

Modeling of Implantation Using Analytical Models



SILVACO



Agenda

- Ion Implantation in Modern Semiconductor Technologies
- Hierarchy of Ion Implantation Models
- Moments (analytic) method
- U. of Texas model implementation in ATHENA
- Multilayer models
- Hierarchy of 2D implant models in ATHENA
- Use of the Moment statement



Ion Implantation in Modern Semiconductor Technologies

- Two trends in the modern semiconductor technologies greatly affect ion implantation processing
 - scaling down of device design
 - decrease of thermal budget and number of masking steps
- The first trend demands shallow junction formation and precise control of vertical and lateral profiles
- The second leads to wider use of high energy (MeV) implants (buried layers, triple well etc.)



Ion Implantation in Modern Semiconductor Technologies (con't)

- Wide variety of implant conditions
 - energies from 1 keV - few MeV
 - high angles (e.g. halo implants, LDD formation without spacer)
 - zero angle instead of traditional 7 degrees to avoid nonuniform doping across the wafer
 - diminishing use of "screen oxide"
 - higher requirements to "damage management" in order to reduce transient diffusion effects
- ATHENA as a generic process simulator must accurately handle all conditions



Hierarchy of Ion Implantation Models

- Ion implantation models are naturally divided into two groups:
 - models applicable to ordered (crystalline) materials
 - models applicable for disordered (non-crystalline) materials
- The only accurate approach to model ion transport in crystalline materials is to follow trajectories of many ions
- Molecular Dynamics method solves the classical mechanics equation of ion motion through crystal which is represented as a cluster of a few hundred or thousand atoms
 - extremely slow
 - used mainly in research (defect formation, etc.)



Hierarchy of Ion Implantation Models (con't)

- Another method is Binary Collision Approximation (BCA) in which collision with only one nearest target atom is considered
 - There are several non-commercial BCA programs (e.g. MARLOWE)
 - They were successfully used to predict channeling effects in ion implantation*
 - All commercial implementations were either not accurate enough to predict fine crystalline effects or prohibitively slow to be used in 2D practical applications
 - Details of BCA implementation in ATHENA are discussed in the workshop “Fast Monte Carlo Simulation of Ion Implantation”



Hierarchy of Ion Implantation Models (con't)

- Ion transport through disordered materials is accurately described by Boltzman transport equation
- There are three different methods of solving the Boltzman equation for ion implantation:
 - direct solution method
(used so far only in 1D-mode (SSuprem3))
 - Monte Carlo method
(many implementations, TRIM from IBM is the most popular)
 - method of moments
(used in all commercial process simulators)
- This workshop focuses on moments method, its extension, its implementation and use within ATHENA framework



Moments (Analytic) Method

- Moments method is widely used in statistics for construction of highly asymmetrical distribution
- Almost 100 years ago statistician Pearson found a distribution function based only on four moments
- More than 30 years ago Lindhard et.al. developed first range theory for ion implantation by transforming Boltzman transport equation into series of equations for moments of implant distribution
- More than 20 years ago Hofker et.al. suggested to use Pearson distribution function for implant profiles
- Between 10 and 20 years ago several tables of ion implant moments were calculated or compiled. Later they were used in process simulators



Moments (Analytic) Method (con't)

- In the moments (or analytic) method, the ion implant distribution $f(x)$ is constructed from its moments specified as:

$$R_p = \mu_1$$

projected (or longitudinal) range

$$\Delta R_p = \sqrt{\mu_2}$$

longitudinal standard deviation or straggling

$$Sk = \gamma = \mu_3 / \Delta R_p^3$$

longitudinal skewness (or gamma)

$$\beta = \mu_4 / \Delta R_p^4$$

longitudinal kurtosis (or beta)

Where

$$\mu_1 = \int_{-\infty}^{\infty} x f(x) dx$$

$$\mu_i = \int_{-\infty}^{\infty} (x - R_p)^i f(x) dx, \quad i=2,3,4 \dots$$



Moments (Analytic) Method (con't)

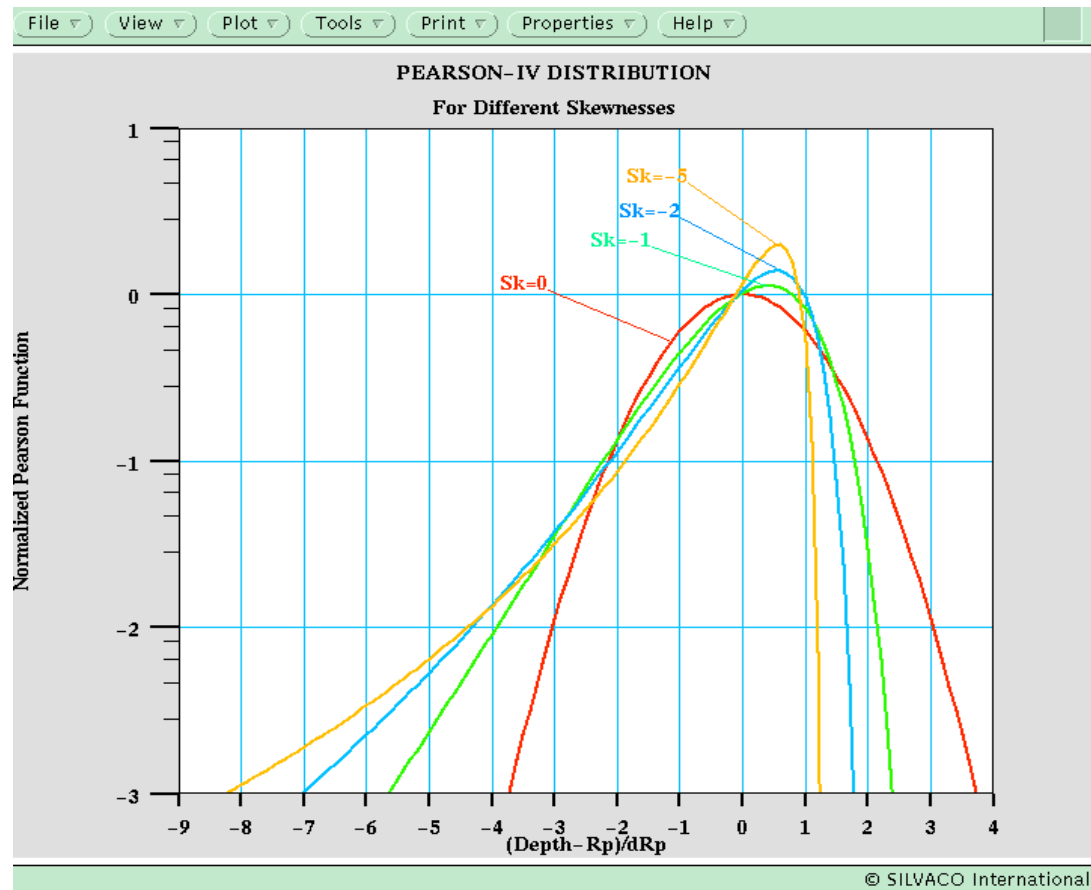
- Pearson distribution functions are solutions of a simple differential equation:

