

DISSERTATION

Miniaturization Problems in CMOS Technology: Investigation of Doping Profiles and Reliability

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Chapter 3

Simulation of Ion Implantation

There are two methods, the analytical and the Monte Carlo method, which are commonly used in modern TCAD tools for the simulation of ion implantation processes. Mainly increasing accuracy requirements due to the continued downscaling of device dimensions necessitate the transition from the simple analytical simulation of ion implantation to the particle-based Monte Carlo simulation for more and more applications. This chapter outlines fundamental modeling concepts required for the physically based simulation of doping profiles.

The basic idea of the analytical approach is that the doping profile can be approximated by a statistical distribution function [42, 45–47]. This function depends on a set of parameters which can be expressed by characteristic parameters of the implanted dopant distribution, for instance, the mean projected range R_p . The characteristic parameters, the so-called moments, can be extracted from Monte Carlo calculation results or from measured doping profiles. One-dimensional distribution functions can be combined to multi-dimensional profiles by a convolution method which takes a dose matching rule and numerical scaling into account. The analytical simulation of profiles requires relatively little CPU-time, even in two and three dimensions.

Due to the simplicity of the underlying concept, analytical implantation tools cannot accurately predict doping profiles for complex targets, for instance, multilayer targets or advanced devices with junction depths in the range of a few nanometers. In a compound target like SiGe, range predictions will be still worse, because the doping profiles additionally depend on the germanium fraction of the alloy. In contrast to that, the physics-based Monte Carlo method uses an atomistic approach and, therefore, is able to simulate the channeling effect and the accumulation of point defects during the implantation process in crystalline targets, as well as, e.g., shadowing effects arising from mask edges [15, 17, 42]. The Monte Carlo method imitates the implantation process by computing a large number of individual ion trajectories in the target. The three-dimensional device structures can be complex, with the only limitation being the computer memory size which must hold all the interaction details of the target. The underlying physical models are applicable for a wide range of implantation conditions without the need for an additional calibration.

One drawback of the Monte Carlo method are long computing times, which is the main reason why the use of Monte Carlo implantation tools is usually avoided in technology optimization. However, the capability of accurately predicting doping profiles can significantly reduce the development time for a new CMOS technology. In particular next generation technology nodes in the deep sub-100nm regime will put high demands on the accuracy of TCAD tools.

3.1 Physical Models

This chapter outlines the fundamental physics associated with the penetration of energetic ions into solids. The moving ions lose energy to the solid, create point defects, and after stopping they produce the final distribution in the target. The Monte Carlo modeling of ion implantation allows the incorporation of arbitrarily complex physical models at an atomic level.

3.1.1 Stopping of Ions in Solids

An ion which penetrates into a target loses energy constantly to the sea of electrons. It may go many atomic layers, before there is a collision with a target atom which is hard enough to displace that atom and create an interstitial and vacancy pair. The energy required to push a target atom just far enough from its lattice site so that it cannot pop back into its empty site is the *displacement energy* E_d , which is approximately 15eV in silicon. Fig. 3.1 shows different scenarios which can arise for ions shot into a crystalline target material.

Assume an incident ion with atomic number Z_1 and energy E has a collision with a target atom of atomic number Z_2 . After the collision the incident atom has energy E_1 and the struck atom has energy E_2 . A *displacement* occurs if $E_2 > E_d$, so that the atom Z_2 has enough energy to leave the site. A *vacancy* occurs if both $E_1 > E_d$ and $E_2 > E_d$. Both atoms then become moving atoms of the cascade. If $E_2 < E_d$, then the atom Z_2 does not have enough energy and it will vibrate back to its site releasing E_2 as *phonons*. If $E_1 < E_d$, $E_2 > E_d$, and $Z_1 = Z_2$, then the incoming atom remain at the site and the collision is called a *replacement collision* with E_1 released as phonons. This type of collision is common in single element targets with large recoil cascades. If $E_1 < E_d$, $E_2 > E_d$, and $Z_1 \neq Z_2$, then Z_1 becomes an *interstitial atom*.

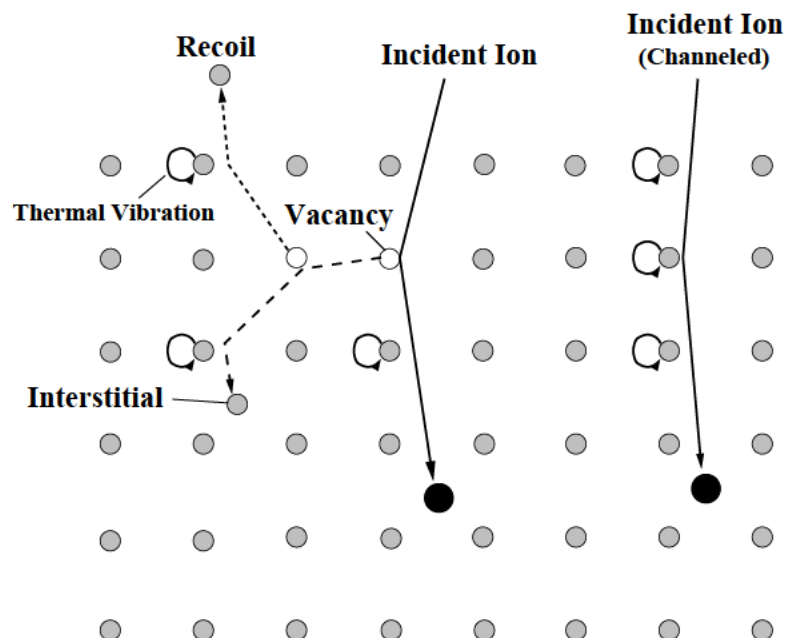


Figure 3.1: The incident ions 'make way' for themselves by knocking the target atoms out of their lattice sites, whereas recoil cascades are generated.

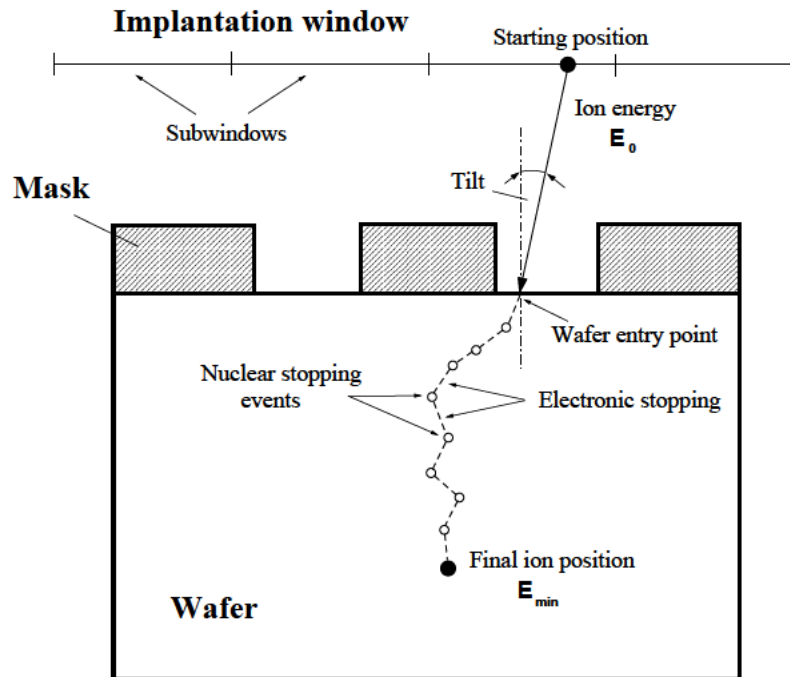


Figure 3.2: Principle of the Monte Carlo simulation method.

Ziegler et al. have demonstrated in [16] that the Monte Carlo calculation of ion trajectories is a very feasible way for accurately simulating the final ion distribution in crystalline silicon. Typically, Monte Carlo programs calculate a large number of individual particle trajectories in a target. Each particle history begins with a random starting position within the implantation window, a given direction, and an ion beam energy E_0 . Fig. 3.2 depicts that a particle changes its direction as a result of nuclear collision events and moves in straight free-flight-paths between collisions. The kinetic energy of the particle is reduced as a result of nuclear and electronic energy losses, and the history is terminated either when the energy drops below a specified value E_{min} or when the particle leaves the simulation domain. The rate at which an ion loses energy depends on the target atom density N_T (in cm^{-3}) and on the nuclear and electronic stopping powers $S_n(E)$ and $S_e(E)$ (in eVcm^2),

$$\frac{dE}{dx} = -N_T [S_n(E) + S_e(E)] . \quad (3.1)$$

The nuclear and electronic stopping powers are assumed to be independent and both are in general functions of energy.

3.1.2 Binary Collision Approximation

The interaction of the moving ion with an atomic nucleus of the target (nuclear stopping) can be treated as an elastic collision process, whereas the interaction with the electrons can be treated as an inelastic process without any scattering effects (electronic stopping). The binary collision approximation (BCA) assumes that only two charged particles, the moving ion (atomic number

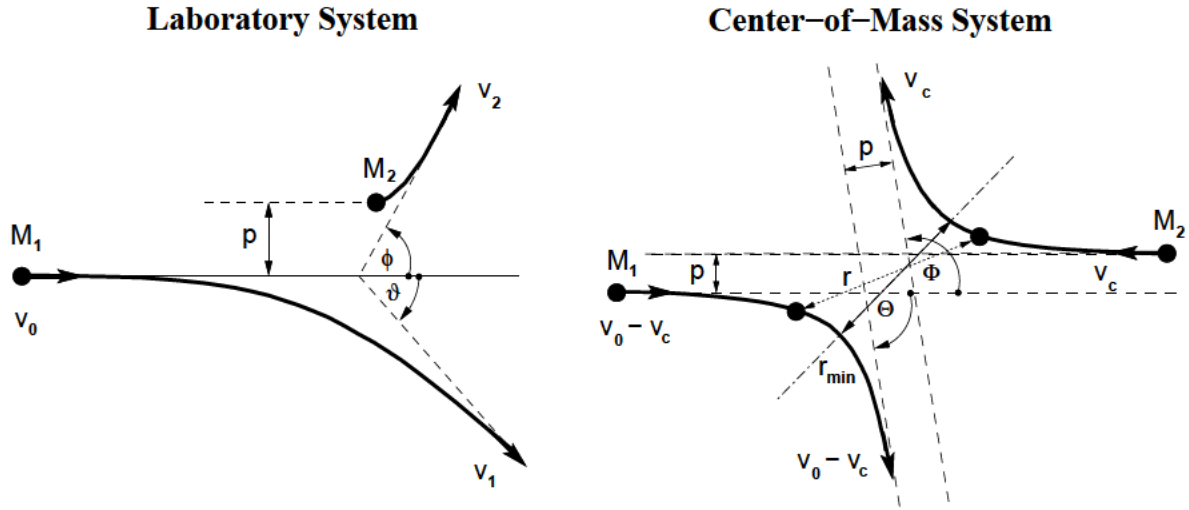


Figure 3.3: Classical two particle scattering process in the laboratory system and in the center-of-mass system.

