Monte Carlo Simulation of Ion Implantation Profiles Calibrated for Various Ions over Wide Energy Range

Kunihiro SUZUKI*, Yoko TADA*, Yuji KATAOKA*, and Tsutomu NAGAYAMA**

***Abstract*—Monte Carlo simulation is widely used for predicting ion implantation profiles in amorphous targets. Here, we compared Monte Carlo simulation results with a vast database of ion implantation secondary ion mass spectrometry (SIMS), and showed that the Monte Carlo data sometimes deviated from the experimental data. We modified the electron stopping power model, calibrated its parameters, and reproduced most of the database. We also demonstrated that Monte Carlo simulation can accurately predict profiles in a low energy range of around 1 keV once it is calibrated in the higher energy region.**

***Index Terms*—Ion implantation, database, amorphous, monte carlo, electron stopping power**

I. INTRODUCTION

Ion implantation is a standard technology to dope substrates in Si VLSI processes. The ion implantation profiles in Si substrates are generated based on a vast database of ion implantations in commercial simulators [1]. However, the database cannot predict profiles accurately when there are no experimental data or only poor data. Recently, various ions such as C, N, and F have been used to suppress transient enhanced diffusion in the subsequent annealing processes [2-4]. Therefore, theoretical evaluation of these profiles is invoked.

Extensive theoretical studies have been done on ion implantation profiles in an amorphous Si (aSi) substrate. Good reviews of this subject are described in ref. [5]. The interaction between incident ions and substrate atoms is composed of two mechanisms: one is the interaction between ions and the nucleus of the substrate atom and another is the interaction with the electrons of the target atoms, which are treated as independent mechanisms. These mechanisms can be directly implemented into Monte Carlo simulation such as SRIM [6] and a Monte Carlo simulator basically based on the same models in SRIM is also implemented in a commercial simulator [1], and is used optionally when the experimental data are poor. The calibration of the Monte Carlo simulation has been done focusing on a limited number of experimental data.

We established a secondary ion mass spectrometry (SIMS) ion implantation database over wide ion implantation conditions [7]. This database enables us to verify the accuracy of the Monte Carlo simulation over a wide range of ion implantation conditions of various ions and a wide energy range between 1 and 2000 keV. We sometimes used data in crystalline Si (cSi), since the profiles around the peak region are almost the same as the ones in aSi.

The ion implantation energy regions at around 1 keV are frequently used to realize shallow junctions. Recently, accurate SIMS evaluation has been demonstrated [8,9], which enables us to robustly compare the theory with experimental data in this low energy region.

II. EXPERIMENT

We deposited around 1 μm of aSi by low pressure chemical vapor deposition at 550 °C on Si substrates, or formed an amorphous layer by post Ge ion implantation. We verified that the profiles near the peak and surface regions in these amorphous layers are almost the same as

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the profiles in cSi substrates. Therefore, we also used the profiles in cSi neglecting the channeling tail region.

We evaluated ion implanted impurity concentration profiles using SIMS. In the SIMS measurement, the primary ions were raster scanned over a wide area, and secondary ions were collected from the central small area using electronic gating to avoid edge effects. The depth calibration of the measured profile was done using a Dektak 2A surface profilometer, and the concentration scale was adjusted to the as-implanted dose. The standard SIMS measurement conditions are shown in ref. [7] and that for shallow profiles are described in ref. [9].

III. Calibration of Monte Carlo Simulation

We will briefly explain the physics of ion implantation. A detailed description can be found in ref. [5].

In a nuclear interaction, a binary interaction is assumed. The energy transferred from the incident atom to the target atom T_{2f} is given by

$$T_{2f} = \frac{4M_1M_2}{\left(M_1+M_2\right)^2}\sin^2\left(\frac{\Phi}{2}\right)T_{1i} \quad (1)$$

where T_{1i} is the incident atom energy, and M_1 and M_2 are the incident and target atom mass number, respectively. Φ is the scattering angle calculated using Ziegler-Litmark-Biersak universal potential model [5].