$$\frac{Df(x)}{dx} = \frac{(x-a) + (x)}{b_0 + b_1x + b_2x^2}$$

- The shape and characteristics of the function $F(x)$ could be quite different depending on discriminant of quadratic function in the right-side of the equation
- Function $f(x)$ does not have discontinuities and has a "bell" shape only when the discriminant is positive (the quadratic equation does not have any roots). In this case $f(x)$ is referred as Pearson-IV function
- In terms of skewness (Sk) and kurtosis (β), this means that for each absolute value of Sk exists a critical value of β above which all profiles are nice Pearson-IV function (Figure page 11)



Moments (Analytic) Method (con't)



Pearson-IV distribution for different skewnesses.

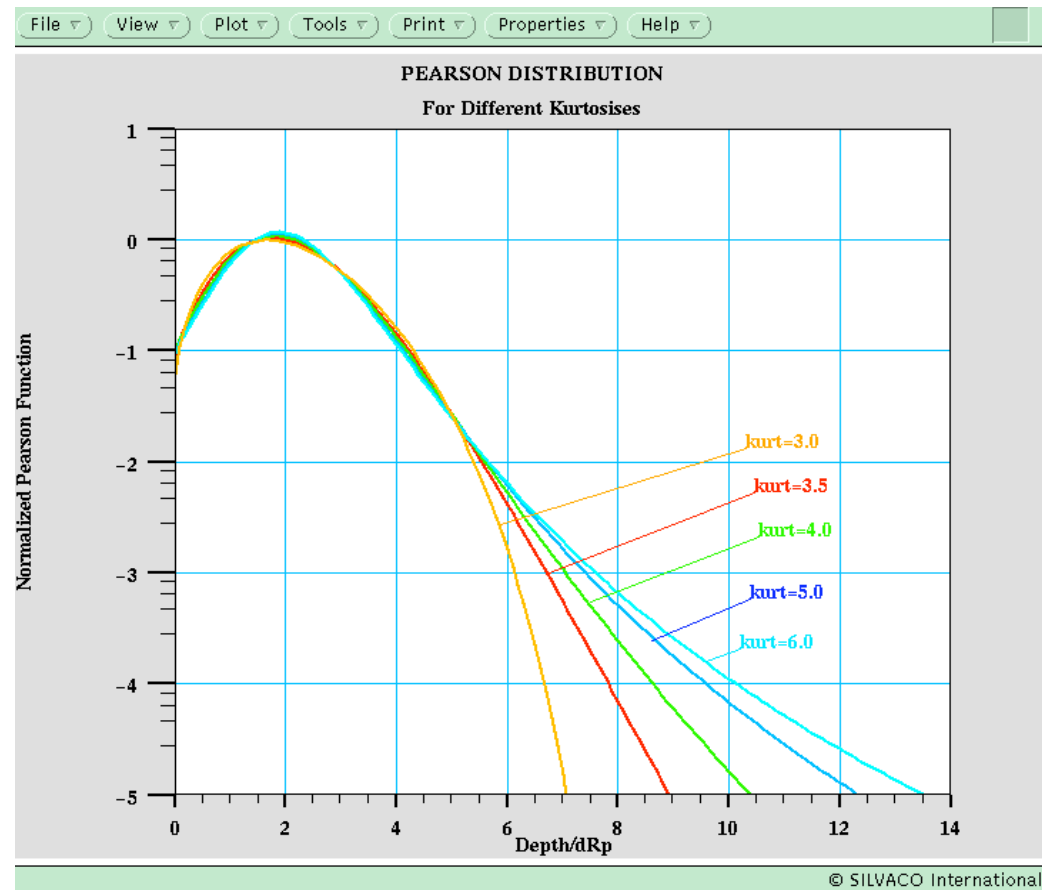


Moments (Analytic) Method (con't)

- Skewness is a measure of asymmetry of the profile, so $Sk=0$ corresponds to a symmetrical profile
- A special case of $Sk=0$ and $\beta =3.0$ corresponds to Gaussian distribution function
- The sign of Sk determines direction of the profile tail
- The kurtosis determines "length of the tail"
- The figure on page 13 shows the Pearson functions with positive $Sk=0.5$ and different kurtosises
- All functions in Figure 2 with $\beta \geq 3.5$ belong to Pearson-IV type
- Pearson function with $\beta =3.0$ for non-zero Sk must have a discontinuity. But in this specific case the point of discontinuity is located at $x<0$, e.g outside the material surface



Moments (Analytic) Method (con't)



Pearson distribution for different kurtosises.



Moments (Analytic) Method (con't)

- Capabilities of the moment method:
 - applicable to completely disordered materials (amorphous)
 - needs improvements to handle multilayered structures (this will be discussed later)
 - could give quite accurate profiles when crystal effects are not very pronounced
 - polycrystalline materials
 - partially disordered crystals during high dose implant
 - implant through an amorphous layer
 - it is as accurate as accurate the moments calculated or extracted from the experimental profile
 - could serve as a first approximation for ~ 7 degrees implants into crystalline materials
 - not applicable for ~ 0 degrees, low and moderate dose implants into single crystals without or with very thin overlaying amorphous material



U. of Texas Model Implementation in ATHENA

- As we just concluded, standard method of moments has many limitations and completely fails when channeling effects are an important part of the implantation process
- Only finely tuned BCA programs could address these effects from the first principles
- A semi-empirical method capable of simulating 1D-profiles with channeling tails has been developed by Al Tasch et.al. in U. of Texas in Austin. We will refer to the method as UT-Model.
- In the UT-Model, the implant concentration is calculated as a linear combination of two Pearson functions (Figure page 16):

