Proposal of a point-source model for highly-accurate analytical 3D calculation of ion implanted dopant profiles

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***Abstract*: A point-source model of ion implantation for 3D simulation is proposed for the first time. Implanted ion profile is calculated by integrals, over implanted surface, of point-source implanted profiles which are calculated by a well-tuned Monte Carlo simulation and are then reconstructed by analytical functions considering various channeling directions. The significance of the proposed model is demonstrated by remarkable accuracy of lateral profiles along the masked surface.**

I. INTRODUCTION

Ion implantation is one of the key processes in LSI fabrication, and its simulation of implanted ion profile is very important for accurate device simulation. With decreasing device feature size, dopant profiles in lateral direction have gained much more importance since they affect such characteristic like puchthroughs, short-channel effects of deep submicron devices. There are two approaches for implantation simulation. Well-tuned Monte Carlo simulation (***MCS***)[1-3] is excellent in accuracy and can deal with 3D profiles. Even with modern fast computers, however, slow calculation speed prohibits extensive use of ***MCS***. On the other hand, analytical simulation (***AS***) [4-6] is fast and is used daily by device developers.

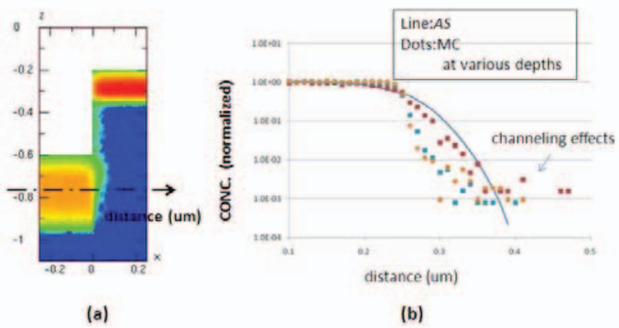

Fig.1 : B profile implanted at 20keV with a dose yielding no crystalline damage, simulated by well-tuned MC. (a):Cross section, (b):Lateral profile.

AS of implanted ion profiles started in 1D[4]. Its accuracy was easily checked by dopant profiles using SIMS. For 2D and 3D simulations, it is quite natural that lateral spread of ions is extended from established 1D profiles. Some statistical function like Gaussian distribution is assumed in lateral direction, and is tried to fit to ***MCS***. However, lateral spread of implanted ions often shows depth dependency, and no single decay length can explain lateral profiles. Moreover, ion channeling in oblique channeling direction makes the lateral profile quite complicated. Fig.1 demonstrates these situations, and shows simulated substrate structures and lateral profiles at various depths. Normalized lateral profile does not show any depth-dependency by ***AS***. On the other hand, ***MCS*** indicates that lateral spread depends on the depth. Moreover, channeling effects are clearly seen. It seems there is no possible way to accommodate these situations for traditional ***AS***.

When we think of ion implantation process, it is quite natural that implanted ion profiles are summation of point-source implantation over implanted surfaces. If we can find out 3D expression of point-source-implanted ion profiles, the following integrals are simple, and do not include any ambiguity. The calculation is 3D in nature. The deficiency may be that there is no experimental technique to verify point-source implanted ion profiles. However, ***MCS*** well-tuned to 1D depth profile by blanket implantation could be the substitute of experiments. Hobler et al [7] already pointed out this possibility and studied point-source response. But their work did not consider channeling in all the three major crystalline directions, <100>, <110> and <111>, with no further study.

In this paper, we propose a point-source simulation model (***PSS***) of ion implantation for 3D simulation for the first time. Apparently most difficult case, no-tilted B implantation on oxide-free crystal silicon, is tried. Well-tuned ***MCS*** is used as a reference [8]. We have succeeded in analytical representation of point-source implanted profiles. The accuracy of the new model is demonstrated in masked 3D profiles.

II. Models

Fig.2 illustrates the proposed model. Ion implantation to the planer substrate is considered as an integration of point-source implantation over implanted surface. If we know the point-source ion profile and represent this profile by some mathematical functions, then integration is an easy task. The problem may be there is no experimental technique to obtain point-source ion profiles. However, well-tuned Monte Carlo simulation can be the substitute of experiments.