On the other hand, Lindhard proposed an electron stopping power of

$$S_e = r_e 1.21\times10^{-16} Z_1^{7/6}\frac{Z_1Z_2}{\left(Z_1^{2/3}+Z_2^{2/3}\right)^{3/2}}\frac{1}{\sqrt{M_1[g]}}\sqrt{E[eV]}\ \left[eV\,cm^2\right] \quad (2)$$

where Z_1 and Z_2 are the incident and target atomic number, respectively [10]. r_e is a fitting parameter. We implemented the above physics in our own Monte Carlo simulator.

Fig. 1 shows the comparison of SIMS and Monte Carlo data with r_e of 1. We obtained good agreement between Monte Carlo and SIMS data for As profiles, and close agreement for P profiles, but significant deviation for B profiles.

Fig. 2 compares SIMS and Monte Carlo B data with various r_e. The profile becomes shallower with increasing r_e. We can obtain close agreement of peak position as well as the overall shape of the profile with r_e of around 1.5.

Fig. 3 compares various energy-dependent ion SIMS profile data with the Monte Carlo simulation with optimized r_e. We obtained a good agreement between SIMS and the Monte Carlo data for any ions of B, As, P, In, Sb, Ga, Ge, Si, N, F, and C. It is noteworthy that we can fit the data with a single r_e over a wide energy range. The value of r_e is not far from 1 and it is 1 in many cases. Table 1 summarizes r_e in a periodic table form. r_e is apt to decrease towards the right-hand side and also down the table although the physical reason is not clear. Therefore, we can predict the profiles in an amorphous layer using a Monte Carlo simulation with a default r_e deduced from the table and we can further improve the accuracy if we tune r_e with a few experimental data.

Low energy ion implantation of around 1 keV is frequently used to realize shallow junctions. There is no cri-

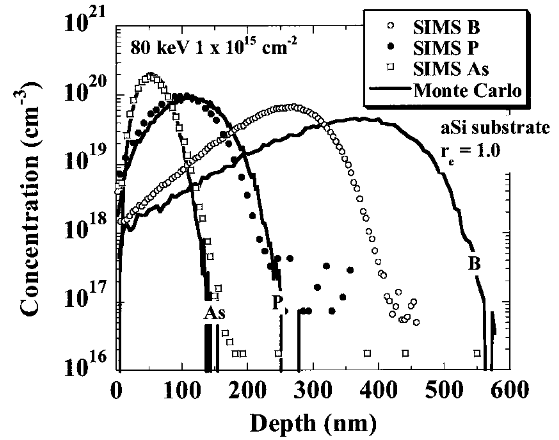


Fig. 1. Comparison of Monte Carlo simulation with B, P and As ion implantation profiles in aSi.

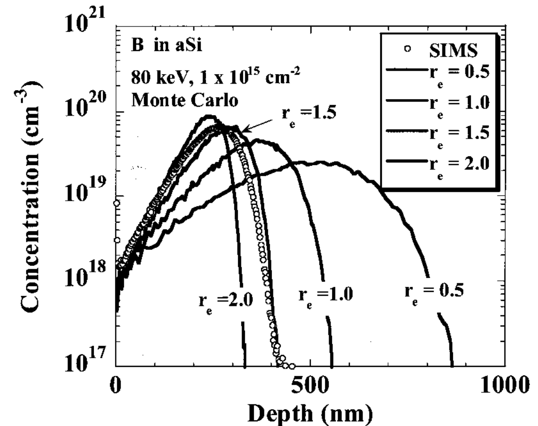


Fig. 2. Comparison of Monte Carlo simulation with B ion implantation profiles in aSi with various r_e.

