# Analysis of Ion Implantation Profiles for Accurate Process/Device Simulation: Analysis Based on Quasi-Crystal Extended LSS Theory

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Ion implantation profiles are sometimes needed in cases where the implantation conditions are not covered by existing databases or novel materials are being used. Although profiles can be derived by Monte Carlo simulation, it can take a long time to trace the trajectories of tens of thousands of ions. My coworkers and I have proposed an extended LSS (Lindhard, Scharff, and Schiøtt) theory that predicts profiles almost instantaneously but with comparable precision to Monte Carlo simulation. Although it works for profiles in amorphous layers, it cannot predict profiles in the crystalline materials used in practice. Therefore, we proposed a quasi-crystal extended LSS theory (QCLSS) in which parameters corresponding to the characteristic channeling phenomena in crystalline materials are implemented with a semi-empirical model and linked to the extended LSS theory. This can provide nearly instantaneous predictions of the implantation profiles of novel ion species in novel crystalline substrates. By applying the QCLSS theory to  $Si_{1-x}Ge_x$ substrates (which have recently been the focus of much study), we constructed a database for the implantation of B, As, and P ions in substrates with arbitrary values of composition ratio x.

### 1. Introduction

In the development of cutting-edge devices, it is sometimes necessary to use new materials or perform ion implantation with new ion species. Constructing a database for the prediction of such profiles can be a costly and time-consuming process. What is needed is a technique that can provide rough profile information even for combinations of ions and substrates for which little experimental data is available.

The implantation profiles of new types of ion in new types of substrate can be predicted by Monte Carlo simulation. In Monte Carlo simulation, nuclear interactions and electron interactions are considered as two-body problems involving an injected ion and a single substrate atom.<sup>1)-3)</sup>

Nuclear interactions are considered on

the basis of the system shown schematically in **Figure 1** (a). The energy  $T_n$  lost by an ion of energy E as a result of these interactions is expressed by

$$T_{n} = \frac{4M_{1}M_{2}}{(M_{1} + M_{2})^{2}} \cos^{2} \left( \int_{r_{\min}}^{\infty} \frac{b}{r^{2}\sqrt{1 - \frac{V(r)}{E_{c}} - \frac{b^{2}}{r^{2}}}} dr \right) E, \quad (1)$$

where  $M_1$  and  $M_2$  are the mass numbers of the ion and substrate atom, respectively, r is the distance between an ion and a substrate atom,  $r_{\min}$  is the minimum distance between them,  $E_c$  is the energy of the ion in the barycentric coordinate system, V(r) is the interaction potential between an ion and a substrate atom and is set empirically so as to reproduce large amounts of experimental data, and b is the collision parameter set by generating



Figure 1 Interactions between incident ions and substrate atoms.

a random number for each collision in the Monte Carlo simulation.

Electron interactions are modeled as changes in the electron behavior within the region of overlap between the electron clouds of an ion and a substrate atom, as shown in **Figure 1 (b)**. An electron interaction is assumed to reduce the ion's energy by  $T_{e}$ . The interactions between electrons are calculated using the average value obtained using a wide variety of different values of *b*. The energy lost by ions per unit length of travel is called the electron stopping power  $S_{e}$ . This widely used parameter is obtained from the following formula.<sup>1)</sup>

$$\begin{split} S_e &= \int T_e 2\pi b db \\ &= 1.21 \times 10^{16} Z_1^{\frac{1}{6}} \frac{Z_1 Z_2}{(Z_1^{\frac{2}{3}} + Z_2^{\frac{2}{3}})^{\frac{3}{2}}} \frac{1}{\sqrt{M_1[\mathrm{g}]}} \sqrt{E[\mathrm{eV}]} \left[ \mathrm{eV} \, \mathrm{cm}^2 \right], \, (2) \end{split}$$

where  $Z_1$  and  $Z_2$  are the atomic numbers of the ions and substrate atoms, respectively. The interactions between ions and substrate atoms are a function of the atomic number and mass number. Consequently, combinations of incident ions and substrate atoms can be accounted for by plugging the corresponding values of  $M_1$ ,  $M_2$ ,  $Z_1$ , and  $Z_2$  into this formula. Monte Carlo simulation can take some time to implement because tens of thousands of ion paths must be tracked to reduce statistical errors. Recent advances in computer technology have made it possible to perform these calculations within a few minutes, which is good enough to allow the technique to be used in practice. However, since it does not produce the sort of instantaneous results that can be provided by an ion implantation database, the Monte Carlo approach is impractical for situations such as an investigation of dozens of different implantation conditions.