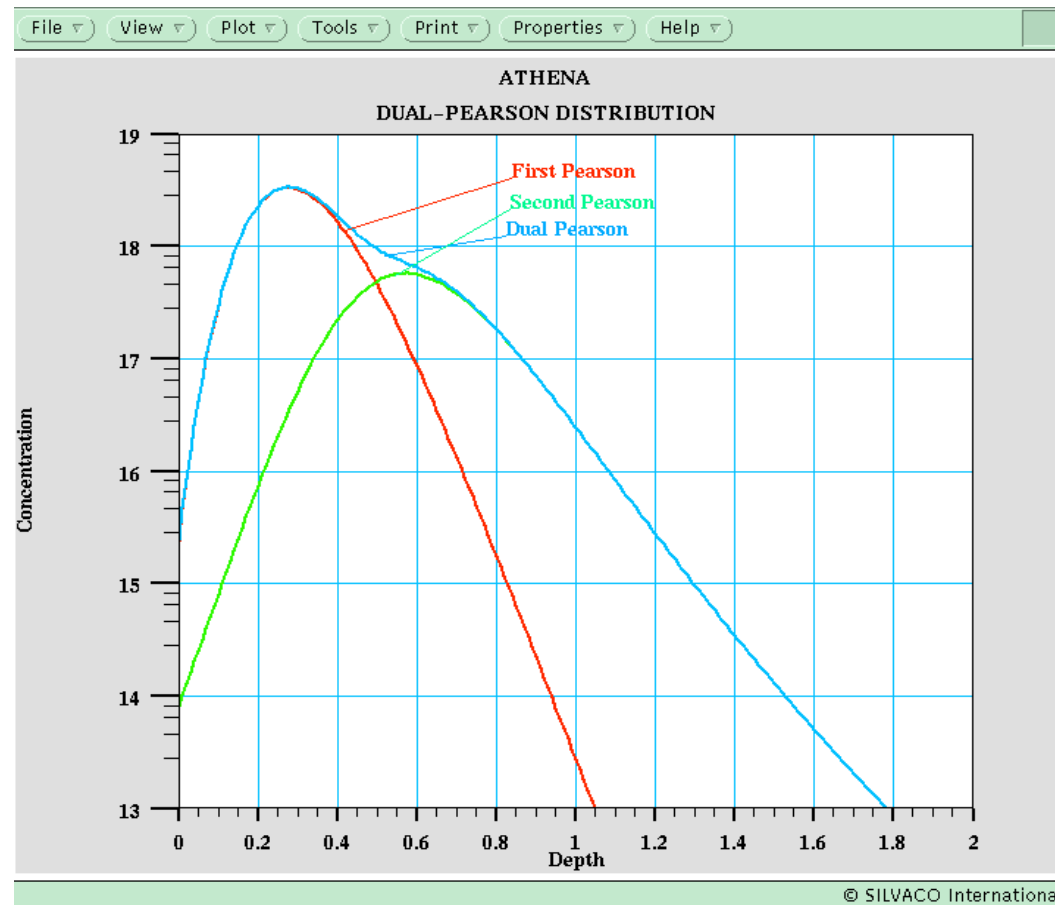
$$C(x) = D*[R f_1(x) + (1-R)* f_2(x)],$$

D is implantation dose

R is a dose ratio



U. of Texas Model Implementation in ATHENA (cont.)



Dual-Pearson distribution.



U. of Texas Model Implementation in ATHENA (con't)

- Each profile is described by 9 parameters: 4 moments for the first Pearson function, 4 moments for the second Pearson function, and the ratio R
- Al Tasch and his coworkers performed a very large amount of implants and SIMS profile measurements from which 9 parameters were extracted and gathered into look-up tables*
- They also devised and thoroughly checked a special interpolation procedures which allow to calculated profiles for conditions which do not coincide with tabulated ones
- The range of validity for UT-Model look-up tables is shown in the next table

*References

1. A.F. Tasch et al., J. Electrochem. Soc., 136, p.810, 1989.
2. K.M. Klein et al., J. Electrochem. Soc., 138, p.2102, 1991.
3. P.Gupta et al., Mat. Res. Soc. Symp. Proc., p.235, 1992.



U. of Texas Model Implementation in ATHENA (con't)

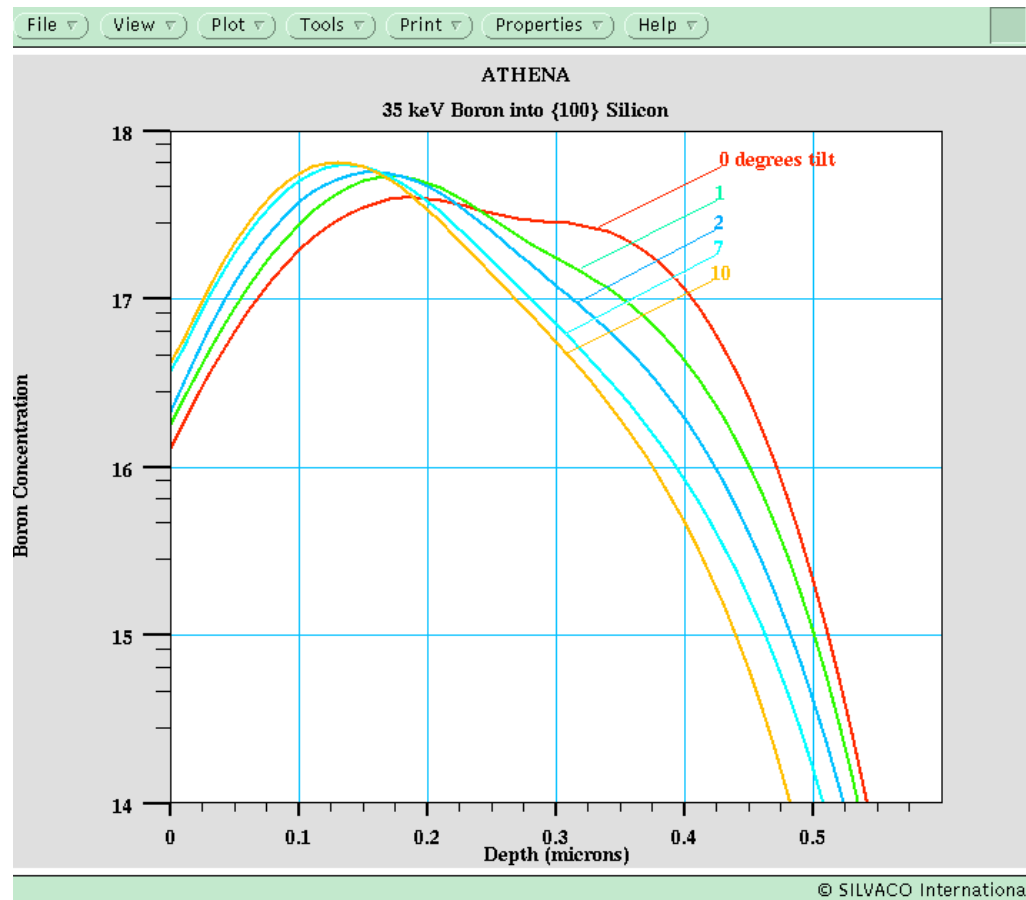
Ions	Energy (keV)	Dose (cm ^{**} -2)	Tilt angle (degrees)	Rotation angle (degrees)	Screen Oxide (Angstroms)
B	1-80(1)	1e13-8e15	0 - 10	0 - 360	native oxide -500(2)
BF2	15-65(1)	1e13-8e15	0 - 10	0 - 360	native oxide
As	1-180(3)	1e13-8e15	0 - 10	0 - 360	native oxide
P	10-180(3)	1e13-8e15	0 - 10	0 - 360	native oxide

Table 1. Range of validity for University of Texas models in *ATHENA*.