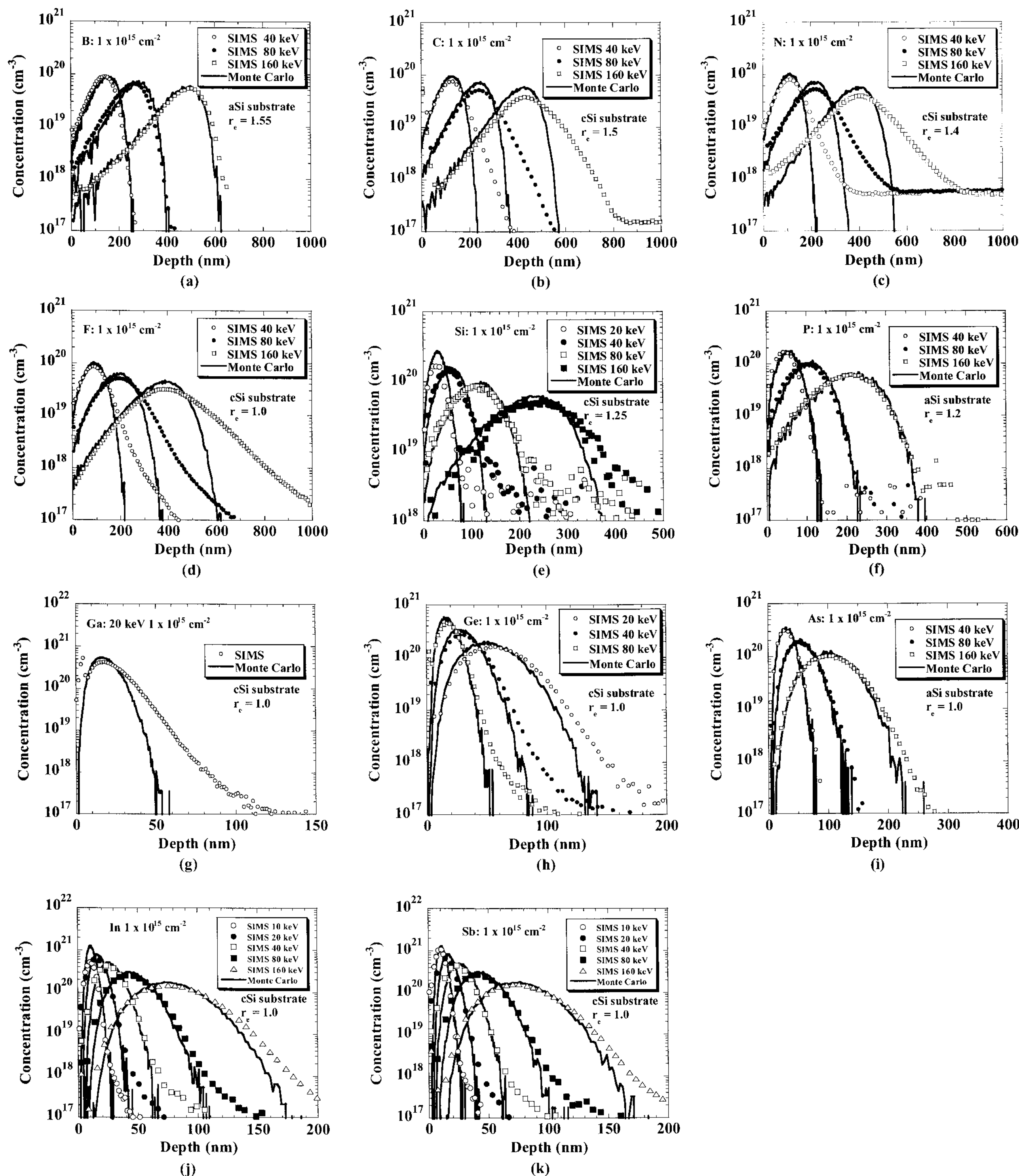


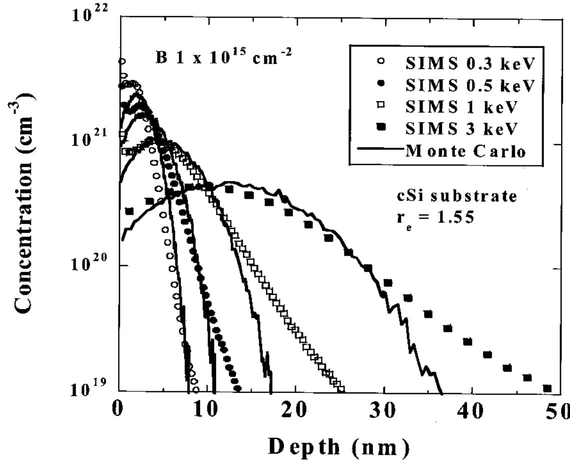
Fig. 3. Comparison of Monte Carlo simulation with various ion implantation profiles with optimized re. (a) B, (b) C, (C) N, (d) F, (e) Si, (f) P, (g) Ga, (h) Ge, (i) As, (j) In, (k) Sb.

tical point at this energy region from the standpoint of physics. However, SIMS reaches its resolution limit in this energy region. Recently, fundamental SIMS measurement mechanisms have been understood, and their accuracy have also been improved [8,9]. Therefore, it is interesting to compare the SIMS data with the calibrated Monte Carlo simulation.

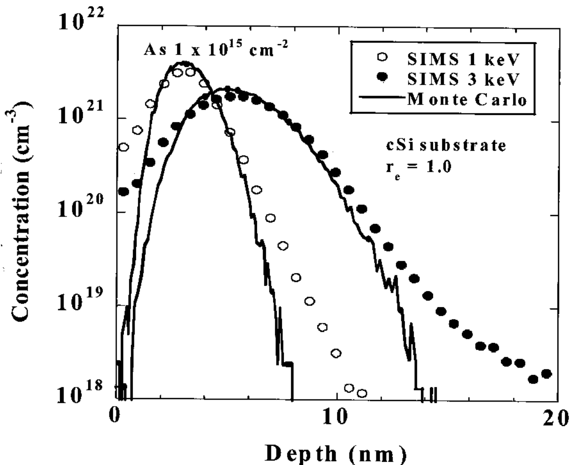
Fig. 4 compares the SIMS B and As profiles and Monte Carlo simulation. The SIMS B and As profiles near the peak region agree well with the Monte Carlo data. Therefore, the Monte Carlo simulation calibrated in the energy range of around few 10 keV can also predict the profiles

Table 1. Summary of r_e.

B	C	N	F
1.55	1.5	1.4	1.0
	Si	P	
	1.25	1.2	
Ga	Ge	As	
1.0	1.0	1.0	
In		Sb	
1.0		1.0	



(a)



(b)

Fig. 4. Comparison of Monte Carlo simulation with low energy ion implantation profiles. (a) B, (b) As.

in the energy range of around 1 keV.

IV. Calibration of Monte Carlo Simulation Extended to High Energy Region

Lindhard's S_e model of equation (2) assumes the interaction between the electron cloud of ions and substrate atoms. However, the electron cloud of incident ions is stripped at high energy regions. Therefore, Lindhard's model becomes invalid at high energy regions. The corresponding critical velocity v_c can be roughly evaluated as [10]

$$v_c = Z_1^{2/3} v_0 \tag{3}$$

where v_0 is the Bohr speed. Therefore, the corresponding critical energy is

$$E = \frac{M_1}{2}\left(Z_1^{2/3} v_0\right)^2 \tag{4}$$

giving values of about 2, 10, and 29 MeV for B, P, and As, respectively. Ion implantation of a few MeV is sometimes used to form wells in CMOS processes. Therefore, we should be careful about B implantation in the MeV energy region.

Fig. 5 compares B and P SIMS data in the Monte Carlo simulation with Lindhard's S_e model. SIMS and Monte Carlo results agree well at 400 keV for B and P. However, Lindhard's model predicts much shallower B profiles at 2 MeV, while it is still accurate for P. Therefore, we cannot apply Lindhard's S_e model in energy regions exceeding equation (4), and need a different one.