On the other hand, the LSS (Lindhard, Scharff, and Schiøtt) theory can produce similar results by using the same electron and nuclear interactions as Monte Carlo simulation.<sup>4)–7)</sup> This theory is based on the idea of using probability functions instead of tracing the paths of individual ions as in Monte Carlo simulation. It provides an integral equation that should match the ion implantation profile. This equation can be computed almost instantaneously, but approximations must be made when it is being solved. So far, these approximations have lacked precision, and it has not been possible to reproduce the precision of Monte Carlo simulation. As a result, the LSS theory is currently not used in any simulator.

In response, my coworkers and I proposed an extended LSS theory that makes more accurate approximations and can perform nearly instantaneous calculations that give results of comparable accuracy to those of Monte Carlo simulation.<sup>8),9)</sup> Since it does not consider channeling phenomena that occur in crystalline substrates that are actually used in VLSI (verylarge-scale integrated circuit) processes, we later proposed another theory called the quasicrystal extended LSS theory (QCLSS), which is linked to the extended LSS theory by modeling these phenomena empirically.10,11 QCLSS can provide nearly instantaneous predictions of ion implantation profiles in cases where there is insufficient data. These predictions can be produced in roughly the same amount of time as needed to generate profiles based on information stored in a database.

In this paper, I first review the extended LSS theory and then describe the QCLSS theory.

## 2. Extended LSS theory

A schematic illustration of the implantation

range of ions with energy E according to the extended LSS theory is shown in **Figure 2**. We postulate a probability function that gives particular values to the range R along the beam direction and the projected ranges  $R_p$  and  $R_{\perp}$  perpendicular and parallel to the implantation plane. Here, I present an analysis for R that can be derived relatively simply and a simple explanation of how existing models can be extended. A detailed derivation can be found in Reference 8).

When ions are implanted with energy E, the probability that they will achieve a range Ris denoted by P(E,R), where the stochastic mean value of R is defined as

$$\langle R(E) \rangle = \int_0^\infty R P(E,R) dR$$
 (3)

For both nuclear and electron interactions, it has been shown that  $\langle R(E) \rangle$  should confirm to the following integral equation.<sup>1)</sup>

$$\frac{1}{N} = \int [\langle R(E) \rangle - \langle R(E - T_n) \rangle] d\sigma_n 
+ \int [\langle R(E) \rangle - \langle R(E - T_e) \rangle] d\sigma_e ,$$
(4)

where N is the atomic density of the substrate,  $T_n$  and  $T_e$  are the interaction energy losses, and



Definition of LSS theory parameters.

 $\sigma_n$  and  $\sigma_e$  are the corresponding collision crosssection areas. These integral equations cannot be solved directly, so approximations are used. For example, the term  $\langle R(E - T_n) \rangle$  representing the range of ions with energy of  $E - T_n$  is approximated by a certain number of terms from a Taylor expansion as

$$\langle R(E-T_n) \rangle \approx \langle R(E) \rangle - \frac{d \langle R(E) \rangle}{dE} T_n + \frac{1}{2} \frac{d^2 \langle R(E) \rangle}{dE^2} T_n^2 - \frac{1}{6} \frac{d^3 \langle R(E) \rangle}{dE^3} T_n^3,$$
 (5)

which can then be reduced to a differential equation. The solution  $\langle R(E) \rangle^{(1)}$  of the first-order Taylor expansion of integral equation (4) is given by

$$\frac{1}{N} = \frac{d\left\langle R(E)\right\rangle^{(1)}}{dE} \left[S_n(E) + S_e(E)\right].$$
(6)

The solution  $\langle R(E) \rangle^{\scriptscriptstyle (2)}$  of the second-order Taylor expansion is given by

$$\frac{1}{N} = \frac{d\left\langle R(E)\right\rangle^{(2)}}{dE} \left[S_n(E) + S_e(E)\right] \\ -\frac{1}{2} \frac{d^2 \left\langle R(E)\right\rangle^{(2)}}{dE^2} \left[\Omega_n^2(E) + \Omega_e^2(E)\right].$$
(7)

And the solution  $\langle R(E) \rangle^{(3)}$  of the third-order Taylor expansion is given by

$$\frac{1}{N} = \frac{d \left\langle R(E) \right\rangle^{(3)}}{dE} \left[ S_n(E) + S_e(E) \right] 
- \frac{1}{2} \frac{d^2 \left\langle R(E) \right\rangle^{(3)}}{dE^2} \left[ \Omega_n^2(E) + \Omega_e^2(E) \right] 
+ \frac{1}{6} \frac{d^3 \left\langle R(E) \right\rangle^{(3)}}{dE^3} \left[ \Lambda_n^3(E) + \Lambda_e^3(E) \right].$$
(8)