NOTE: From *Simulation Standard*, December 1996.



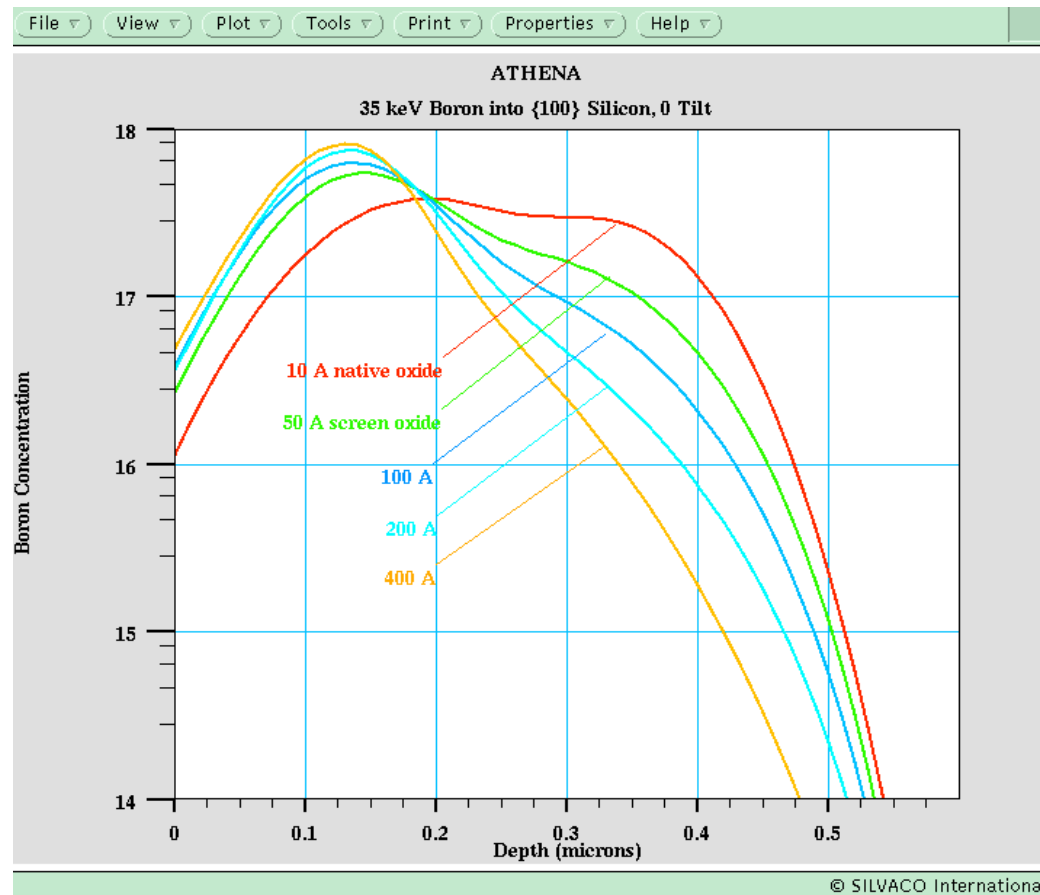
U. of Texas Model Implementation in ATHENA (con't)



35 keV boron into {100} silicon.



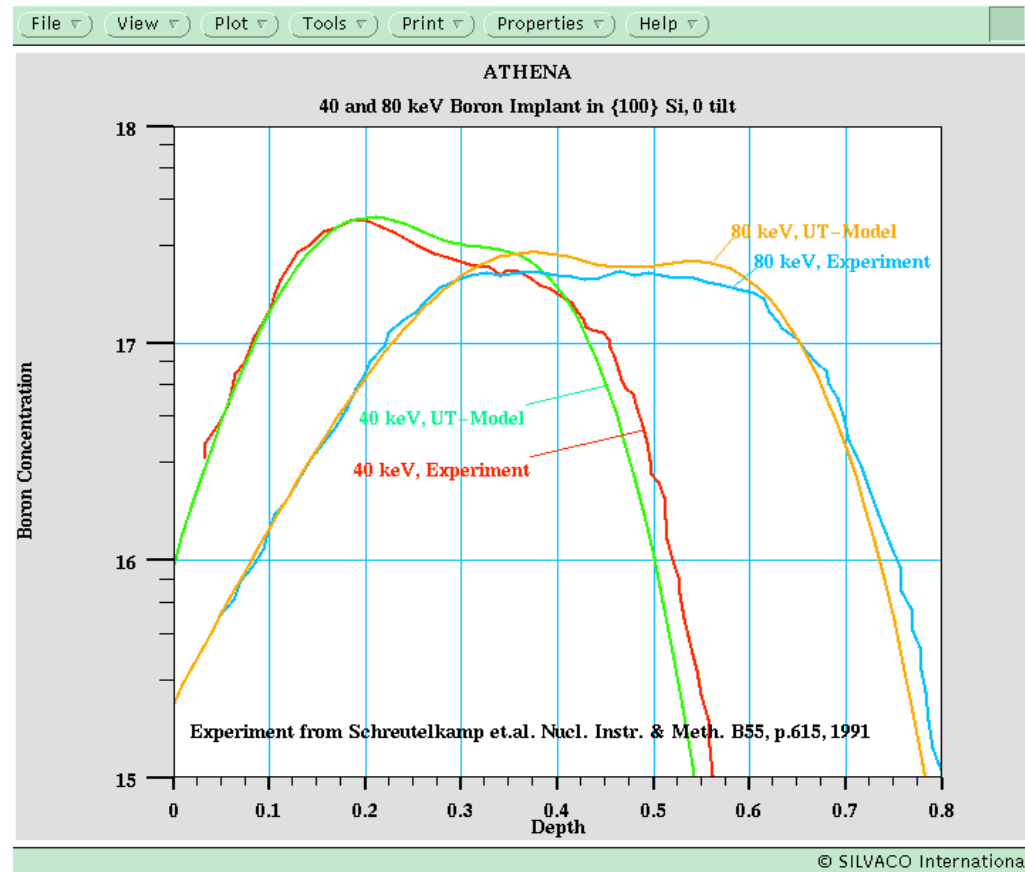
U. of Texas Model Implementation in ATHENA (con't)



35 keV boron into {100}, 0 tilt.