Z_1 , mass M_1 , kinetic energy E_0) and one target atom (atomic number Z_2 , mass M_2) are involved in one scattering process. While the moving particle M_1 passes and is deflected, the stationary particle M_2 recoils or at least activates thermal lattice vibrations. The distance between the incident direction and the stationary particle is the impact parameter p . Fig. 3.3 shows the scattering variables in a two-body collision. The unknown velocities v_1 , v_2 and directions ϑ , ϕ from the incident direction after the collision event can be found from the conservation of energy (3.2) and momentum (3.3), (3.4) in the laboratory system.

$$\frac{1}{2} M_1 v_0^2 = \frac{1}{2} M_1 v_1^2 + \frac{1}{2} M_2 v_2^2, \quad (3.2)$$

$$M_1 v_0 = M_1 v_1 \cos \vartheta + M_2 v_2 \cos \phi, \quad (3.3)$$

$$0 = M_1 v_1 \sin \vartheta + M_2 v_2 \sin \phi. \quad (3.4)$$

For solving this two-body problem it is convenient to transform the scattering process from the laboratory coordinates to the center-of-mass coordinate (CM) system of ion and target atom. In Fig. 3.3, the CM system moves with constant velocity v_c to the right. Equation (3.5) defines v_c in such a way that the total momentum of the CM system becomes zero. The basic reason for this transformation is that the CM system reduces any two-body problem to a one-body problem, because the total momentum of the particles is always zero and the paths of the two particles are symmetric as shown in Fig. 3.3. The single particle has the initial kinetic energy E_c (3.6) and moves with a reduced mass M_c (3.7) and velocity v_c in a stationary potential $V(r)$ which is centered at the origin of the CM coordinates.

$$M_1 v_0 = (M_1 + M_2) \cdot v_c, \quad (3.5)$$

$$E_c = \frac{M_2}{M_1 + M_2} \cdot E_0, \quad (3.6)$$

$$M_c = \frac{M_1 M_2}{M_1 + M_2}. \quad (3.7)$$

Ziegler derives the particle scattering path by using Lagrangian mechanics in polar coordinates in [17]. The result is the famous “scattering integral” (3.8) which allows to evaluate the scattering angle Θ in the CM system. The angle Θ depends on the energy E_c , the interatomic potential $V(r)$, and the impact parameter p . The distance of minimum approach between the two particles is denoted as r_{min} (see Fig. 3.3), which is determined by the real root of the denominator in (3.8).

$$\Theta(p, E_c) = \pi - 2p \int_{r_{min}}^{\infty} \frac{dr}{r^2 \sqrt{1 - \frac{V(r)}{E_c} - \frac{p^2}{r^2}}} . \quad (3.8)$$

The inverse transformation leads to the scattering angle ϑ of the ion (3.9), the angle ϕ of the recoil (3.10), and the loss in energy of the ion, ΔE , which is equal to the recoil energy (3.11).

$$\tan \vartheta = \frac{\sin \Theta}{\frac{M_1}{M_2} + \cos \Theta} , \quad (3.9)$$

$$\cos \phi = \sin \frac{\Theta}{2} , \quad (3.10)$$

$$\Delta E = \frac{4 M_1 M_2}{(M_1 + M_2)^2} \cdot \sin^2 \frac{\Theta}{2} \cdot E_0 . \quad (3.11)$$

The scattering integral (3.8) cannot be calculated analytically for interatomic screening potentials and a numerical integration would be too time-consuming, since a simulated ion undergoes typically 100 to 1000 collisions. Solutions to this problem are to use an analytical approximation formula or a lookup table method. The used method is of critical importance in terms of accuracy and efficiency for the Monte Carlo calculation.

Interatomic Potential

The only non-trivial quantity in equation (3.8) is the interaction potential $V(r)$ between the ion and the target atom. The potential $V(r)$ is a repulsive Coulomb potential between the two positively charged nuclei, which is screened by surrounding electrons. The effect of the electrons is described by a dimensionless screening function $\Phi(r)$ which is less than one.

$$V(r) = \frac{Z_1 Z_2 q^2}{4 \pi \epsilon_0 r} \cdot \Phi(r) . \quad (3.12)$$

Z_1 and Z_2 are the atomic numbers of the involved particles, q is the elementary charge, and ϵ_0 is the dielectric constant. Well-known older screening functions are the Bohr potential [48], the Thomas-Fermi potential [49], the Moliere [50], and the Lenz-Jensen approximation [51]. Ziegler, Biersack, and Littmark performed the calculation of the interatomic potentials for 522 atom pairs. Based on these calculations they could derive the *universal screening potential* which is suitable for arbitrary atom pairs [17].

$$\Phi(x) = 0.1818 e^{-3.2x} + 0.5099 e^{0.9423x} + 0.2802 e^{-0.4029x} + 0.02817 e^{-0.2016x} , \quad (3.13)$$

$$x = \frac{r}{a_U} \quad \text{with} \quad a_U = 0.8854 \frac{a_0}{Z_1^{0.23} + Z_2^{0.23}} \quad (\text{\AA}) . \quad (3.14)$$

The equation (3.13) for the universal screening function $\Phi(x)$ consists of four fitted exponential terms and uses the scaled radius x as its argument. Ziegler, Biersack, and Littmark introduced

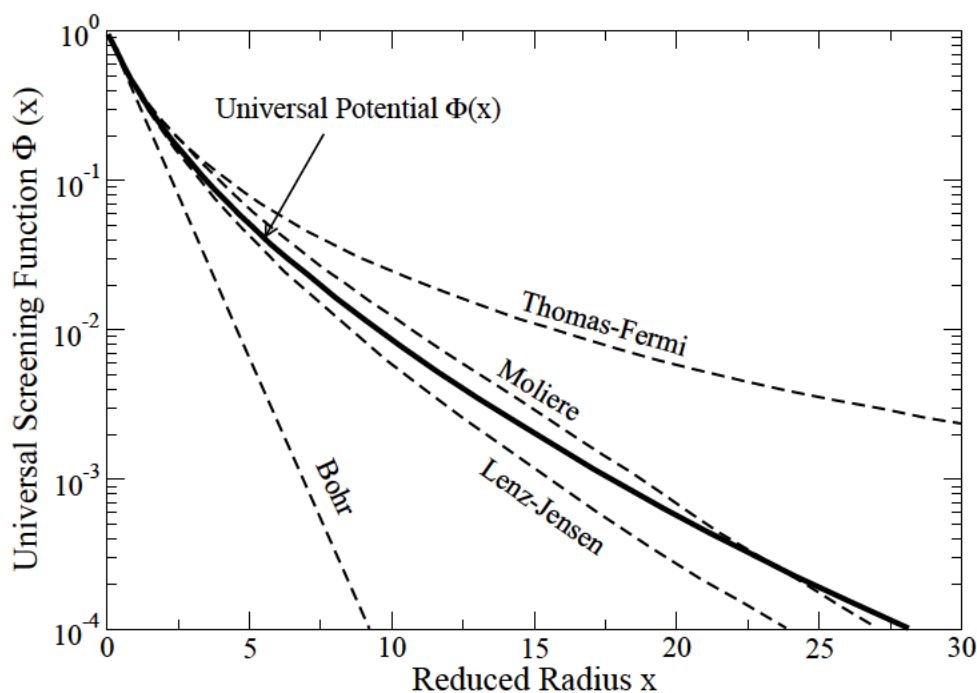


Figure 3.4: Universal screening potential and other approximations.

the scaled radius x according to (3.14), where r is the real radius, a_U is the universal screening length, and $a_0 = 0.529\text{\AA}$ is the Bohr radius. In the literature the universal potential is known as Ziegler-Biersack-Littmark (ZBL) potential.

Lattice Vibrations

Thermal vibrations displace the lattice atoms from their ideal lattice positions and they have been identified as source of the dechanneling mechanism, unless the crystalline target contains considerable damage [52, 53]. The approximation of a spherically symmetric Gaussian distribution $f(\Delta x, \Delta y, \Delta z)$ can be used to describe the displacement of atoms from their rest position.

$$f(\Delta x, \Delta y, \Delta z) = \frac{1}{\sqrt[3]{2\pi\sigma^2}} \cdot \exp\left(-\frac{\Delta x^2 + \Delta y^2 + \Delta z^2}{2\sigma^2}\right). \quad (3.15)$$

The standard deviation σ of the atomic displacement $\sqrt{\Delta x^2 + \Delta y^2 + \Delta z^2}$ from the rest position can be adjusted according to the *Debye theory* [54], which is in good agreement with X-ray diffraction experiments [55]. This theory uses an empirical parameter, the Debye temperature

Method	Θ_D (K)	σ (Å) at 300K
Specific heat	645	0.065
Channeling experiment	490	0.083
Simulation of ion implantation	450	0.090

Table 3.1: Debye temperature Θ_D and corresponding average vibration amplitude σ .

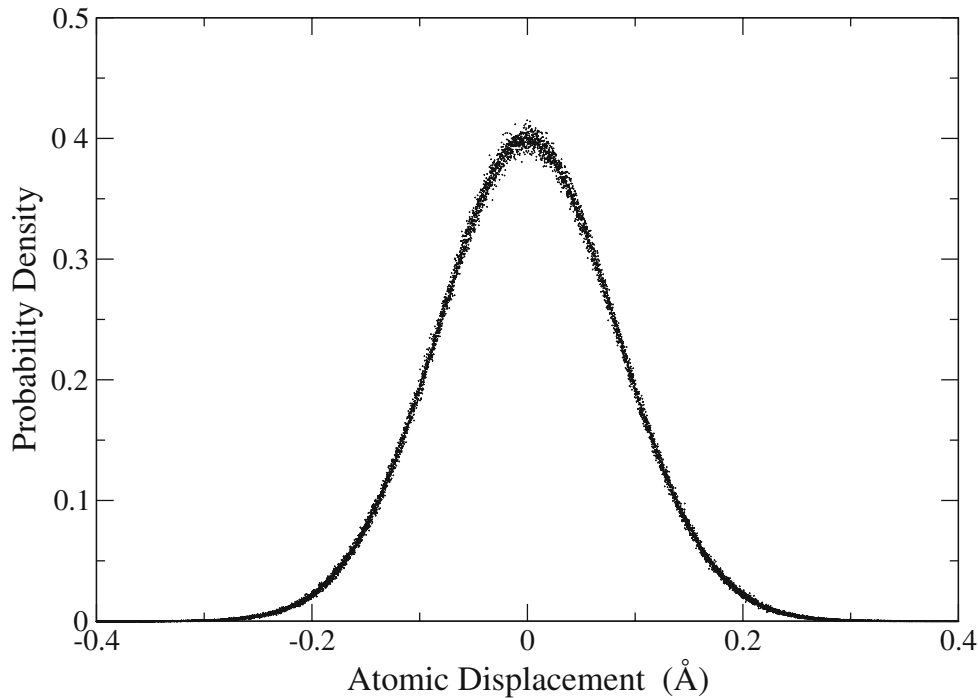


Figure 3.5: Gaussian distribution of the atom vibration amplitudes in MCIMPL-II.

