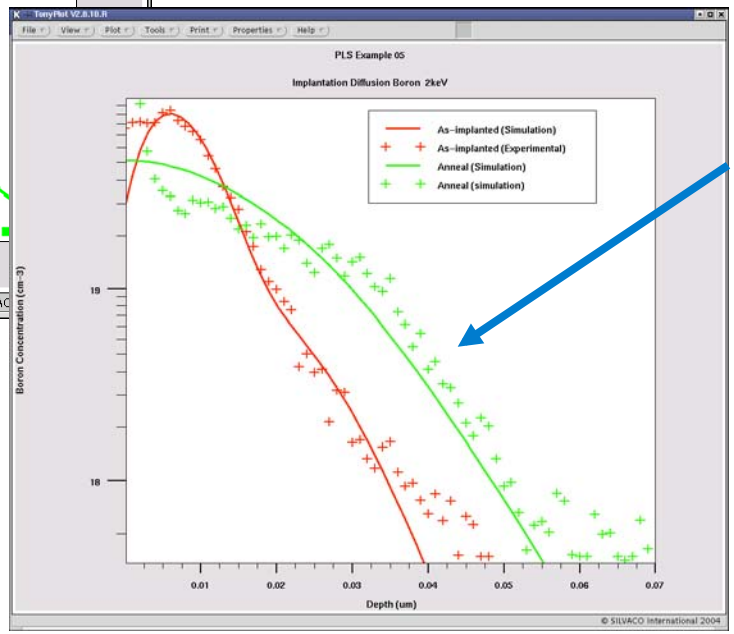
  experimental setup: 800°C/30 min

Full PLS Model Simulations on Implantation/ Diffusion



- PLS model simulation of boron diffusion after implantation at medium (20keV) and low (2keV) energy implantation

Prediction of the inactivation of dopant at the concentration pic



Simulation of rapid thermal anneal

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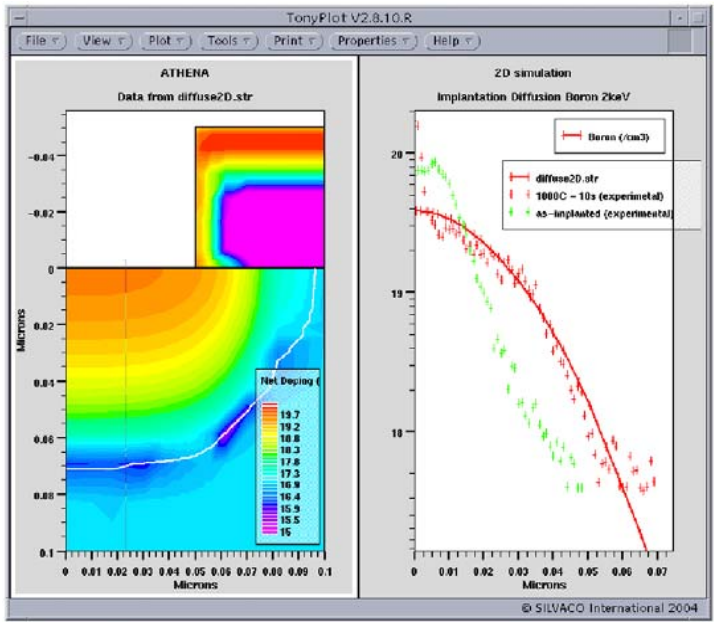
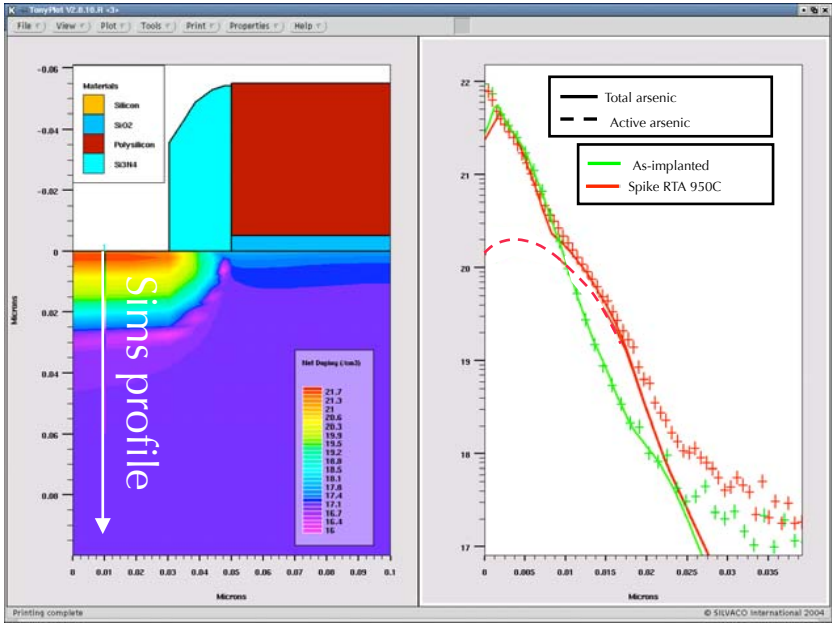
PLS Model in 2D