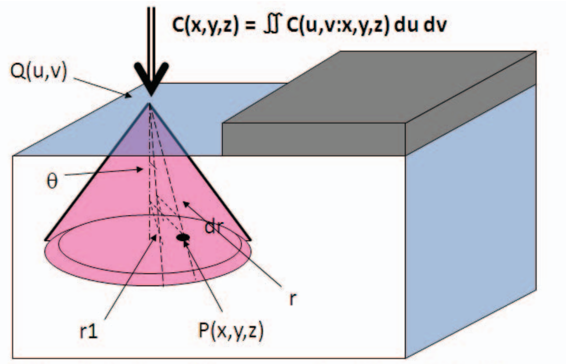

Fig.2 : Illustration of the proposed model. Implanted ion Distribution is calculated by integrals of point-source profile over implanted surface.

In this work, MC simulation model in HyEnexss is used. Its accuracy for simulation 1D depth profile by blanket implantation was already demonstrated in ref.[8] and one of the examples is shown in Fig.3.

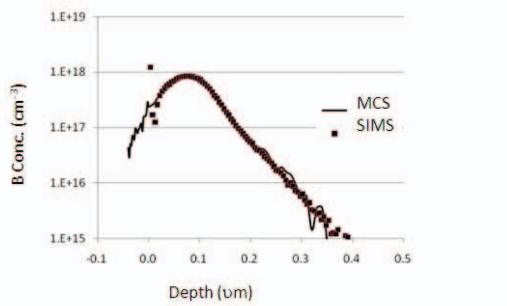

Fig.3:Comparison with our MCS results with experiments. Boron was implanted at 30keV onto SiO2-covered Si.

Using HyEnexss, point-source implanted B profile with tilt angle being 0 is simulated at 20keV with dose causing no crystalline damage effects. Cross-sectional ion profiles are shown in Fig.4(a)-(d). Fig.4(a) shows cross section at {100} plane. Ions, which suffered nuclear scattering around the center can find channeling directions, <100> perpendicular to the original ion direction of [001]. Thus, relatively higher B concentration is observed in lateral direction near the surface. Fig.4(b) shows cross section at {110} plane. <111> direction is oblique to original ion direction and higher concentration is found in oblique direction. Channeling in <110> direction

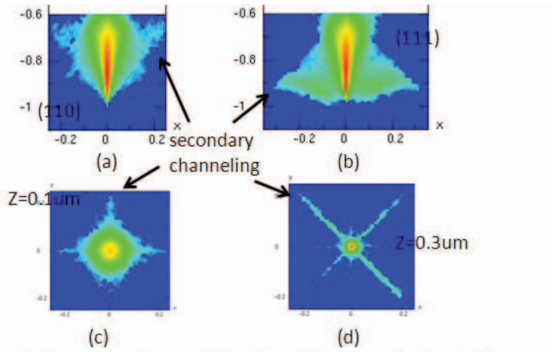

Fig.4 : Cross-section profiles of point-source implanted boron. (a):(110)plane, (b):(111)plane, (c)planer view at the depth of 0.1um, and (d) planer view at the depth of 0.3um.

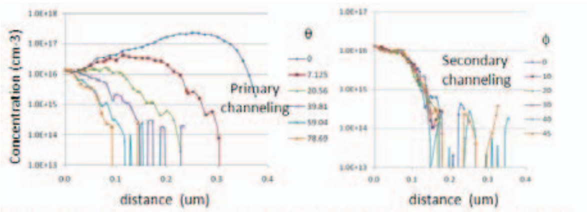

Fig.5 : 1D profiles starting at the implantation point to various directions. (a): θ-dependency, and (b): ϕ-dependency