Θ_D , which can be determined with the aid of specific heat measurements [56], by channeling experiments [57], or by comparison of simulated profiles with SIMS data [58], as summarized in Table 3.1 for silicon at a wafer temperature of 300K.

Fig. 3.5 shows a sample size of 10000 atom vibration amplitudes which are used for the Monte Carlo calculation of ion trajectories in MCIMPL-II. The simulator uses an average vibration amplitude $\sigma = 0.083\text{\AA}$ according to a Debye temperature of 490K to model the motion of the atoms in silicon. Note that the random variates from the Gaussian distribution presented in Fig. 3.5 are derived from a random-number generator which produces uniformly distributed random variates in the interval $[0, 1]$. The fast *polar method* is used to generate originally random variates in pairs from the normal distribution contained in the interval $[-\infty, \infty]$ with mean $\mu = 0$ and standard deviation $\sigma = 1$, as described in [59].

3.1.3 Electronic Stopping Power

The electronic stopping power of the target is complicated and not fully understood up to now, since several physical processes contribute to the electronic energy loss [16]:

- Direct kinetic energy transfer to target electrons, mainly due to electron–electron collisions.
- Excitation of band- or conduction-electrons (effect on weakly bound or non-localized target electrons).
- Excitation or ionization of target atoms (effect on localized electrons).
- Excitation, ionization, or electron-capture of the projectile.

The electronic stopping models used for Monte Carlo implantations into silicon can be classified as non-local or local. While non-local models assume that the electronic energy loss is independent of the relative positions of the ion and the target atoms [16, 60], local models take such a dependence into account, using either the impact parameter of the collisions [61] or the local electron concentration along the ion path [62]. Hobler et al. proposed an empirical electronic stopping model for the implantation into crystalline silicon [63], which is based on the Lindhard electronic stopping model and an impact parameter approach.

In the Hobler model the total electronic energy loss ΔE is composed of a non-local part which dominates in the case of large impact parameters (channeling ions) and a local part which is considered at every collision.

$$\Delta E = \Delta E_{nl} + \Delta E_{loc} . \quad (3.16)$$

The non-local part ΔE_{nl} is proportional to the path length ΔR traveled by the ion between two nuclear collision events in a target material with atomic density N .

$$\Delta E_{nl} = N S_e \Delta R \cdot \left[x_{nl} + x_{loc} \left(1 + \frac{p_{max}}{a} \right) \exp \left(-\frac{p_{max}}{a} \right) \right] . \quad (3.17)$$

The local part ΔE_{loc} is exponentially proportional to the impact parameter as proposed by Oen and Robinson in [61].

$$\Delta E_{loc} = x_{loc} \frac{S_e}{2 \pi a^2} \exp \left(-\frac{p}{a} \right) . \quad (3.18)$$

The term in equation (3.17) containing x_{loc} approximates the local electronic energy loss due to collisions with impact parameters larger than p_{max} . The electronic stopping power S_e is assumed to be velocity proportional in (3.19). Lindhard et al. proposed the expression (3.20) for the coefficient k [60], which considers the properties of the ion species and the target material.

$$S_e = k_{corr} k \sqrt{E} , \quad (3.19)$$

$$k = 8 \pi \hbar a_0 \sqrt{2} \cdot \frac{Z_1^{\frac{7}{6}} Z_2}{\left(Z_1^{\frac{2}{3}} + Z_2^{\frac{2}{3}} \right)^{\frac{3}{2}} \sqrt{M_1}} . \quad (3.20)$$

Z_1 and M_1 are the charge and the mass of the implanted particle, Z_2 is the atomic charge in single-element targets, a_0 is the Bohr radius, and E the kinetic energy of the particle. The *Lindhard correction factor* k_{corr} is used to empirically adjust the strength of the electronic stopping. The *screening length* a is expressed by the value $\frac{a_U}{0.3}$ in [61], where a_U is the screening length used for the interatomic screening potential in (3.14). Hobler et al. multiplied the length by a *screening pre-factor* f according to

$$a = f \cdot \frac{a_U}{0.3} . \quad (3.21)$$

The parameters x_{nl} and x_{loc} are the non-local and the local fraction of the total electronic stopping power which requires the relation (3.22) to hold.

$$x_{nl} + x_{loc} = 1 . \quad (3.22)$$

Dopant species	Energy limit (MeV)
Arsenic	194.1
Boron	2.2
Phosphorus	28.0

Table 3.2: Energy limits for the velocity proportional electronic stopping power [42].

The non-local fraction x_{nl} depends on the energy E and can be modeled by a power law,

$$x_{nl} = y_{nl} \cdot E^q, \quad (3.23)$$

where the empirical parameters y_{nl} and q are the *non-local pre-factor* and *non-local power*. Lindhard indicated that the electronic stopping power S_e is only proportional to the ion velocity up to a maximal energy which is shown for some important ion species in Table 3.2.

The drawback of the empirical Hobler model is that many parameters have to be fitted, in particular for crystalline materials. Hobler has demonstrated for boron implantations in crystalline silicon [64] that the accuracy of the empirical model is better than that of the purely electron-density-based model. The Hobler model requires less additional computational effort since the impact parameter which is used by the BCA algorithm to determine the nuclear energy loss can be applied to calculate the electronic energy loss. Both the nuclear and the electronic stopping powers depend on the energy and contribute to the total stopping. Fig. 3.6 demonstrates the slowing down of boron ions with an initial energy of 40keV. Note that the nuclear stopping has its maximum at 3keV and the electronic stopping dominates for higher energies.

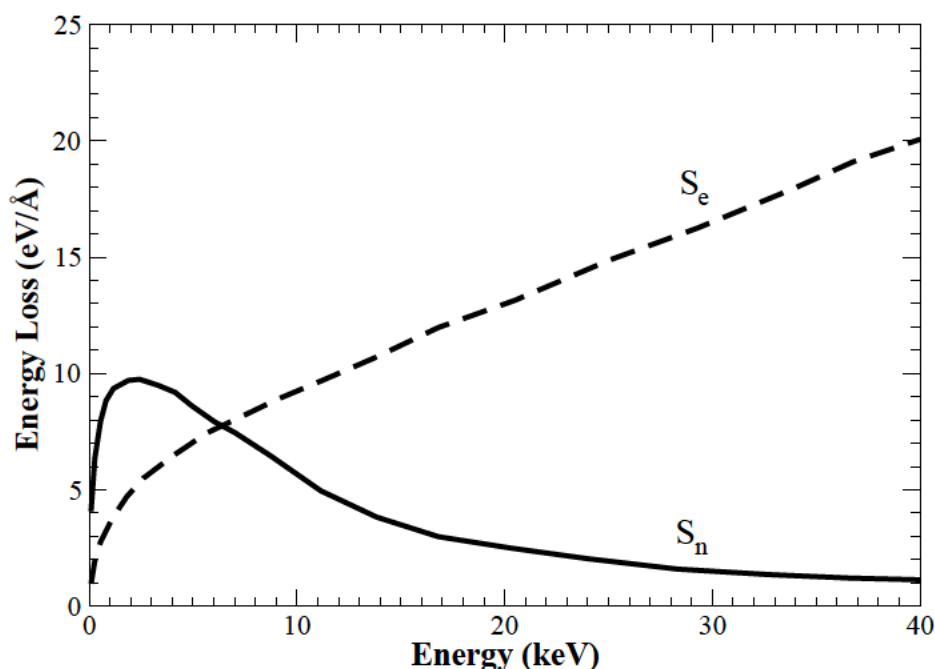


Figure 3.6: Average nuclear and electronic stopping powers $S_n(E)$ and $S_e(E)$ for a 40keV boron implantation into silicon, analyzed with MCIMPL-II.

Summarizing, it can be said that the electronic stopping is dominant for higher energies, lighter ions, and under channeling conditions.

3.1.4 Damage Generation

The nuclear stopping process of energetic ions in crystalline targets displaces atoms from their lattice sites. If the ion implantation dose is high enough, a continuous amorphous layer can be formed in a silicon wafer beneath the surface. A so-called *Frenkel pair* or *Frenkel defect* is formed when a displaced target atom forms an interstitial and leaves a vacancy behind at its original lattice site [29]. The point defects in the target accumulate during the implantation process and influence the trajectories of subsequently implanted ions. In addition, the generated point defects cause a transient enhanced diffusion (TED) effect of dopant atoms during the RTA annealing process. Due to the fact that it is difficult to measure damage concentrations in crystals, the simulation of implantation induced point defects as well as the identification of amorphized regions in the device are very beneficial for modern CMOS process engineering.

The generation of point defects can be modeled by the analytical *modified Kinchin-Pease model* or by the computationally intensive *Follow-Each-Recoil method*.

Modified Kinchin-Pease Model

The modified Kinchin-Pease model assumes that the number of displaced atoms (Frenkel pairs) in a collision cascade is a function of the transferred energy ΔE from the ion to the primary recoil atom [65, 66]. In this theory, the defect producing energy E_ν is obtained from the kinetic energy of the primary knock-on recoil, reduced for the electronic loss by all recoils comprising the cascade. The recoils themselves are not individually followed in this computationally fast approach. It was found in [63] that experimental results can be well described by the modified Kinchin-Pease model together with a model for point defect recombination. The defect recombination which takes place in a recoil cascade can be modeled empirically by using the local point defect concentration.