In the above differential equations,

$$S_{n,e}(E) = \int T_{n,e} d\sigma_{n,e} \tag{9}$$

$$\Omega_{n,e}^{2}(E) = \int T_{n,e}^{2} d\sigma_{n,e}$$
(10)

$$\Lambda^3_{n,e}(E) = \int T^{3}_{n,e} d\sigma_{n,e}.$$
(11)

These terms are calculated from the interaction potentials. It thus follows that the number of terms in the Taylor expansion corresponds to the order of the resulting differential equation. Mathematically, only the first-order differential equation has an analytical solution. The results obtained by solving the differential equation of this first-order Taylor expansion correspond to the analytical solution of the original LSS theory.<sup>1)</sup> From differential equation (6), which is derived from the first term of the Taylor expansion, we can derive the following well-known formula for  $\langle R(E) \rangle$ .

$$\langle R(E) \rangle^{(1)} = \frac{1}{N} \int_{0}^{E} \frac{dE}{S_n(E) + S_e(E)}$$
 (12)

However, the second-order differential equation (7) cannot be solved analytically. Therefore, the solution is assumed to be of the form

$$\left\langle R(E)\right\rangle^{(2)} = \left\langle R(E)\right\rangle^{(1)} + \Delta_R^{(2)}(E), \tag{13}$$

where  $\Delta_R^{(2)}(E)$  is a very small term. Substituting this into Equation (7), we obtain

$$\begin{split} \frac{1}{N} &= \frac{d\left[\left\langle R(E)\right\rangle^{(1)} + \Delta_R^{(2)}(E)\right]}{dE} \left[S_n(E) + S_e(E)\right] \\ &- \frac{1}{2} \frac{d^2 \left[\left\langle R(E)\right\rangle^{(1)} + \Delta_R^{(2)}(E)\right]}{dE^2} \left[\Omega_n^2(E) + \Omega_e^2(E)\right] \\ &\approx \frac{d\left\langle R(E)\right\rangle^{(1)}}{dE} \left[S_n(E) + S_e(E)\right] \\ &+ \frac{d\Delta_R^{(2)}(E)}{dE} \left[S_n(E) + S_e(E)\right] \\ &- \frac{1}{2} \frac{d^2 \left\langle R(E)\right\rangle^{(1)}}{dE^2} \left[\Omega_n^2(E) + \Omega_e^2(E)\right]. \end{split}$$
(14)

Here,  $\Delta_R^{(2)}(E)$  is ignored in the second-order differential terms. From the differential equation of the first-order Taylor expansion [Equation (6)], the term  $\frac{1}{N}$  on the left hand side cancels out the first term on the right hand side, so Equation (14) can be simplified to

$$0 = \frac{d\Delta_{R}^{(2)}(E)}{dE} \left[ S_{n}(E) + S_{e}(E) \right] -\frac{1}{2} \frac{d^{2} \langle R(E) \rangle^{(1)}}{dE^{2}} \left[ \Omega_{n}^{2}(E) + \Omega_{e}^{2}(E) \right].$$
(15)

The second term of Equation (15) can be calculated from the first-order perturbation solution, so the original second-order differential equation (7) becomes a first-order differential equation in  $\Delta_R^{(2)}$ , from which we can obtain the following analytical solution for  $\Delta_R^{(2)}$ .

$$\Delta_{R}^{(2)}(E) = \int_{0}^{E} \frac{1}{S_{n} + S_{e}} \frac{\Omega_{n}^{2} + \Omega_{e}^{2}}{2} \frac{d^{2} \langle R(E') \rangle^{(1)}}{dE'^{2}} dE'$$
(16)

The third-order solution can be written as

$$\left\langle R(E)\right\rangle^{(3)} = \left\langle R(E)\right\rangle^{(2)} + \Delta_R^{(3)}(E),$$
 (17)

and by applying a similar perturbation approximation, we arrive at the following formula.

$$\Delta_{R}^{(3)}(E) = \int_{0}^{E} \frac{1}{S_{n} + S_{e}} \left[ \frac{\Omega_{n}^{2} + \Omega_{e}^{2}}{2} \frac{d^{2} \Delta_{R}^{(2)}}{dE'^{2}} + \frac{\Lambda_{n}^{3} + \Lambda_{e}^{3}}{6} \frac{d^{3} \langle R(E') \rangle^{(2)}}{dE'^{2}} \right] dE' \quad (18)$$

Integral equations for  $R^m$ ,  $R_p^m$ , and  $R_{\perp}^m$  and their cross terms are derived in the same manner,



Figure 3 Relationship between  $\beta$  and  $\gamma^2$ .

and an analytical solution is obtained by applying the same perturbation approximation as for R. In this way, analytical solutions for the moments  $R_p$ ,  $\Delta R_p$ , and  $\gamma$  necessary for ion implantation profiles were derived for the first time.