Arsenic



Boron implanted at 2 keV – $10^{14}cm^{-2}$ and annealed at 950°C – 10s

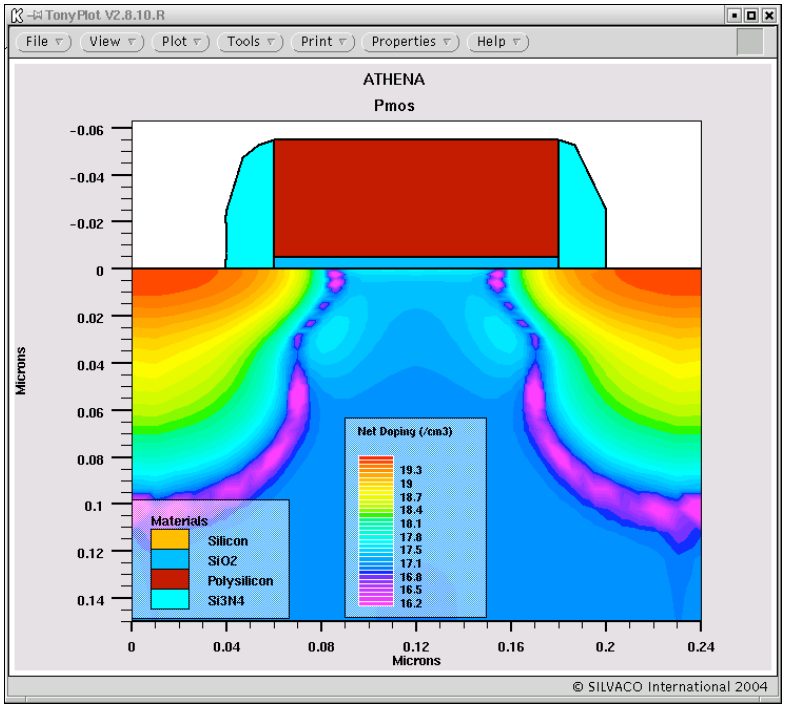
Boron



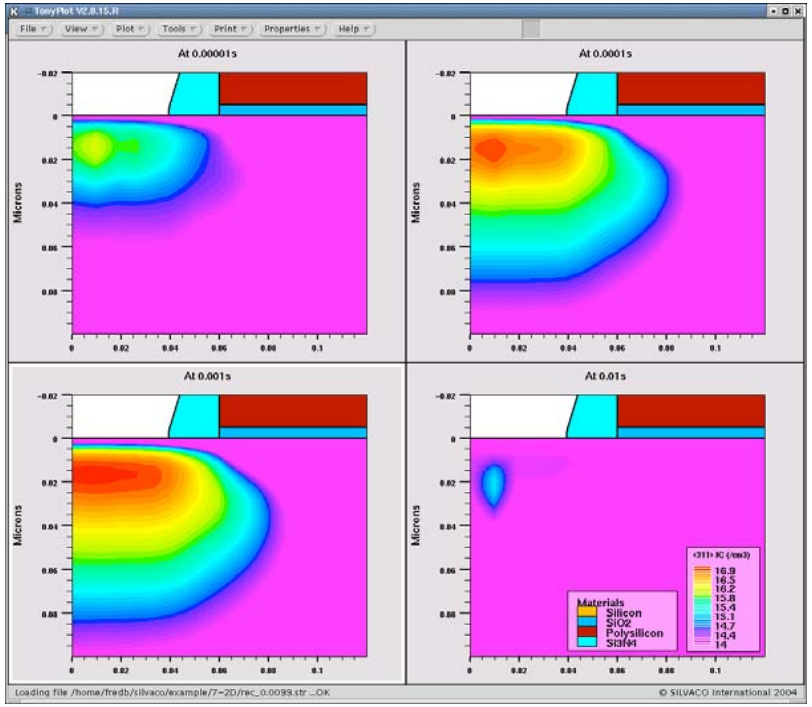
Arsenic implanted at 2 keV – $10^{14}cm^{-2}$ and spike-annealed at 950°C with a ramp up estimated at 100°C/s.

PLS Model in 2D

Boron + Arsenic halo



<311> defects



Conclusion and Future Development

- Conclusion:
  - Fully integrated in SILVACO tools
  - Full physical model with ability to perform advanced simulations
  - Possibility to easily add more equations to take into account more phenomena
- Ongoing development:
  - Fully coupled with BCA implantation simulation with interstitial and vacancy profiles as initial conditions
  - Taking into account other impurities such as Carbon or Fluorine
  - Simulation of defect engineering: formation of Vacancy Clusters