The electronic energy loss is calculated according to Lindhard's theory [67] using the analytical approximation of Robinson [68] to the universal function $g(\varepsilon_d)$. The "damage energy" E_ν is calculated from the initial energy ΔE of the primary recoil by

$$E_\nu = \frac{\Delta E}{1 + k_d \cdot g(\varepsilon_d)} , \quad (3.24)$$

$$k_d = 0.133745 \cdot \frac{Z^{\frac{2}{3}}}{M^{\frac{1}{2}}} , \quad (3.25)$$

$$g(\varepsilon_d) = 3.4008 \varepsilon_d^{\frac{1}{6}} + 0.40244 \varepsilon_d^{\frac{3}{4}} + \varepsilon_d , \quad (3.26)$$

$$\varepsilon_d = 0.0115 (\text{eV})^{-1} \cdot Z^{-\frac{7}{3}} \cdot \Delta E , \quad (3.27)$$

where Z and M are the atomic number and mass of the recoil atoms, and the reduced energy ε_d is a dimensionless quantity. The number of generated Frenkel pairs ν_{gen} in a recoil cascade can be calculated from the energy E_ν using a constant displacement efficiency $\kappa = 0.8$ in the

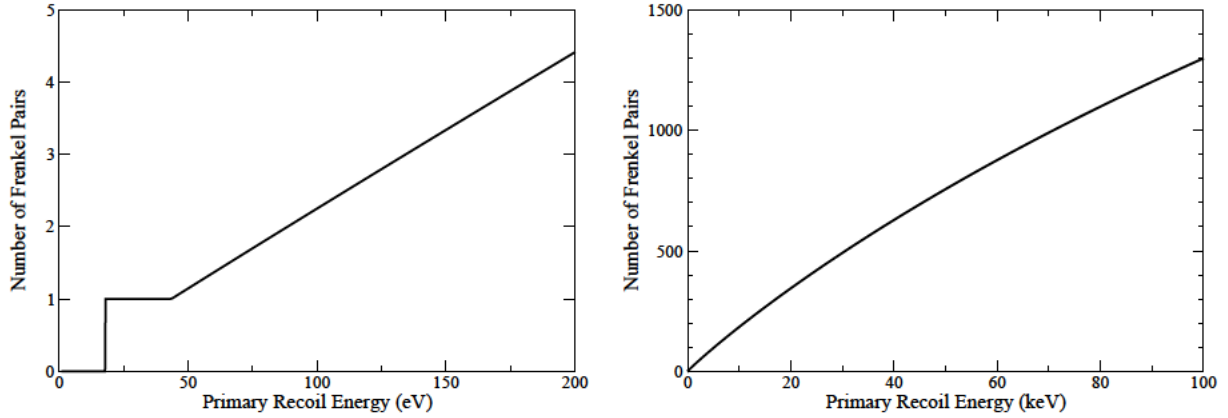


Figure 3.7: Number of Frenkel pairs generated by a primary knock-on atom in silicon assuming $E_d = 15\text{eV}$, plotted for two different energy ranges.

modified Kinchin-Pease damage generation formula, given by

$$\nu_{gen} = 0 \quad \text{for } E_\nu < E_d, \quad (3.28)$$

$$\nu_{gen} = 1 \quad \text{for } E_d \leq E_\nu < 2.5 \cdot E_d, \quad (3.29)$$

$$\nu_{gen} = \frac{\kappa E_\nu}{2 E_d} \quad \text{for } E_\nu \geq 2.5 \cdot E_d. \quad (3.30)$$

The primary recoil atom produces only lattice vibrations if the damage energy E_ν is below the displacement energy E_d . The curves in Fig. 3.7 show the number of produced point defects ν_{gen} for damage cascades in silicon as a function of the transferred energy ΔE without considering pre-existing point defects, as calculated by the modified Kinchin-Pease model.

The recombination between interstitials and vacancies has to be taken into account in order to realistically calculate the produced amount of point defects [63]. The recombination within a collision cascade can be described by a constant fraction f_{rec} of Frenkel pairs surviving the spontaneous self-annealing process due to beam-induced heating of the wafer. If ν_{gen} is the number of point defects generated in a recoil cascade, then the average number of point defects surviving recombination within the cascade is given by $\nu_{gen} \cdot f_{rec}$. The correction parameter f_{rec} depends on the ion species since heavy ions produce damage more efficiently by overlapping of large cascades than lighter ions. A light ion produces typically small cascades due to small transfer energies, where recombination becomes more likely. The recombination with point defects of previously generated damage cascades can be included by an additional factor f_{pre} which depends on the recombination probability p_{rec} defined in (3.33). The average number of stable point defects ν_{st} is linked to the number of generated point defects ν_{gen} according to

$$\nu_{st} = \nu_{gen} \cdot f_{rec} \cdot f_{pre}, \quad (3.31)$$

$$f_{pre} = (-1)p_{rec}^2 + (+1)(1 - p_{rec})^2 = 1 - 2p_{rec}, \quad (3.32)$$

$$p_{rec} = \frac{N_V + N_I}{4 N_{sat}}. \quad (3.33)$$

The factor f_{pre} is obtained by considering the four possible cases for a Frenkel pair having survived recombination within the recoil cascade. In the first case, the generated Frenkel pair (both components) recombines with a pre-existing Frenkel pair, which reduces the total number of Frenkel pairs by one. The probability for this process is p_{rec}^2 . In the second case, which occurs with the probability $(1 - p_{rec})^2$, the generated Frenkel pair survives, resulting in an additional Frenkel pair. In the third and forth case either the interstitial or the vacancy survives while the other one recombines, resulting in no change of the total Frenkel pair number. Adding this changes with their probabilities yields $(1 - 2p_{rec})$ as the net average fraction of point defects surviving recombination with previously generated point defects. The recombination probability p_{rec} is proportional to the concentration of already existing vacancies and interstitials and it has a species dependent saturation level N_{sat} as given in (3.33). Assuming equal local concentrations of vacancies and interstitials, $N_V = N_I$, the probability p_{rec} has to be equal to the probability of survival $(1 - p_{rec})$ at the saturation concentration, leading to $p_{rec} = 0.5$ for $N_V = N_{sat}$. Substituting (3.32) and (3.33) into (3.31) and assuming $N_V = N_I$, the number of stable point defects ν_{st} are finally obtained by

$$\nu_{st} = \nu_{gen} \cdot f_{rec} \cdot \left(1 - \frac{N_V}{N_{sat}}\right). \quad (3.34)$$

In principle, the displaced atoms can be placed on tetrahedral interstitial sites (tetrahedral interstitial model) [69], on random positions (random model) [70], or on random positions within spheres around the tetrahedral interstitial sites. In [63], Hobler et al. placed the silicon interstitials on random positions within the maximum impact parameter p_{max} from the ion path in the plane perpendicular to the ion's direction of motion. From the comparison of simulations and experiments they found that the silicon interstitials are rather randomly distributed in the crystal lattice than located at tetrahedral interstitial sites.

Follow-Each-Recoil Method

The modified Kinchin-Pease model can only estimate the number of vacancies produced in a collision cascade and, therefore, this damage model assumes the same local concentration for the interstitials. There is a small offset between the local vacancy and interstitial concentrations, since a vacancy stays at the position where the recoil has been generated whereas an interstitial typically comes to rest somewhere slightly deeper in the target. This results in an interstitial profile with its peak at a slightly deeper position than the peak of the corresponding vacancies. The Follow-Each-Recoil method calculates the trajectories of all recoiling atoms in a collision cascade. In the full cascade simulation, the nuclear and electronic loss of a recoil is calculated in the same way as for an implanted ion just with different physical properties. This approach requires a tremendous computational effort, since a cascade can be in the range of thousand displaced atoms in silicon, as demonstrated for high energies of the primary recoil in the right plot of Fig. 3.7. The advantage of the Follow-Each-Recoil method is that the location of the interstitials can be accurately calculated as well as pollution effects can be estimated. A pollution occurs in a semiconductor device, for instance, if implanted ions push oxygen atoms from an isolation layer into the active area of the device [71].

3.2 Monte Carlo Implantation with MCIMPL-II

For a rigorous study of doping profiles for advanced semiconductor devices it is mandatory to consider crystalline materials and arbitrary three-dimensional geometries. The Monte Carlo ion implantation simulator MCIMPL-II was used for the simulation of doping profiles throughout this thesis. Therefore, a brief description of the simulator is presented in this section. The simulator has been developed on the basis of MCIMPL [15] at the Institute for Microelectronics. In contrast to its predecessor, MCIMPL-II has a flexible object-oriented architecture and uses the functionality of the Wafer-State-Server library [72]. MCIMPL-II can be easier extended to new materials, while MCIMPL was originally just designed for the implantation into silicon. Hobler started the project in 1986 by implementing the fundamental physical models and by calibrating the models for the most important dopant species used in silicon technology [73]. Stippel extended the simulator to three dimensions [74] and Bohmayr implemented the Trajectory-Split method [75]. Hössinger included the Follow-Each-Recoil method in MCIMPL [42]. When he designed MCIMPL-II, he replaced the simple data management of MCIMPL by a better handling of the simulation data for a fast point location in heavily non-planar device structures [76]. In the scope of this work, the postprocessing of raw Monte Carlo data in MCIMPL-II was improved, and a grid-generator was implemented to allow a fast simulation of one-dimensional doping profiles which is particularly necessary for calibration purposes.

3.2.1 Basic Features and Principle of Operation

The current status is that MCIMPL-II can be used for one- and three-dimensional implantation applications. Two-dimensional applications can be modeled by using two-and-a-half dimensional device geometries with a small depth dimension. The simulator can handle arbitrarily shaped device structures including overhang structures. The simulated structure can be composed of several amorphous and crystalline material segments. Various amorphous materials can be simulated, for instance, SiO_2 , Si_3N_4 , TiN , or TaN , which are typically used in CMOS processing. Several crystalline material segments can also be used in one simulation domain with the restriction that the crystal orientation has to be identical in all segments. In this work the simulator has been extended from crystalline silicon to $\text{Si}_{1-x}\text{Ge}_x$ alloys of arbitrary germanium content in the range from silicon to germanium. Polycrystalline materials are treated as amorphous materials in which the crystalline structure of the grains is neglected. This is not really a restriction, since low-resistivity polysilicon for gates or interconnects is usually processed by deposition of amorphous silicon, followed by high-dose ion implantation doping, and finishing annealing.

The Monte Carlo calculation of ion trajectories in crystalline targets uses substantially only two random processes. The first one is applied to achieve equally distributed starting points of ion trajectories within the implantation window and the second one is used to imitate the thermal vibrations of the target atoms. While the simulated ion moves through the target the simulator uses locally either a crystalline or an amorphous model for searching the next collision partner of the ion. The application of the amorphous model in crystalline targets is performed with a certain probability which depends on the amount of already generated damage in the crystal. Thus the transition from the crystalline to the amorphous state of a region is taken into account, which is caused by the accumulation of point defects during the implantation process. Note that the Monte Carlo simulation of ion implantation without consideration of

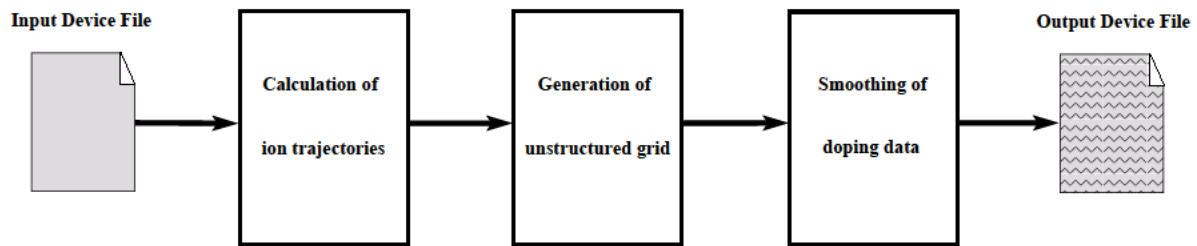


Figure 3.8: Schematic diagram of the Monte Carlo simulation with MCIMPL-II.

damage is a static problem where the passage of time plays no role. In consideration of damage accumulation over time the Monte Carlo simulation becomes dynamic. In order to improve the performance, the simulator uses histogram cells aligned on an orthogonal grid to count the number of implanted ions and of generated point defects. The doping or damage concentration within a cell is obtained by the number of particles contained in the cell divided by the volume of the cell. However, the ion implantation process is accurately simulated by computing a large number of individual ion trajectories in the target. Being based on appropriately scaled random numbers, the results obtained with the Monte Carlo method are never exact, but they converge to the characteristics of the underlying physical models by increasing the number N of simulated ions. The statistical error of Monte Carlo results vanishes for a sample size $N \rightarrow \infty$.