C(r,θ,ϕ)	Components
= (non-channeling)	: $C_{Na}(r,\theta)$
+ (local channeling)	: $C_{Nc}(r,\theta)$
+ (primary channeling)	: $C_{Cp}(r, p_0,\omega)$
+ (secondary channeling)	: $C_{Cs}(r,p_i,\omega)$

$$= C_{Na}(r,\theta) + C_{Nc}(r,\theta) + C_{Cp}(r, p_0,\omega) + \Sigma\, C_{Cs}(r,p_i,\omega)$$

p_0 : primary channeling direction
p_i : secondary channeling direction
ω : solid angle

Fig.6 : Construction of point-source implanted profiles.

seems to be not so large. Fig.4(c) and(d) show planer view at the depths of 0.1μm and 0.3μm, respectively. Secondary channeling is dominated in <100> direction at the depth of 0.1μm, while it is dominated in <111> direction at the depth of 0.3μm. In other directions, the secondary channeling effects are not large.

In order to represent these ion profiles by mathematical functions, spherical coordinates are the first choice. 1D profiles starting from implantation point to various directions are extracted. From the symmetry of the diamond structure, profiles for 0< ϕ <45 are sufficient. Fig.5 shows examples of 1D profile: Fig.5(a) at ϕ =0 with parameter of θ, and Fig.5(b) at θ =25 degree with parameter of ϕ. Secondary channeling effects are clearly seen in <100> (ϕ =0) and (111) (ϕ =45) planes.

These profiles are assumed to be the sum of those depending on the following effects, respectively(Fig.6).

(1) Random collisions with nuclei:$C_{Na}(r,\theta)$.
(2) Minor local channeling effects: $C_{Nc}(r,\theta)$.
(3) Primary channeling effects due to ion implantation being done in the main channeling direction;<001>: $C_{Cp}(r,p_0,\omega)$.
(4) Secondary channeling effects in a major channeling direction,<100>, <110>, and <111>: $C_{Cs}(r,p_i,\omega)$.

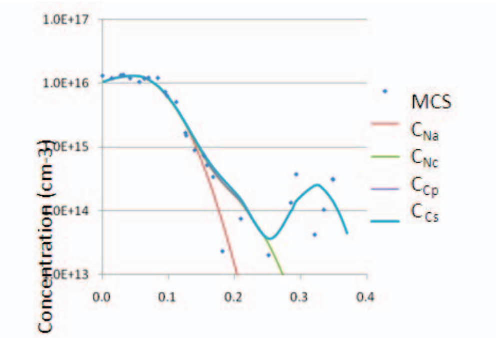

Fig.7 : An example of fitting result to 1D profile at θ=27degree and ϕ=45 degree.

Here, we represent each profile by Half-Gaussian, and 4 parameters, Rp, C_0, σ_1 and σ_2 of each Half-Gaussian are extracted depending on θ and ϕ.

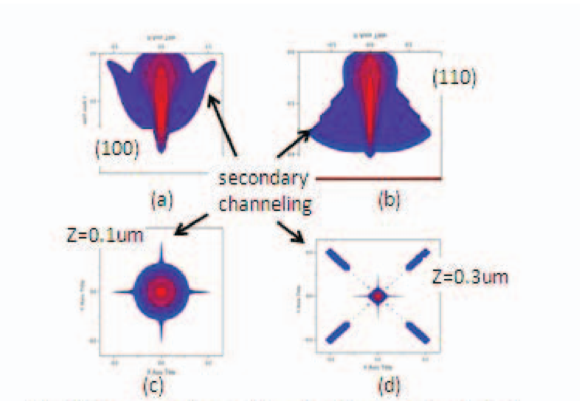

Fig.8 : Cross-section profiles of point-source implanted boron calculated by the proposed model., corresponding to Fig.4. (a):(100)plane, (b):(110)plane, (c)planer view at the depth of 0.1um, and (d) planer view at the depth of 0.3um.

There are 16 parameters for each direction. In order to reduce the number of parameters, these parameters are approximated by some smooth function of θ and ϕ.

Fig.7 shows an example of fitting results. First, $C_{Na}(r,\theta)$. is extracted by referring to implantation to amorphous Si. Then, $C_{Nc}(r,\theta)$. is extracted by referring to implantation to crystalline Si. For ϕ-value other than 0 and 45 degrees, no major channeling effects are assumed. Finally, parameters for primary and secondary channeling directions are extracted.