Ziegler utilized the linear response method and treated this phenomenon universally [5]. He evaluated S_e of H S_e^1 for various substrate atoms and summarized it as an empirical form of

$$S_e^1 = C_1 E^{C_2} + C_3 E^{C_4} \tag{5}$$

where C_1, C_2, C_3, C_4 are given in a Table for corresponding substrate atoms. S_e for the other ions are assumed to be related as

$$S_e^{Z_1} = Z_1^{\,2} \zeta_{Z_1}^2 S_e^1 \tag{6}$$

where $\zeta_{Z_1}^2$ expresses the order of the stripping of the electron cloud and its detailed description can be found in ref. [5]. Ziegler used a different S_e model for low energy regions given by

$$S_e^{Z_1}(E) = S_e^{Z_1}(E_c)\left(\frac{E}{E_c}\right)^{0.45} \tag{7}$$

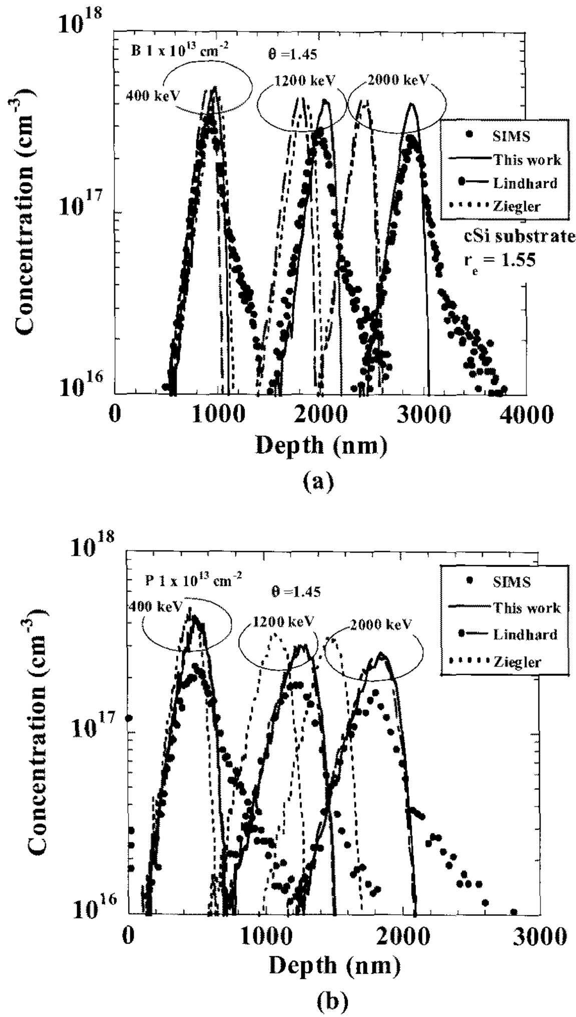


Fig. 5. Comparison of Monte Carlo simulation with B and P ion implantation profiles at high energy region. (a) B, (b) P.

where E_c is the critical energy to switch the model and is given by

$$\frac{E_c}{M_1} = 25\ keV/amu \tag{8}$$

and $S_e^{Z_1}(E_c)$ can be evaluated from the model given by

$$S_e^{Z_1}(E_c) = Z_1{}^2 \zeta_{Z_1}^2(E_c) S_e^1(E_c) \tag{9}$$

Therefore, Ziegler's model is proportional to $E^{0.45}$ in this low energy region, which has similar dependence to Lindhard's one.

Fig. 5 also compares SIMS and Monte Carlo with Ziegler's S_e models. Ziegler's model predicts a better B profile than Lindhard's model at 1200 keV, but it is still not accurate enough. On the other hand, Ziegler's model predicts worse P profiles than Lindhard's model at 1200 and 2000 keV. Although Ziegler's model is based on physics with some empirical treatment, it is not enough to reproduce the experimental data as it is. One possible approach to improving the accuracy is to tune various parameters in Ziegler's model. However, it is not a simple model to handle. We prefer to use a simpler approach as shown in the following.