The principle of simulator operation can be grouped into the following three sections:

- Initialization of the internal data structures
- Physical Monte Carlo simulation of ion trajectories
- Transfer of the doping data to an unstructured grid

The input device structure for implantation is provided as a file in the WSS (Wafer State Server) format [77], which contains all geometry and material information of the simulation domain. Thereby the dimension of the simulation is specified by the input WSS file. Additionally, the input file can contain implantation data from previous implantation steps. The implantation conditions and simulation parameters, for instance, the desired number of simulated ions are specified by user defined command-line parameters. A description of the simulator command-line interface is provided in [42]. Fig. 3.8 shows schematically the simplified simulation data flow from the input file to the output file. The simulation is started by initializing the histogram for the Monte Carlo simulation. When histogram cells are set up, they are initialized with data from previous implantation steps and they are continuously updated when damage is generated by an ion. Thereby damage accumulation from several ion implantation steps is automatically considered as well as damage accumulation within a single implantation step. The incoming dopant ions are slowed down due to the nuclear and electronic stopping power of the target material. The final position of an implanted ion is reached where it has lost its kinetic energy. After performing the Monte Carlo calculation of all ion trajectories, the dopants, vacancies and interstitials are stored in histograms. A sophisticated smoothing algorithm based on the Bernstein polynomial approximation [78] is applied in order to reduce the statistical fluctuation of raw Monte Carlo results. The smoothed data are then translated from the internal orthogonal

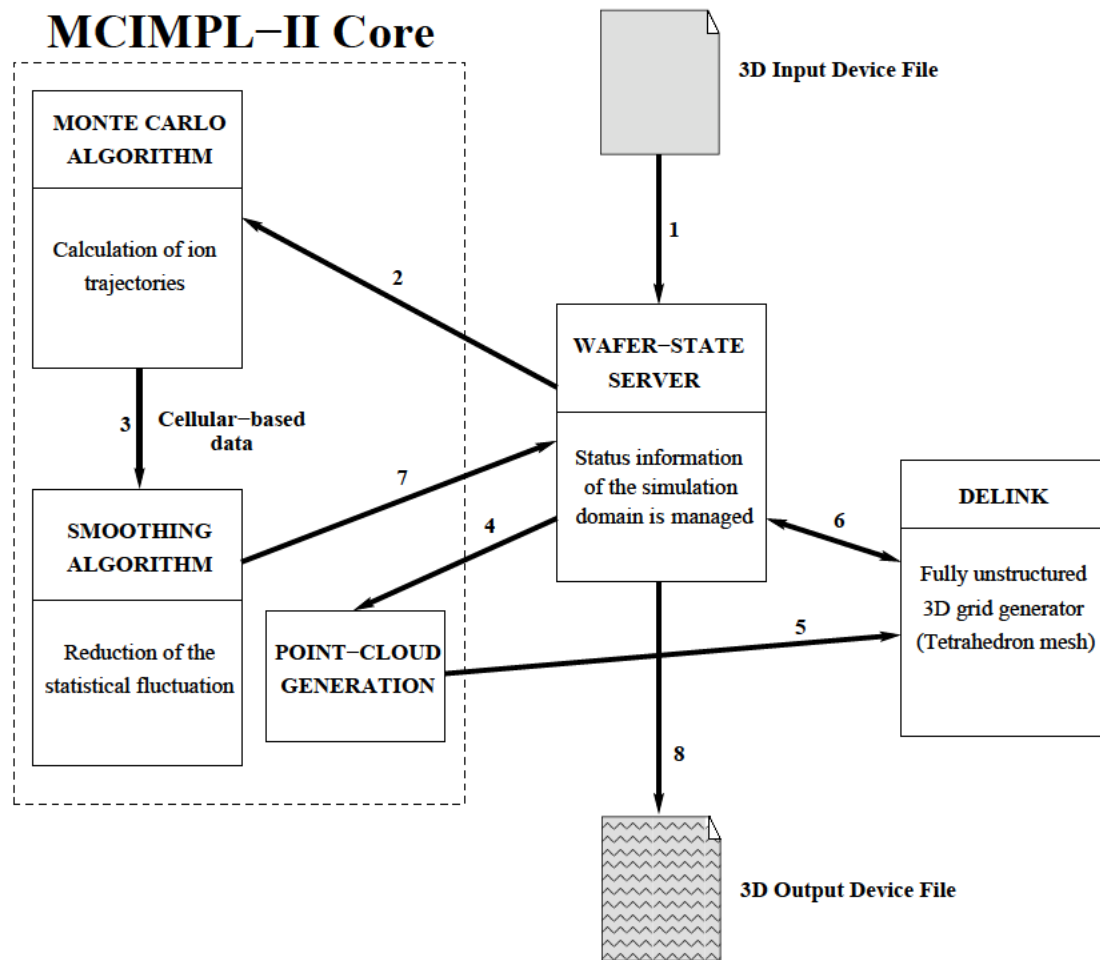


Figure 3.9: Flow of data between the linked software components of MCIMPL-II, consisting of MCIMPL-II Core, Wafer-State-Server, and DELINK.

grid to an unstructured destination grid. The resulting output file contains the smoothed doping and damage profiles which include the implantation results of all already performed implantation steps. This WSS file can then be visualized for analysis purposes and/or it can be used as input file for the subsequent simulation of annealing processes.

The simulator makes use of the Wafer-State-Server functionality not only for reading a WSS file (geometry and attributes request) or WSS file writing (attributes update), but there is also a continuous interaction during the simulation. When an ion moves through the simulation domain, the simulator requires the material type information at the current position of the ion in order to select the appropriate model for the next collision event. The Wafer-State-Server performs a point location and delivers the desired information to the simulator core unit. Lastly, the Wafer-State-Server provides a gridder interface to integrate different grid generators with the simulator. Fig. 3.9 shows the data flow during the three-dimensional simulation of ion implantation in a more detailed way including the Wafer-State-Server and the three-dimensional unstructured grid generator DELINK [79]. A brief description of the Wafer-State-Server based simulation environment and the WSS file format is provided in Appendix A.

3.2.2 Calculation of Ion Trajectories

The core of the simulator performs the calculation of ion trajectories in a three-dimensional manner independent of the dimension of the simulated device structure. An ion trajectory is simulated by successively applying nuclear and electronic stopping processes that slow down the ion motion (as described in Section 3.1). Therefore it is necessary to locate atomic nuclei of the target which collide with the ion projectile. After finding the location of the next collision partner, the parameters of the nuclear and electronic stopping models are determined. The partner dependent parameters for the stopping models are the mass and charge of the target atom, the impact parameter, and the free flight path length between two nuclear collisions. Several physical and numerical models are involved in the trajectory calculation. Each material segment of the simulation domain has assigned its own set of models.

A model set consists primarily of four models selected from the following model classes:

- Partner selection model
- Nuclear scattering model
- Electronic stopping model
- Damage generation model

Initial Conditions

The starting points of the ions are equally distributed within a rectangular implantation window lying in a plane somewhat above the surface of the simulation domain. But instead of selecting the starting points completely randomly, the implantation window is divided into equally sized subwindows and one ion starts from each subwindow. The position of the ion within the subwindow is randomly chosen. This procedure for determining the starting points provides a better statistical equidistribution of the points. Another advantage is that this procedure allows to define a time step for a transient simulation in a very convenient way, which is required for the parallelization of the trajectory calculation. The calculation of the ion trajectories for all subwindows is performed within one time step.

The initial momentum of an ion is determined by the implantation conditions *energy*, and *tilt and twist angles*. In addition a *divergence of the ion beam* can be specified. When a three-dimensional simulation is performed, the simulator assumes that the wafer rotation (twist angle) of 0° is parallel to the x-axis, which means according to the definition of the tilt and twist angle (see Section 2.2.3) that the y-axis is parallel to the primary flat of the wafer.

Selection of Collision Partners

Two different selection strategies exist for crystalline and amorphous materials. In crystalline materials the atoms are placed around their crystal lattice sites due to thermal vibrations. The selection of the target atom which takes part in the next nuclear scattering process is depicted in the left sketch of Fig. 3.10. The ion is located at the beginning of the free flight path L . The actual collision partner among the potential atoms in the direction of motion is that atom which

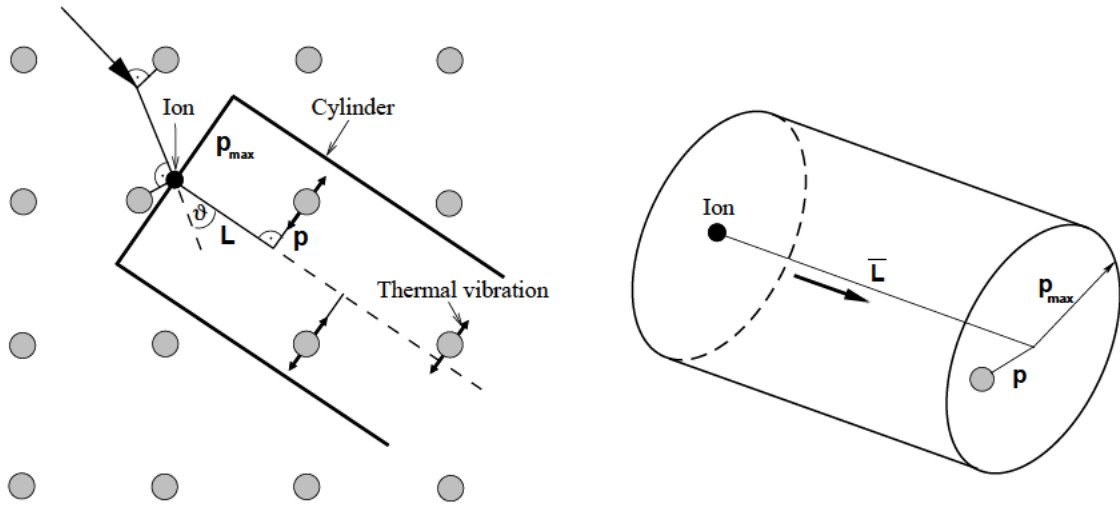


Figure 3.10: Searching for the next collision partners in crystalline materials (left) and cylinder which determines the partner in amorphous targets (right).

leads to the smallest positive free flight path length with an impact parameter p smaller than p_{max} . The maximum impact parameter p_{max} is in the order of magnitude of half of the lattice constant. If two collision partners would lead to almost the same free flight path lengths, the two partners are treated simultaneously based on the BCA method. In this multiple collision the sum of the momenta transferred to the target atoms in individual binary collisions with neighboring atoms is assumed to be the total momentum transferred to the crystal.