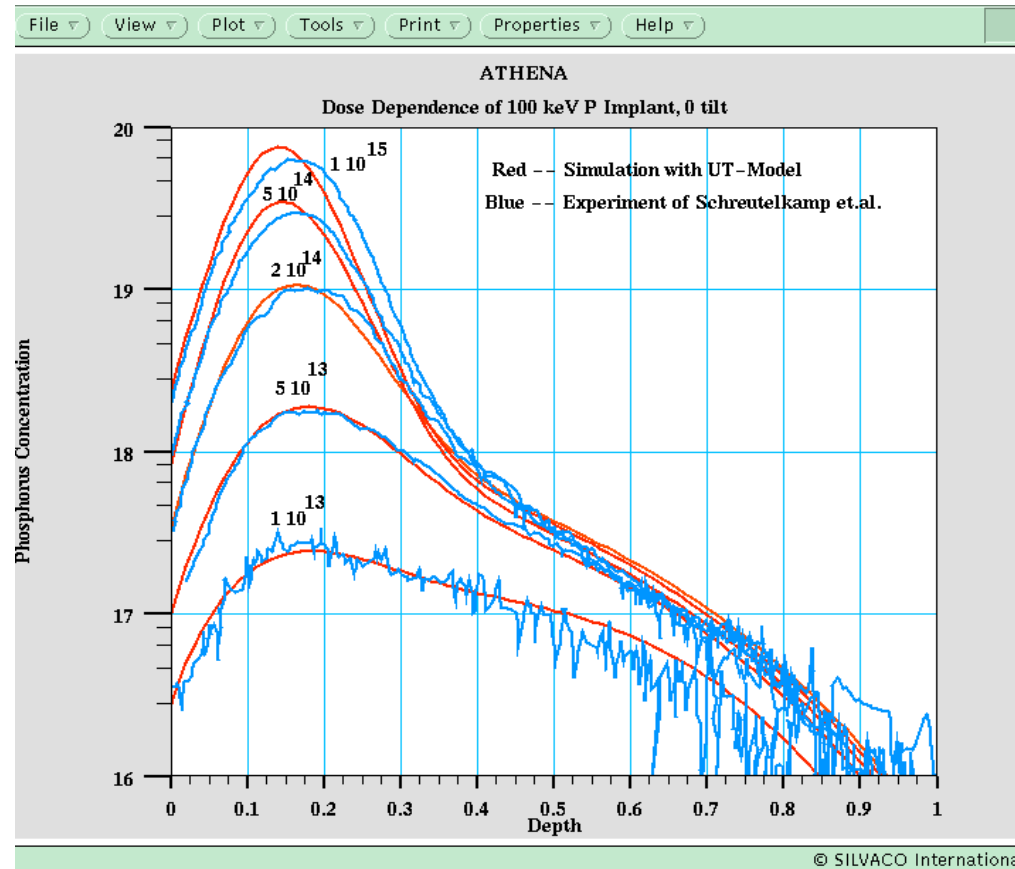
U. of Texas Model Implementation in ATHENA (con't)



40 and 80 keV boron implant in {100} Si, 0 tilt.



U. of Texas Model Implementation in ATHENA (con't)



Dose dependence of 100 keV P implant, 0 tilt.



U. of Texas Model Implementation in ATHENA (con't)

- Conclusions on the UT-Model:
 - UT-Model is now default implantation model in ATHENA
 - Unless parameter "amorphous" is specified, ATHENA will search for solution in UT-tables
 - If implant parameter combination is outside the limits outlined in Table 1, ATHENA will use single Pearson tables
 - Screen oxide thickness "S.OXIDE" should be specified by the user in the IMPLANT statement
- Implementation of the UT-Model allows ATHENA users to accurately and quickly simulate critical implantation steps



Multilayer Models

- As we stressed earlier, the method of moments is derived with condition that material is homogeneous and does not have any internal boundaries.
- However, in almost all practical cases ion implantation goes through regions of different materials (oxide, nitride, silicides, etc.)
- All materials have different range moments, therefore some corrections should be applied when calculating profiles in multilayered structures
- There are several approaches to solve this problem. In all the methods the combine thickness of overlaying layers x_t is substituted by effective thickness of the current material x_{eff}
- This means that in order to calculate a portion of the profile within a second or any subsequent layer, the Pearson function corresponding to the layer's material should be shifted by $x_{eff} - x_t$



Multilayer Models (con't)

- In the default dose matching model (parameter MATCH.DOSE), x_{eff} is calculated from

$$\int_0^{x_{\text{eff}}} C_i(x) dx = \sum_{k=1}^{i-1} D_k$$

- This means that x_{eff} is such thickness of the current material which would absorb the portion of implant dose equal to the sum of the doses placed into all overlaying layers



Multilayer Models (con't)