Bethe derived an electron stopping power model which is valid at high energy regions where the electron cloud is completely stripped as [11]

$$S_e(E) = \left(\frac{q^2}{4\pi\varepsilon_0}\right)^2 \frac{2\pi M_1 Z_2 Z_1^2}{m_e E} \ln\left(\frac{4m_e E}{I\, M_1}\right) \tag{10}$$

where q is the electron charge, ε_0 is the permittivity in vacuum, m_e is the electron mass, and I is the average electron excitation energy, and is given by an empirical form as [12]

$$I = \begin{cases} 11.2 + 11.7Z_2 & \text{for } Z_2 \le 13 \\ 52.8 + 8.71Z_2 & \text{for } Z_2 > 13 \end{cases} \tag{11}$$

In Bethe's model, ions are assumed to be naked, that is, their electron cloud is completely stripped. This assumption is valid when the ion speed is much larger than the one of equation (3).

Fig. 6 shows the dependence of various S_e models on energy for B and P in Si substrate. It can be seen that Ziegler's model is almost the same as Lindhard's model at low energies and the same as Bethe's model at high energies, which is plausible from the standpoint of physics. Note that Ziegler's S_e model for P is higher than Lindhard's model in the MeV energy range, and this should induce a deviation between the Monte Carlo results using Ziegler's model and the SIMS data in Fig. 5 (b).

We propose to combine Lindhard's model with Bethe's model as follows.

First of all, Bethe's model is invalid in low energy regions, and we modify it not to influence Lindhard's model in low energy regions. The energy where Bethe's model has a maximum value can be evaluated from $\partial S_e/\partial E = 0$, and we obtain

$$E = eE_r \tag{12}$$

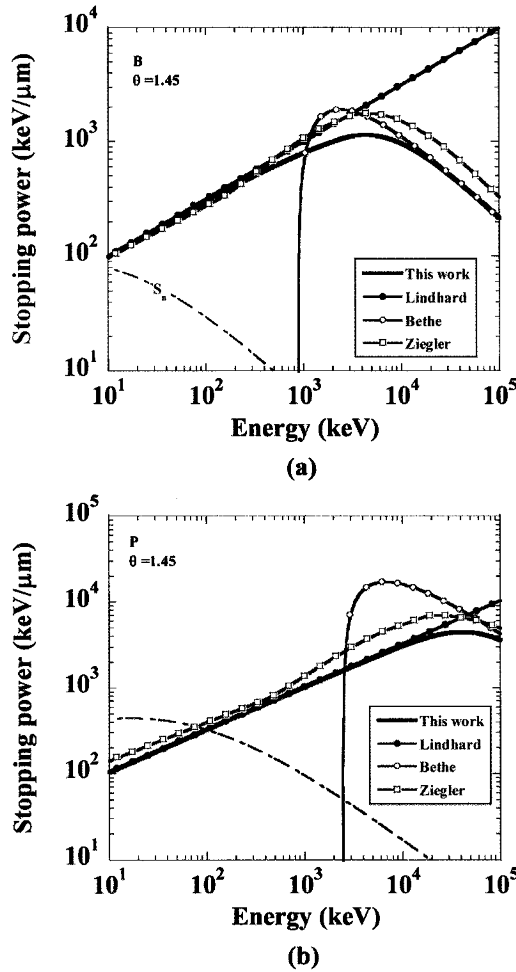


Fig. 6. Energy dependence of electron stopping power with various θ. (a) B, (b) P.

where e is the base of natural logarithm, and

$$E_r = \frac{M_1}{4m_e} I \tag{13}$$

We modify Bethe's model $S_{e_mB}(E)$ as

$$S_{e_mB}(E) = \begin{cases} \left(\frac{q^2}{4\pi\varepsilon_0}\right)^2 \frac{2\pi M_1 Z_2 Z_1^2}{m_e e E_r} & for\ E \le eE_r \\ \left(\frac{q^2}{4\pi\varepsilon_0}\right)^2 \frac{2\pi M_1 Z_2 Z_1^2}{m_e E} \ln\left(\frac{E}{E_r}\right) & for\ E > eE_r \end{cases} \tag{14}$$