The amorphous partner selection model is based on the fact that the atoms in amorphous materials are approximately equally distributed. Therefore only the material density has to be considered by a cylinder with a radius of the maximum impact parameter p_{max} and a length of the average free flight path $\bar{L}$ (as shown in Fig. 3.10) which contains one target atom. The average free flight path is defined according to

$$p_{max}^2 \cdot \pi \cdot \bar{L} = \frac{1}{N_T}, \quad (3.35)$$

where N_T is the atom density in the target. This model uses a constant flight path length $\bar{L}$ and the collision partner is placed in a circular area with the radius p_{max} on a plane perpendicular to the direction of motion with the distance $\bar{L}$ from the actual ion position. The actual amorphous impact parameter p is calculated by using the realization X_i from the set of uniformly distributed random numbers $X_1, \dots, X_n$ in the interval $[0, 1]$ according to

$$p = p_{max} \cdot \sqrt{X_i}. \quad (3.36)$$

The maximum impact parameter p_{max} is determined only by the target atom density:

$$p_{max} = \frac{1}{\sqrt[3]{N_T}}. \quad (3.37)$$

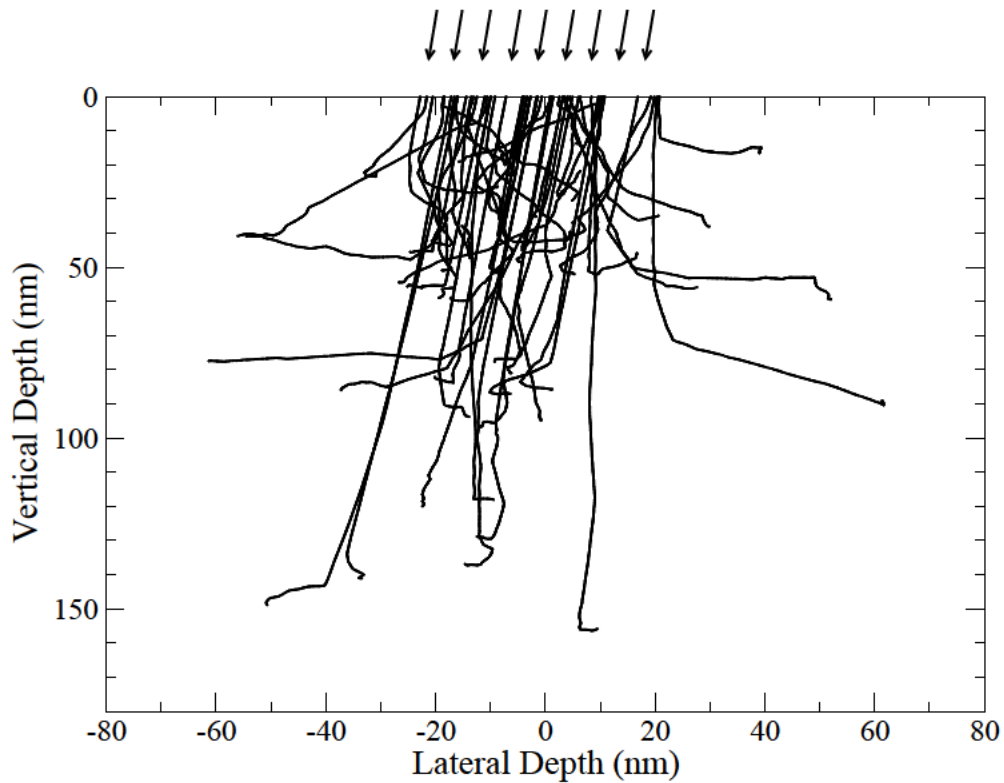


Figure 3.11: Monte Carlo simulation of 50 boron trajectories in crystalline silicon using an energy of 10keV and a tilt of 7° .

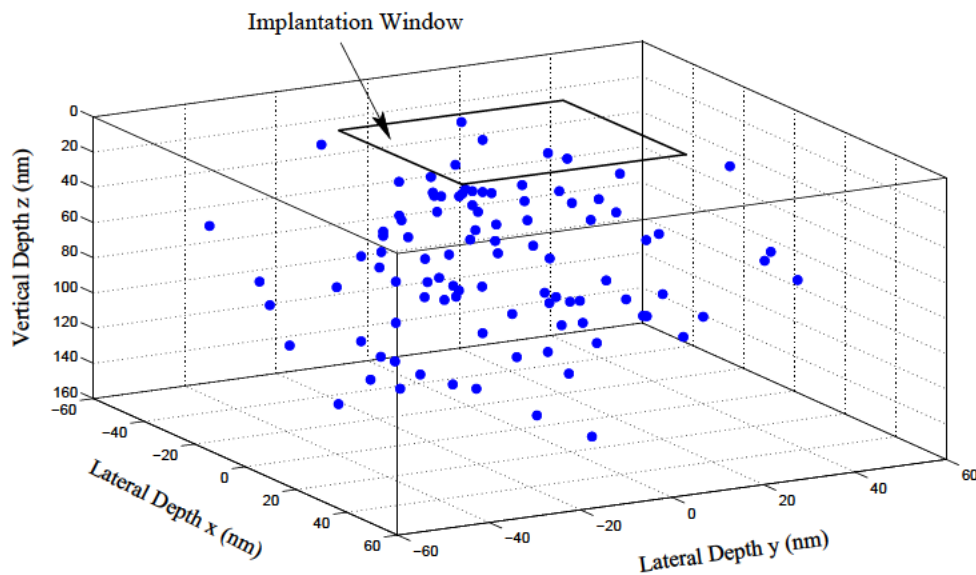


Figure 3.12: Final position of 100 boron atoms implanted with 10keV into silicon.

Nuclear Stopping Process

The nuclear stopping process is simulated with the physical BCA model which is based on the universal ZBL potential (as described in Section 3.1.2). The BCA model contains no tunable parameters and can be applied to all materials. The elastic two-particle scattering process is approximated by its asymptotic behavior and the ion is placed at the closest distance to the collision partner (which is equal to the impact parameter) before the nuclear scattering event. The center-of-mass scattering angle Θ is obtained from a lookup table as a function of the reduced impact parameter $\tilde{p}$ and the reduced energy $\tilde{E}$ which are defined as

$$\tilde{p} = \frac{p}{a_U} , \quad (3.38)$$

$$\tilde{E} = \frac{a_U}{Z_1 Z_2 e^2} \cdot E_c , \quad (3.39)$$

where the universal screening length a_U (3.14) and the transformed energy E_c (3.6) are used. The calculated ion trajectories presented in Fig. 3.11 show the change of the flight direction of ions due to heavy ion-atom collisions (small impact parameter) as well as the retention of the flight direction as ions travel along crystalline channels. The atomic-scale distances between nuclear collision events produce continuously plotted trajectories (every trajectory point

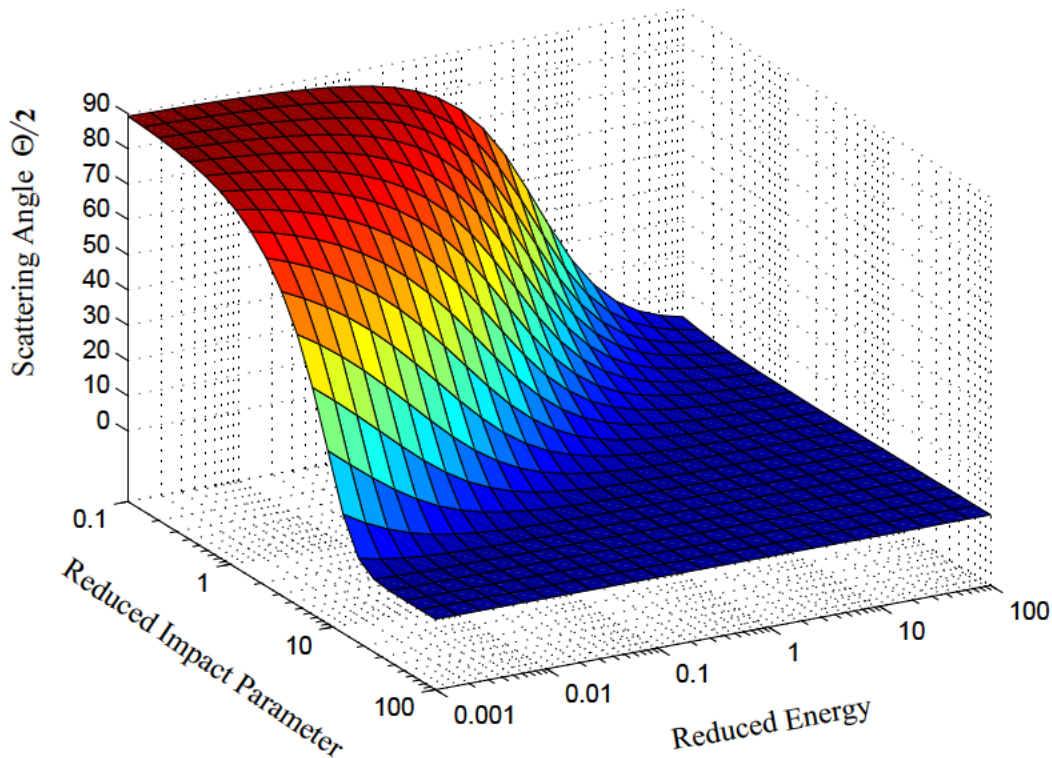


Figure 3.13: Tabulated scattering angle as a function of the scaled quantities impact parameter and energy.

corresponds to a single collision event). Fig. 3.12 shows the simulated distribution of 100 boron atoms in crystalline silicon which are implanted from the implantation window using the same implantation conditions as for the visualized trajectories in Fig. 3.11. The three-dimensional visualization of the tabulated scattering angle is presented in Fig. 3.13 by using a bicubic spline interpolation. The table values of the scattering angle are stored in a data file for 28 energy values and 17 impact parameter values. The surface plot $\Theta(\tilde{p}, \tilde{E})$ revealed that a small impact parameter $\tilde{p}$ and a low energy $\tilde{E}$ of the ion produces strong nuclear scattering ($\Theta/2 \approx 90^\circ$) for a binary collision event while channeling of ions occurs at large impact parameters or at high energies ($\Theta \approx 0^\circ$). The scattering angles of the ion and of the recoil in the laboratory system are calculated from the center-of-mass scattering angle Θ by (3.9) and (3.10), and the transferred energy to the primary recoil atom of a collision cascade is obtained by (3.11).