For Pearson profiles, it is necessary to consider moments up to the fourth order  $\beta$ , but these cannot be derived from the LSS integral equation. A plot of  $\gamma$  and  $\beta$  values extracted from the results of Monte Carlo simulations in which B, As, and P ions were implanted into Si and Ge amorphous substrates at energies of 10, 20, 40, 80, 160, and 320 keV is shown in **Figure 3**. For these implantation conditions,  $\gamma^2$  and  $\beta$  lie more or less on a single line expressed by

$$\beta = 2.661 + 1.852\gamma^2. \tag{19}$$

Therefore, we chose to use this formula.

An As ion implantation profile evaluated according to LSS theory is compared with Monte Carlo simulation results in **Figure 4**. The conventional first-order model can provide an accurate representation of only the peak concentration position, while the profile shape differs significantly from the Monte Carlo simulation results.





Comparison of As implantation profiles obtained by Monte Carlo simulation and LSS theory with various levels of approximation.

Figure 4 shows the results of models obtained from the second- and third-order Taylor expansions. The second-order expansion produces a profile roughly similar to the Monte Carlo simulation results, while the third-order expansion matches it closely.

Monte Carlo simulation and extended LSS theory are compared in Figure 5 in terms of how the moments depend on the acceleration energy. The first-order model is sufficiently accurate for calculating  $R_p$ , but produces values for  $\Delta R_p$  that are approximately half as large as they should be. Eliminating the higher-order terms of the Taylor expansion corresponds to ignoring the large angular dispersion of the energy transfer quantities, so a qualitative match tends to be obtained.  $\Delta R_p$  is obtained with sufficient accuracy from the second-order model. This means that the second-order model is sufficient when Gaussian profiles are used. For  $\gamma$ , if we do not use at least the third-order model, then accurate results will not be obtained. This third-order model has been confirmed to match the results of Monte Carlo simulations with various other types of ions.

# 3. Quasi-crystal extended LSS theory

In practice, channeling phenomena occur in crystalline substrates used for VLSI processes, and the resulting profiles cannot be accurately represented with Pearson profiles. The implantation profiles in crystalline substrates are denoted by tail functions.<sup>12)-15)</sup> In a tail function, the parameters characteristic of crystalline materials are L, a, and  $\Phi_{chan}$ . We have proposed a quasi-crystal extended LSS theory (QCLSS) to represent these parameters empirically.<sup>11)</sup> These three parameters are introduced below.

### 1) Parameter L

L corresponds qualitatively to the channeling length measured from position  $R_p$ . Therefore, we postulate that L is associated with range  $R_{\max}$  in a manner expressed by

$$L = \xi_L \left( R_{\max} - R_p \right), \tag{20}$$

where  $\xi_L$  is a constant of proportionality and  $R_{\text{max}}$ is evaluated solely in terms of its interaction with the electron stopping power  $S_e$ :

$$R_{\max} = \int_{0}^{E} \frac{dE}{NS_{e}\left(E\right)}$$
 (21)

For a Si substrate, L is obtained by experiment. The values of  $R_{\text{max}}$  and  $R_p$  can be evaluated from the extended LSS theory. Values of  $\xi_L$  obtained by combining these formulas are shown in **Figure 6**, where  $E_1$  is the energy at which the electron and nucleus stopping powers are equal and  $\xi_L$  is not fixed but varies with the acceleration energy and mass numbers  $M_1$  and  $M_2$  of the ions



Figure 5

Comparison of various moments obtained by Monte Carlo simulation and LSS theory with various levels of approximation.

and substrate atoms, respectively. We have proposed that these parameters are related by the function

$$\xi_{L} = \begin{cases} \frac{0.18}{1 + 0.2 \frac{M_{2}}{2M_{1}}} \ln\left(1000 \frac{E}{E_{1}}\right) & \text{for } \frac{E}{E_{1}} \ge \frac{1}{1000} \\ 0 & \text{for } \frac{E}{E_{1}} < \frac{1}{1000} \end{cases}$$
(22)

and we have confirmed that this function is also applicable to Ge substrates.<sup>10),11)</sup> Equation (22) was not derived physically, but its qualitative significance is described below.