Biersack et al. proposed a similar model with a mathematical trick [13]. Both modified Bethe's models become the original Bethe's model at high energy regions and much larger than Lindhard's model at low energy regions. We propose to combine Lindhard's model and the modified Bethe's model of equation (14) as

$$\frac{1}{S_e} = \left[\left(\frac{1}{r_e S_{eL}}\right)^\theta + \left(\frac{1}{S_{e_mB}}\right)^\theta\right]^{1/\theta} \tag{15}$$

This S_e becomes Lindhard's model at low energy regions, and Bethe's model at high energy regions, as is the case for Ziegler's model. When θ is one, it is the same form of the Biersack's model [13]. θ empirically expresses the transition from Lindhard's model to Bethe's model.

Fig. 7 shows the dependence of the B profile at 2000 keV on θ. A model with θ of 1 predicts a deeper profile, and one with θ of 2 predicts a shallower profile. The model well reproduces the data with θ of 1.45. The dependence of S_e on energy with various θ is shown in Fig. 8. The transition region becomes narrow with the increase of θ.

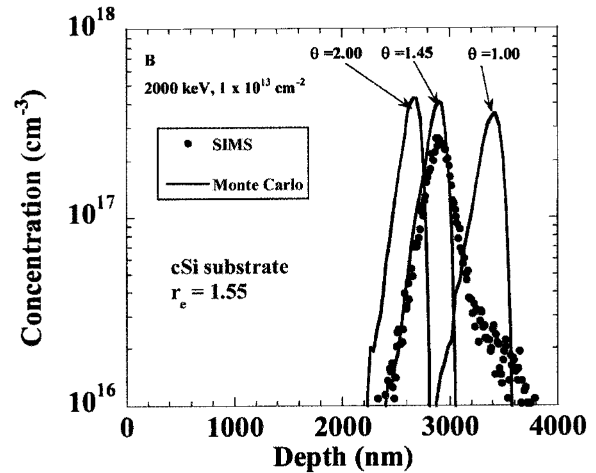


Fig. 7. Comparison of Monte Carlo simulation with B ion implantation profiles at high energy regions with various θ.

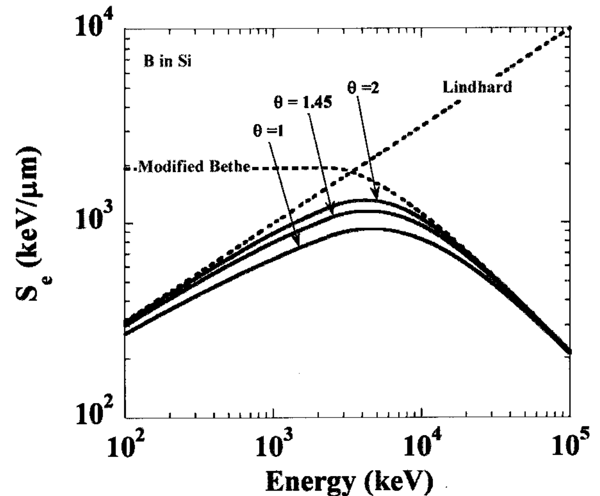


Fig. 8. Dependence of B electron stopping power on θ.

We applied θ of 1.45 to the other energies and ions, and obtained good agreement as shown in Fig. 4. The agreement of SIMS P with the model does not mean that θ of 1.45 is the optimal value for these cases, but the value ensures Lindhard's model is dominant at this energy region. Since the model is empirical, we should find optimal values for each combination of ion and substrates in the energy region of around equation (4) or equation (13).