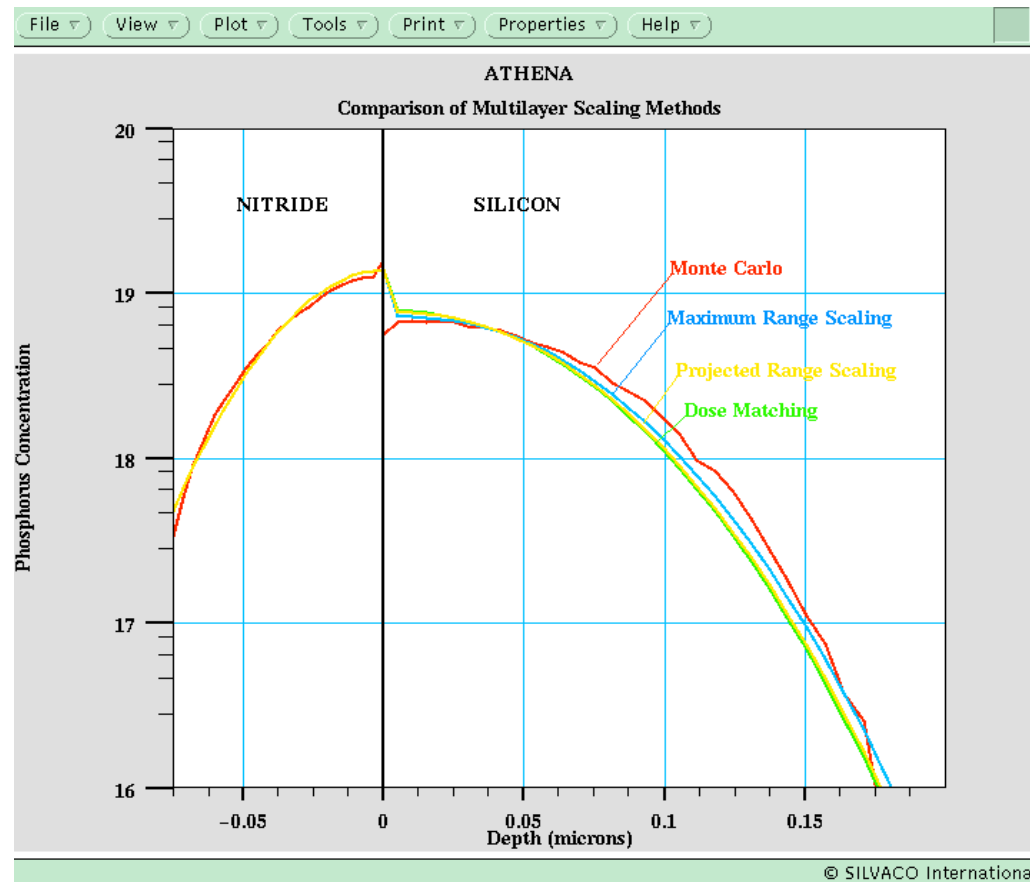
- In the range matching method (parameter RP.EFF), x_{eff} is calculating as:

$$e_{ff} = \sum_{k=1}^{i-1} \frac{t_k}{R_{pk}} R_p$$

- It means that thicknesses of overlaying layers are normalized according projected range ratio
- In the maximal range scaling method (MAX.SCALE) R_p substituted with $R_p + 3 \cdot \Delta R_p$



Multilayer Models (con't)



Comparison of multilayer scaling methods.

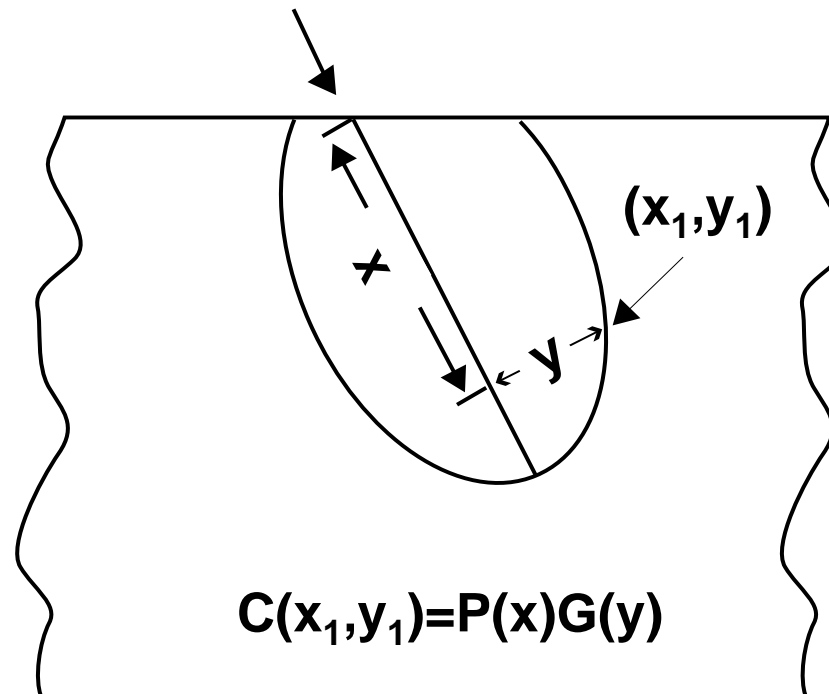


Hierarchy of 2D Implant Models in ATHENA

- Accuracy of 1D implant profile simulation could be confirmed by measurements. There are several though quite difficult and expensive 2D measurement methods. However they are not accurate enough
- Both Monte Carlo and BCA methods are basically three-dimensional. However, it is obvious that number of trajectories increases enormously if high accuracy is needed for 2D or 3D simulations
- First, we need to build a model for the 2D profile of implant into a point (very narrow window see Figure page 28)



Hierarchy of 2D Implant Models in ATHENA (con't)



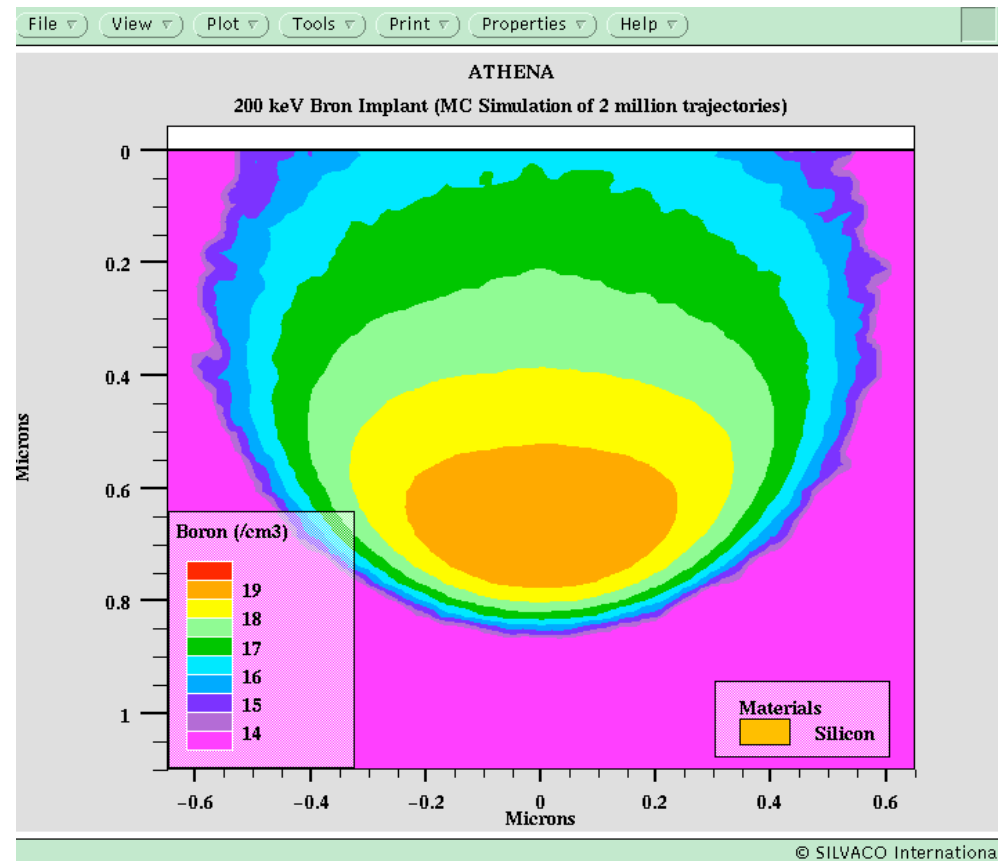


Hierarchy of 2D Implant Models in ATHENA (con't)