Electronic Stopping Process

The electronic stopping process is calculated by using the Hobler model described in Section 3.1.3. The only physical parameter required for this electronic stopping model is the impact parameter which is determined in the BCA model when selecting a collision partner. The model requires for every crystalline material a set of four parameters k_{corr} , a_U , y_{nl} , and q for each ion species (Table 3.3). In contrast to MCIMPL, where there is only one set of parameters per ion species for one target material available (since MCIMPL was originally just designed for the implantation into silicon), the model parameters can be independently calibrated for each ion-target combination in MCIMPL-II. Therefore, different crystalline material segments can be used in one simulation domain. Due to the fact that the model implies a dependence on the charge and the mass of the atoms of the target material, the electronic stopping power is averaged in the case of a compound material like SiGe. The contribution of each atom species is considered according to the stoichiometry of the material. In addition, a special treatment is applied for multiple collisions. While the non-local part of the electronic stopping model is considered only once, the local contribution to the electronic stopping process is calculated once for each binary collision which is part of the multiple collision event.

Ion species	Charge	Mass	k_{corr}	a_U	y_{nl}	q
Boron	5	11.009	1.75	0.450	0.050	0.230
Nitrogen	7	14.006	1.6861	0.4364	0.3177	0.1101
Oxygen	8	15.994	1.55	0.099	3.193E-5	0.97
Fluorine	9	18.998	0.9	0.6586	0.08	0.0
Silicon	14	27.977	1.4	0.4	0.12	0.1
Phosphorus	15	30.994	1.2674	0.4212	0.1447	0.0253
Germanium	32	72.59	1.15	0.3	0.3	0.0
Arsenic	33	74.92	1.1316	0.3056	0.2991	0.0243
Indium	49	114.82	1.1	0.3	0.5	0.0
Antimony	51	120.9	1.1	0.3	0.5	0.0
Xenon	54	131.3	1.1	0.3	0.5	0.0

Table 3.3: Empirical parameters for the electronic stopping process in silicon.

Ion species	f_{rec}	$N_{sat} \text{ (cm}^{-3}\text{)}$
Boron	0.139	$4 \cdot 10^{21}$
Phosphorus	1.0	$2 \cdot 10^{22}$
Arsenic	2.1	$5 \cdot 10^{22}$

Table 3.4: Recombination model parameters for different dopant species in silicon.

Calculation of Damage Production

The calculation of implantation induced point defects in crystalline materials is performed with the computationally efficient modified Kinchin-Pease damage model in combination with the Hobler recombination model as described in Section 3.1.4. The ion species dependent parameters of the empirical recombination model (Table 3.4) are stored in common with the parameters of the electronic stopping model in an ASCII data file. This file contains one data record for each combination of ion species and target material which holds all empirical parameters including the atomic number and atomic mass of the ion species.

Fig. 3.14 compares simulated boron profiles for 20keV channeling implantations in (100) silicon (shown by continuous lines) to SIMS measurements for the doses of 10^{13} , 10^{14} , and 10^{15} cm^{-2} . The one-dimensional profiles were obtained with one million simulated particles using an ion

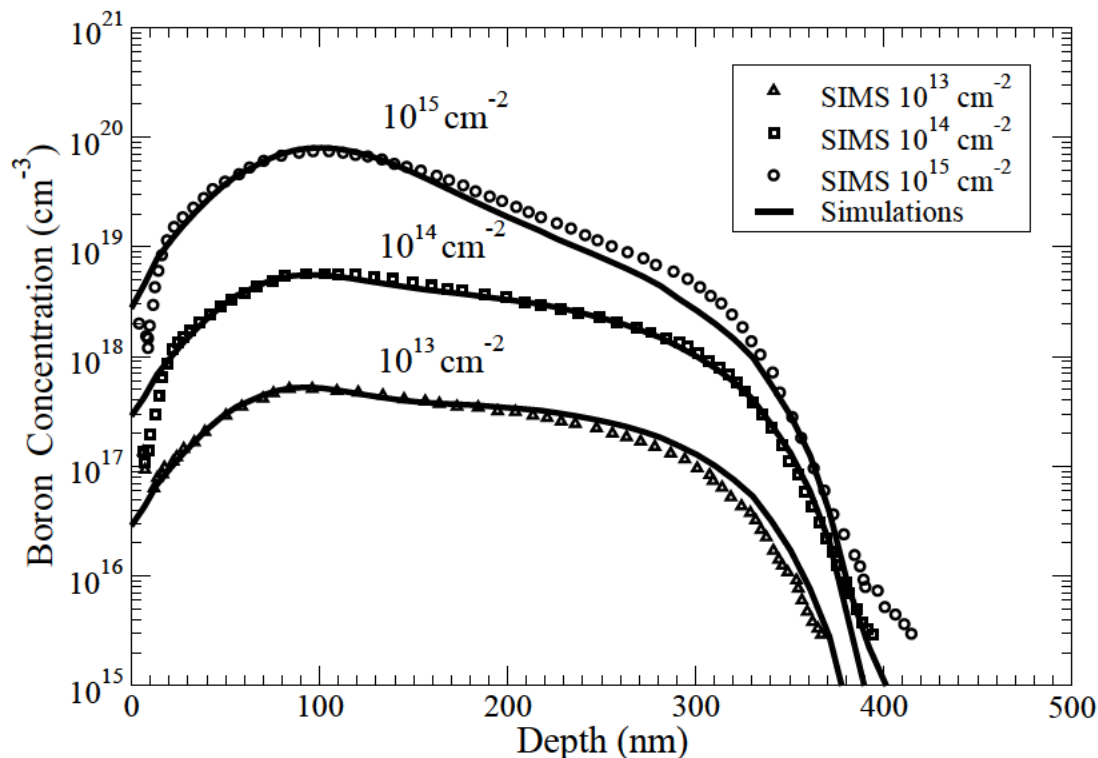


Figure 3.14: Illustration of the dose dependence for boron profiles using an energy of 20keV and a tilt of 0° , simulated with the Kinchin-Pease model.

beam divergence of $\pm 1^\circ$ in the simulations. It can be observed that the shape of the boron profiles is significantly influenced by the produced crystal damage. The accumulation of point defects with increasing implantation dose is well reproduced by the combined damage modeling approach based on the generation and recombination of point defects. It should be noted that the assumption of a native oxide film of 1nm thickness on the wafer surface is necessary to obtain a good agreement between boron simulation results and experimental data.

3.2.3 Speed-up Algorithms

The atomic-scale simulation of ion implantation processes using a Monte Carlo method is one of the most time-consuming computational tasks in semiconductor process simulation. On the one hand side, dramatically shrunk geometries of advanced devices require highly accurate simulation results by computing a very large number of ion trajectories and, on the other hand side, applications with higher implantation energies produce long trajectories in large-volume simulation domains. Three speed-up methods can be employed for the trajectory calculation in three-dimensional applications to get shorter simulation runtimes without losing accuracy:

- Trajectory-Split method
- Trajectory-Reuse method
- Parallelization of trajectory calculation

Trajectory-Split Method

The simulation of ion implantation produces a statistical distribution of the implanted dopant ions (in initial ion direction and lateral), where most of the simulated ions come to rest at a penetration depth close to the projected range in the target. For instance, regions with a dopant concentration of three orders of magnitudes smaller than the maximum concentration are reached just by one of thousand implanted ions. The statistical accuracy of simulation results becomes even worse in regions with lower dopant concentrations, since a reasonable simulation result includes three to five orders of the dopant concentration. At least some implanted particles have to be counted even in histogram cells located in peripheral regions with a very low concentration level of dopants, since no significant information can be derived from a histogram cell which contains only one implanted particle.

The basic idea of the Trajectory-Split method is to increase the number of ion trajectories that end up in regions with a bad statistical representation of dopants by splitting a particle trajectory [42, 80]. The splitting of a particle produces several particles with the same physical properties as the original particle but with a reduced weighting factor. The increase in the number of dopants, vacancies, and interstitials caused by a splitted particle are multiplied with the weighting factor before they are stored in the corresponding histogram. While the simulation of a molecular ion is performed with a weighting factor larger than one to account for statistical identical particles of the same atom species in the molecule [81], the weighting factor has to be below one for a splitted elemental ion to conserve the total implantation dose. The build-up of a trajectory tree is implemented by the full calculation of a primary trajectory and determining of the split points along this trajectory according to various rules. Afterwards a new trajectory

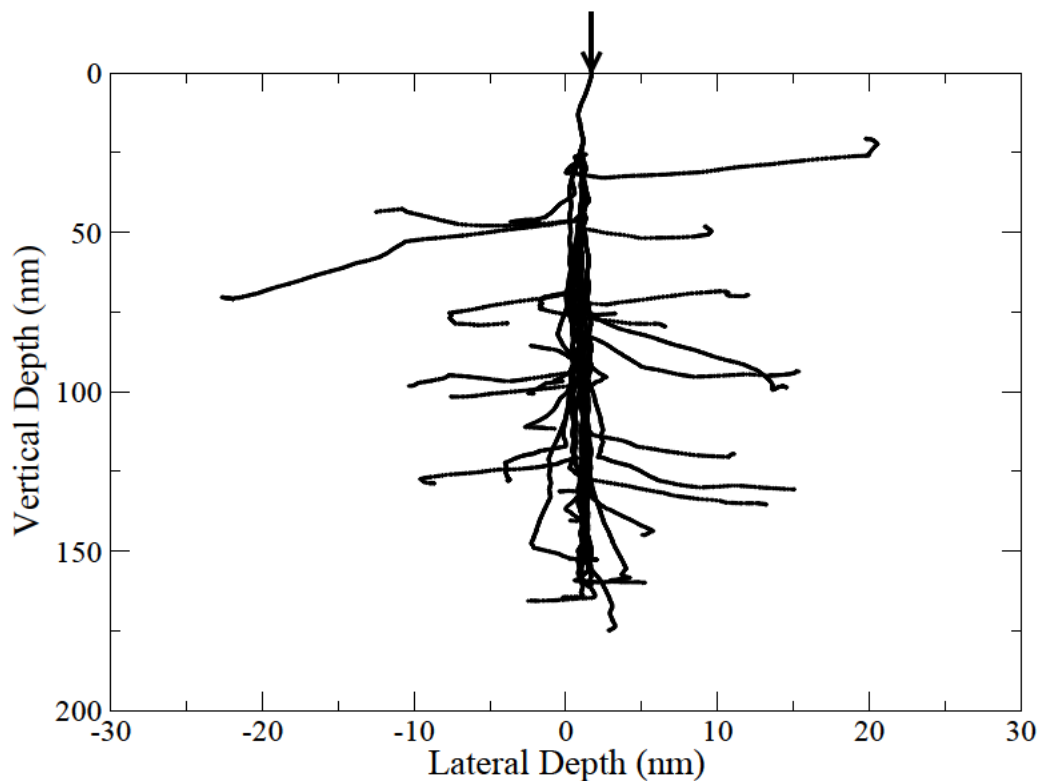


Figure 3.15: Monte Carlo simulation of a boron trajectory tree with a split depth value of 5, an energy of 10keV, and a tilt of 0° in crystalline silicon.

is calculated from every split point up to the end point. In crystalline materials the vibration of the lattice atoms guarantees that two branches of a trajectory tree are not identical after a split point despite equal initial conditions at the split point. The effect of the Trajectory-Split method is that one implanted particle delivers several effective ions which share the same initial part of the trajectory. Therefore less initial ions are required to get a simulation result with the same statistical accuracy. The sharing of parts of a trajectory reduces the average calculation time for trajectories of effective ions. The visualized boron trajectory tree, shown in Fig. 3.15, has a split depth of five, which corresponds to 2^5 trajectories with a particle weight of 2^{-5} . Finally, it should be noted that the Trajectory-Split method is typically applied for crystalline materials to reduce long computation times and to improve the statistical accuracy of doping profiles in the channeling tail region.