The coefficient before the ln term represents the channeling of paths where the ions are angled relative to the beam direction. The ln term indicates that there is a large probability of scattering by nuclei when E is less than  $E_1$ and that the channeling ions are distant from the atomic nuclei and have less stopping power than the average electron stopping power in the amorphous substrate, as shown in Equation (2), when E is greater then  $E_1$ .

2) Parameter a

Parameter a represents the shape of the channeling tail. Although the physical reason

is not clear, its energy dependence can be represented fairly accurately by the following formula for various ion implantation conditions in Si substrates, as shown in **Figure 7**.

$$a(E) = 1 + \frac{1}{1 + \left(\frac{E_1}{E}\right)^4}$$
(23)

We have confirmed that a follows this curve. Specifically, it takes a value of 1 (exponential profile) in the region where the nucleus stopping power is predominant and a value of 2 (Gaussian profile) in the region where the electron stopping power is predominant.

3) Parameter  $\Phi_{chan}$ 

The dose dependence of  $\Phi_{chan}$  for the implantation of P ions into a Si substrate is shown in **Figure 8**. This dependence is qualitatively described below.

 $\Phi_{chan}$  is thought to be associated with the accumulation of damage. When the dose  $\Phi$  is small, the regions of damage formed by ions can be regarded as being independent, so  $\Phi_{chan}$  is proportional to  $\Phi$ . As the dose increases, the damage regions start to overlap and eventually cover the entire surface. Thus, if we ignore



Figure 6 Variation of  $\xi_L$  with energy.



Figure 7 Variation of  $\alpha$  with energy.



Figure 8 Variation of channel dose  $\Phi_{chan}$  with dose.

the intermediate region, we can consider just two regions: a region where damage regions are formed independently by separate ions and a region where the damage regions become saturated. This is expressed by

$$\Phi_{chan} = \begin{cases} \Phi & \text{for } \Phi \leq \Phi_{chansat} \\ \Phi_{chansat} & \text{for } \Phi > \Phi_{chansat} \end{cases}$$
(24)

The saturation channel dose  $\Phi_{chansal}$  is represented by the following empirical formula derived from the profiles of B, As, and P in Si substrates:

$$\Phi_{chansat} = 3.3 \times 10^{13} \left(\frac{M_1}{M_2}\right)^{-1.06} \text{cm}^{-2}.$$
 (25)

Ge and  $Si_{1-x}Ge_x$  have been actively studied. In particular, since the composition ratio of  $Si_{1-x}Ge_x$  is also a parameter, this makes the corresponding database much larger. The results of applying the QCLSS theory to ion implantation profiles in  $Si_{1-x}Ge_x$  substrates with various different values of composition ratio x are shown in **Figure 9**. The theoretical results agree well with experimental data obtained by secondary ion mass spectrometry (SIMS).

In the QCLSS theory, the profiles in  $Si_{1-x}Ge_x$ 



Figure 9 Comparison of QCLSS theoretical results and SIMS experimental results for the effects of Ge content on B implantation profiles in SiGe.

are reproduced without fitting parameters from the relationships between the ions and Si/Ge atoms instead of using physical parameters for the  $Si_{1-x}Ge_x$  material itself. Therefore, we can expect to achieve similar levels of precision for any composition ratio x and not just for the specific values of x used in the experiments. We have demonstrated a database compatible with the application of this theory.<sup>10),11)</sup>

The parameter that determines the amorphous layer thickness is the through dose  $\Phi_{a/c}$ . This has been evaluated experimentally for Si and Ge. As shown in **Figure 10**,  $\Phi_{a/c}$  is expressed empirically in terms of the reduced mass  $M^{*}$ .<sup>10</sup>

$$\Phi_{a_{\lambda}} = 1.71 \times 10^{20} (M^*)^{-4.954} \text{ cm}^{-2}, \qquad (26)$$

where

$$M^* = \frac{M_1 M_2}{M_1 + M_2} \,. \tag{27}$$

For unknown ion/substrate combinations, this can be used to obtain a theoretical estimate of the amorphous layer thickness in the QCLSS theory.



Figure 10

Variation of through dose  $\Phi_{a/c}$  with reduced mass.

### 4. Conclusion

The QCLSS theory can be applied to any combination of ion implantation profiles in crystalline substrates. It covers a wide and practical range of implantation conditions. However, it lacks physical explanation, especially for parameters associated with the crystalline material, so there is still room for improvement.

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