- The simplest approach which is used in most generic process simulators is to multiply a Pearson profile $P(x)$ by Gaussian profile $G(y)$
- Obviously profile in lateral (transversal) direction must be symmetrical, so Gaussian looks like logical selection
- In the simplest approximation standard deviation in $G(y, \Delta Y)$ is constant and equal to so-called averaged lateral stragglings
$$\Delta Y = \left[\int \int f(x,y) y^2 dx dy \right]^{1/2}$$
- However, detailed Monte Carlo simulations (Figure page 31) show that transversal standard deviation could vary with the depth



Hierarchy of 2D Implant Models in ATHENA (con't)



200 keV Boron Implant (MC Simulation of 2 million trajectories)



Hierarchy of 2D implant Models in ATHENA (con't)

- When model FULL.LAT is specified in the IMPLANT statement ATHENA uses parabolic approximation for depth dependence of transversal standard deviation in $G(y, \delta_y(x))$

$$\delta_y(x) = c_0 + c_1(x - R_p) + c_2(x - R_p)^2$$

This parabolic function is the best approximation which could be constructed using spatial moments not higher than the fourth moment in either direction

- Coefficients c_0 , c_1 , and c_2 could be analytically expressed through Y , Sk (lateral third moment or mixed skewness) and β_{xy} (mixed kurtosis)

$$Sk_y = \left\{ \iint_{\infty} f(x,y)(x-R)y^2 dx dy \right\} / (\Delta R_p \Delta Y^2)$$

$$\beta_{xy} = \left\{ \iint_{\infty} f(x,y)(x-R)^2 y^2 dx dy \right\} / (\Delta R_p^2 \Delta Y^2)$$

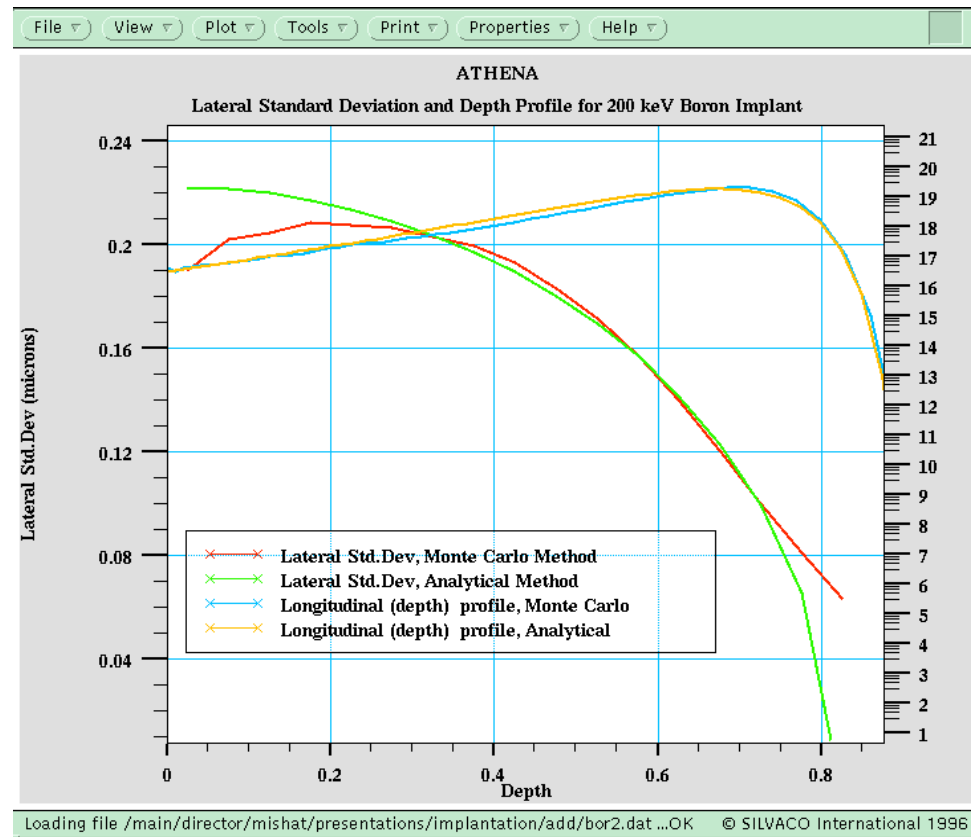


Hierarchy of 2D Implant Models in ATHENA (con't)

- The figure on page 34 compares depth dependence of lateral standard deviation obtained from Monte Carlo Simulation and from parabolic formula of the FULL.LAT Model
- The figure on page 35 shows that FULL.LAT method gives reasonably good agreement with Monte Carlo simulation in the figure on page 36
- If the constant lateral standard deviation is used (Figure page 37) the shape of 2D distribution is wrong.
- The study is now under way in which we analyze how the details of implant distribution shape would affect device characteristics
- It is also important to know in which energy interval FULL.LAT effects are more pronounced