V. SUMMARY

We modified the electron stopping power model by combining Lindhard's model with Bethe's model, and tuned its parameters. We showed that the Monte Carlo simulation can reproduce the ion implanted profiles by tuning a fitting parameter r_e, and showed that r_e is insensitive to energy, and demonstrated to reproduce B, As, P, In, Sb, Ga, Ge, Si, N, F, and C profiles. We also demonstrate that it reproduces the profile at low energy regions such as 0.5 keV B and 1 keV As. Therefore, we can well calibrate Monte Carlo simulation using a few experimental data. We also verified that the combined electron stopping power enables us to reproduce the B profiles in the MeV energy region. Since our model for high energy regions is not based on physics, we should calibrate the corresponding parameter in the other case when the energy is around or exceeds the critical energy.

It should be noted that channeling phenomenon are not considered in this Monte Carlo simulator , and hence this simulator should be used to predict the profiles in the amorphous substrates and also the ones in crystal substrates only near the surface and near the peak concentration region. We should further our work to investigate channeling phenomenon and damage accumulation to accurately predict the junction depth in the crystal substrate.

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REFERENCES

[1] Sentaurus Process http://www.synopsys.com/Tools/TCAD/ProcessSimulation/Pages/SentaurusProcess.aspx

[2] J. C. Hu, A. Chaterjee, M. Mehrotra, J. Xu, W. –T. Shiau, and M. Rodder, "Sub-0.1 mm CMOS source/drain extension spacer formed using nitrogen implantation prior to thick gate re-oxidation," *Symposium on VLSI Tech.*, pp. 488-189, 2000.

[3] Y. Momiyama, K. Okabe, H. Nakao, M. Kojima, M. Kase, and T. Sugii, Extension engineering using carbon co-implantation technology for low power CMOS design with phosphorus- and Boron-extension," *Ext. abs. The 7th International Workshop on Junction Technology*, pp. 63-64, 2007.

[4] S. Mirabera, G. Impellizzeri, E. Bruno, L. Romano, M. G. Grimaldi, F. Priolo, E. Napolitani, and A. Carnera, "Fulorine segregation and incorporation during solid-phase epitaxy of Si," *Appl. Phys. Lett.*, vol. 86, 121905, 2005.

[5] J. F. Ziegler, J. P. Bier sack, and U. Litmark, The stopping and range of ions in solid, *Pergamum*, 1885.

[6] SRIM-2003: http://www.srim.org/

[7] K. Suzuki, R. Sudo, Y. Tada, Miki Tomotani, T. Feudal, and W. Fichtner, "Comprehensive analytical expression for dose dependent ion-implanted impurity concentration profiles," *Solid-State Electronic*, vol. 42, pp. 1671-1678, 1998.

[8] Y. Kataoka and T. Itani, "Ultra-shallow depth profiling by using SIMS and Ion Scattering Spectroscopy," *Surf. Interface Anal.*, vol. 39, pp. 826-831, 2007.

[9] Y. Tada, K. Suzuki, and Y. Kataoka, "Segregation under low-energy oxygen bombardment in the near-surface region," *Applied Surface Science*, vol. 255, pp. 1320-1322, 2008.

[10] J. Lindhard, and M. Scharff, "Energy dissipation by ions in the keV region," *Phys. Rev.*, vol. 124, no. 1, pp. 128-130, 1961.

[11] H. A. Bethe, "Zur theorie des durchgangs schneller korpuskulasstrhlen duruch materie," *Ann. Phys. (Leipzig)*, vol. 5, pp. 325-400, 1930.

[12] P. Dalton and J. E. Turner, "New evaluation of mean excitation energies for use in radiation dosmetry," *Health Physsics Pergamon Press*, vol. 15, pp. 257-262, 1968.

[13] J. P. Biersack and L. G. Haggmark, "A Monte Carlo computer program for the transport of energetic ions in amorphous targets," *Nuclear Inst. And Meth.*, vol. 174, pp. 257-269, 1980.

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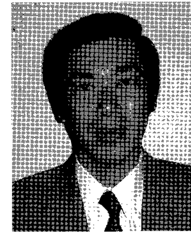

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