III. Applications

First, point-source implanted profile is reproduced by ***PSS*** and cross sections corresponding to Fig.4 are shown in Fig.8(a) -(d). Peculiar shape of B profiles are successfully reproduced by ***PSS***, and secondary channeling effects are clearly seen.

The new model is applied to 3D structure as shown in Fig.9 and compared to ***MCS***. Here, boron ions are implanted to a rectangular hole of thick oxide mask. By ***PSS***, point-source implanted boron profiles as expressed in mathematical functions are integrated over the whole hole area. Depth

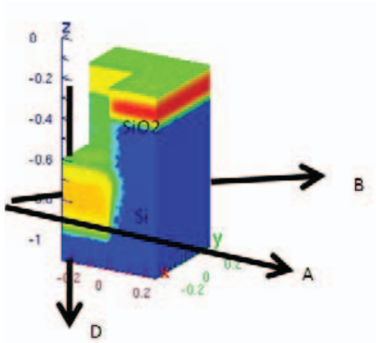

Fig.9 : 3D structure for evaluation of the proposed model. B is implanted at 20keV with dose of 1E13cm-2 to the SiO2-covered (100) Si.

profile (line D) by the new model shows excellent agreements with ***MCS*** as shown in Fig.10. This indicates that the mathematical representation of point-source profile is reasonable. The lateral profile is also compared between ***PSS*** and ***MCS*** along lines A and B in Fig.9. Here, line A lies in {100} plane and line, {110} plane. Fig.11 shows

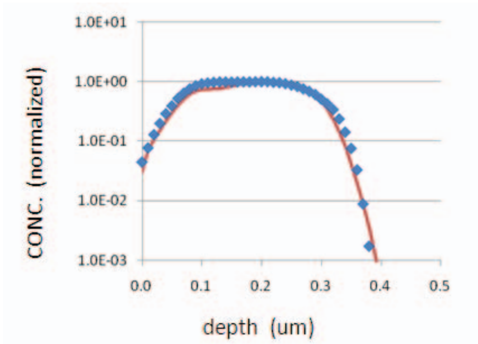

Fig.10 : Comparison of depth profile along line D between ***MCS*** and ***PSS***.

comparisons between ***MCS*** and ***PSS*** at the depth of 0.1 and 0.2 µm. Remarkable agreement between ***PSS*** and ***MCS*** are obtained, and the new model succeeds in simulating depth-dependent non-Gaussian lateral profiles which traditional ***AS*** can never do.

In these calculations, ***MCS*** is done with 1E8 particles and its calculation time is nearly a week on the latest DELL server. On the other hand, calculation time for ***PSS*** is less than 10 minutes on a one-year old mobile PC. Calculation time by ***PSS*** is orders of magnitude faster compared to ***MCS***.

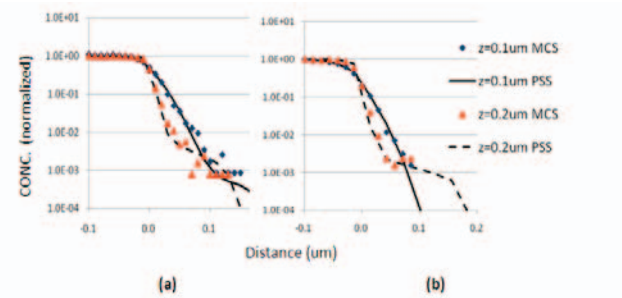

Fig.11 : Comparison of lateral profile along line B between ***MCS*** and ***PSS*** at different depths: (a) in {100} plane and (b) in {110} plane

IV CONCLUSION

A point-source model of ion implantation for 3D simulation is proposed for the first time. The model, taking various channeling effects into account, yields remarkable accuracy in simulating 3D profiles under the mask. Thus, the new model makes it possible to do several orders faster simulation than ***MCS*** without losing the accuracy, and enables extensive use of TCAD tools for optimizing process conditions and extracting maximum yield of deep-submicron devices

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