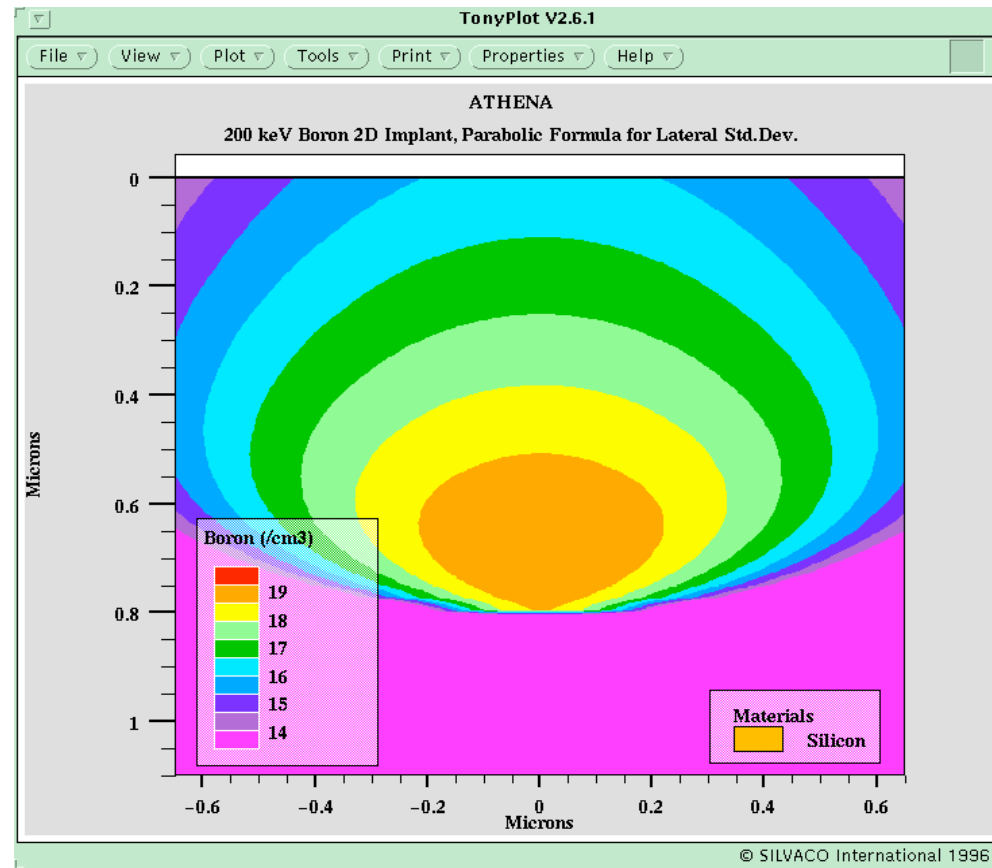
Hierarchy of 2D Implant Models in ATHENA (con't)



Lateral Standard and Depth Profile for 200 keV Boron Implant.



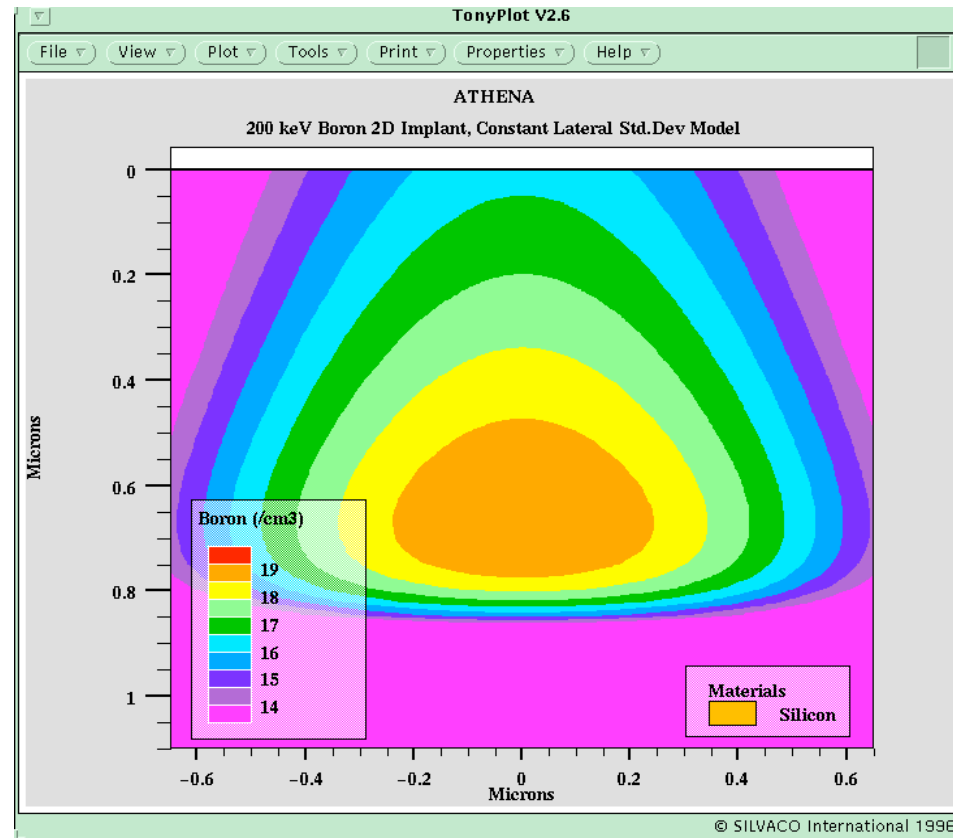
Hierarchy of 2D Implant Models in ATHENA (con't)



200 keV Boron Implant, parabolic formula for lateral Std. Dev.



Hierarchy of 2D Implant Models in ATHENA (con't)



200keV boron 2D implant, constant lateral Std. Dev. model.



Use of the Moment Statement

- The MOMENT statement serves two purposes:
 - set look_up table to be used in the subsequent IMPLANT statement
 - set a set of moments which could be used in the subsequent IMPLANT statement
- 4 different tables could be specified:
 - SVDP_TABLES - default (Al Tasch double Pearson tables)
 - STD_TABLES - tables in old standard format (mainly single Pearson) This type of tables will eventually disappear
 - USR_UT_TAB - user defined tables in the UT format
 - USR_STD_TAB - user defined tables in the old format



Use of the Moment Statement (con't)

- The following parameters can be specified in the MOMENT statement:

ION	Implanted ion (e.g. i.boron, i.bf2, etc)
MATERIAL	Target material (e.g. silicon, material=BPSG)
DOSE	Ion dose (/cm ²).
ENERGY	Ion energy (KeV).
RANGE (or RP)	Projected range (microns).
STD.DEV (or DRP)	Projected Standard Deviation (microns).
GAMMA (or SKEWNESS)	Third longitudinal moment.
KURTOSIS	Fourth longitudinal moment.
LSTD.DEV (or LDRP)	Lateral Standard Deviation (microns).
SKEWXY	Mixed third moment.
KURTXY	Mixed fourth moment.
KURTT	Lateral fourth moment.
DRATIO	Dose ratio for dual Pearson
+ 8 parameters for the second Pearson (SRANGE, etc)	



Conclusion

- Analytical Ion Implantation models allow to accurately simulate key implantation steps of silicon technologies
- The analytical models can be extended by using BCA modeling and moments extraction
- Some critical steps require only Monte Carlo BCA method to be used