Trajectory-Reuse Method

The basic idea of the Trajectory-Reuse method is to use the fact that different regions of the simulation domain behave identical with respect to the trajectory calculation [42]. Therefore it is possible to calculate a trajectory only once and to copy it to other regions. The copying of trajectories can be interpreted as spreading one-dimensional simulation results over a two- or three-dimensional simulation domain as far as possible. In terms of trajectory calculation two

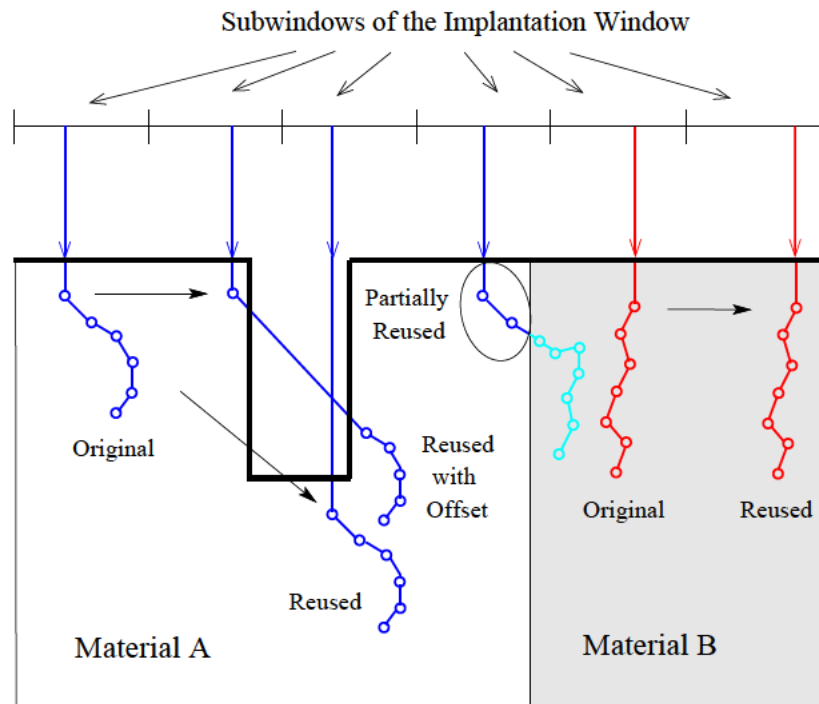


Figure 3.16: Illustration of the Trajectory-Reuse method for two different materials.

regions are considered identical, if all material properties that influence the particle motion are equal along the complete trajectory. In the case of amorphous materials only the density and composition of the material are considered in the simulation, while in the case of crystalline materials the trajectory is also influenced by the damage distribution in the material. Therefore the Trajectory-Reuse method can only be applied to amorphous materials, because regions with an exactly identical damage distribution along the complete trajectory are very improbable. They exist only for an initially undamaged crystal structure.

Fig. 3.16 demonstrates how the Trajectory-Reuse method works for a trench structure and for crossing the boundary between two amorphous materials A and B. As described in Section 3.2.2 the implantation window is subdivided into subwindows and one ion is started from each subwindow during every time step. The Trajectory-Reuse algorithm splits a calculated trajectory which goes through different materials into several sub-trajectories, one for each amorphous material, and stores the obtained sub-trajectories in a list. All parts of a calculated trajectory in crystalline materials are neglected. When the next ion is started, the algorithm searches through the stored trajectory list. The target material of a stored trajectory must be identical to the entrance material of the ion and the ion energy must be less than the energy loss ΔE along a stored trajectory. A new trajectory is calculated and added to the trajectory list, if no suitable trajectory is available in the list.

The Trajectory-Reuse method improves significantly the simulation speed for three-dimensional implantation applications, since large regions of MOS transistor structures are typically composed of amorphous materials. Finally, it should be noted that the performance gain of this method increases with decreasing subwindow size.

Parallelization of Trajectory Calculation

The three-dimensional Monte Carlo simulation of ion implantation requires fairly long simulation run-times to achieve accurate simulation results in complex target structures, which can be in the order of several days on a modern computing environment. The simulation performance can be significantly improved by parallelization of the trajectory calculation. Two parallelization strategies can be used in principle for the trajectory calculation:

- Parallel computing on a cluster of workstations
- Parallel computing on a shared-memory multiprocessor system

A parallelization method based on the Message Passing Interface (MPI) was implemented in MCIMPL [82]. The intention was to perform a distributed simulation on a cluster of workstations which are connected over a slow network. The simulation domain was geometrically distributed among several workstations which have to exchange only a small amount of data during the simulation. Due to the distribution of the memory requirement among several workstations, small workstations could be used for three-dimensional simulations.

However, the current status of the object-oriented simulator MCIMPL-II is that the trajectory calculation is implemented only in a sequential manner. For future work, a powerful parallelization of the simulator can be achieved by using OpenMP based parallel computing on a shared-memory multiprocessor architecture [83]. The OpenMP standard provides a portable standard parallel API specifically for programming shared-memory multiprocessor systems. This standard supports also an *incremental parallelization* by adding compiler directives to the source code. The execution of the simulation program on one multiprocessor workstation ensures a more reliable operation for longer simulation runs compared to a network based MPI solution. The damage accumulation during the simulation has to be considered for parallel computing of trajectories. Only a small error occurs, if the trajectories for all subwindows of the implantation window are computed in parallel using the initial damage distribution of the current time step. At the end of the time step, it has to be ensured that the newly generated damage is updated in the shared internal data structures before proceeding with the next time step.

3.2.4 Postprocessing of Monte Carlo Results

After the calculation of the desired number of ion trajectories, the doping information is stored in histogram cells aligned on an orthogonal grid. Each histogram cell contains a certain number of implanted ions, and the doping concentration within a cell is given by the number of ions divided by the volume of the cell. The statistical nature of the Monte Carlo implantation process produces a statistical fluctuation in the obtained raw cellular doping information. In particular, three-dimensional Monte Carlo implantation results have inherently large variances in the peripheral regions. An advanced smoothing technique based on a Bernstein polynomial approximation has been developed [14, 84–86] in order to transfer the cellular data to an unstructured destination grid which is suitable for the subsequent process simulation step. Finite element simulations are used in the next simulation step to imitate thermal annealing processes which are required to activate the dopants and to eliminate the substrate damage. On the one hand side, the postprocessing procedure performs the necessary interpolation operation, and on the other hand side, it reduces the statistical noise of the obtained doping and damage data.

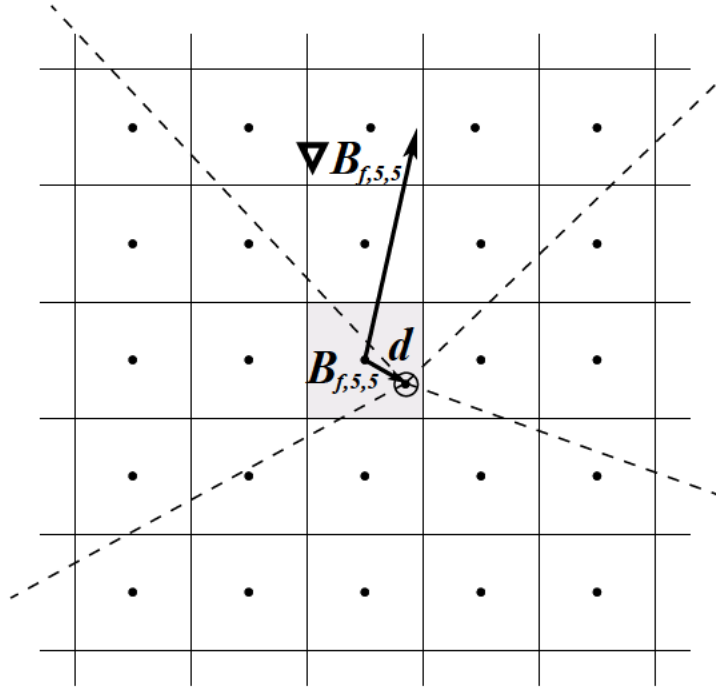


Figure 3.17: Illustration of the smoothing operation performed for one point of the new unstructured grid in a two-dimensional example. The orthogonal lines confine the cells of the internal grid. The four dashed lines denote the unstructured grid, where the new point is marked by a small circle. In the first step the 5^2 sample points are used to calculate the concentration $B_{f,5,5}$ at the middle of the central grey cell. Then the scalar product of the gradient $\nabla B_{f,5,5}$ and the offset vector d is calculated to estimate a value for the delta concentration.

Advanced Smoothing Algorithm

The postprocessing procedure starts by invoking the mesh generator DELINK [79] and passing over a point cloud in common with all interfaces and surfaces present on the Wafer-State-Server to discretize the doping distribution. As a result, the mesh generator produces a tetrahedral mesh which is approximately aligned to the surface and which is fine enough to resolve the doping profile. This mesh is handed over to the Wafer-State-Server where the doping information is added to the points (Fig. 3.9). Therefore, the Wafer-State-Server calls the Bernstein approximation operation provided by the MCIMPL-II core module for each point of the new mesh.

The smoothing of the Monte Carlo result is performed by approximating the doping concentration value for a grid point of the unstructured grid by means of Bernstein polynomials defined in a cubical surrounding space [85]. The Bernstein polynomial $B_{f,n,n,n}(x_1, x_2, x_3)$ approximates a function f of 3 variables, where $n \in \mathbb{N}$ are the concentration sample points in each dimension. The Bernstein approximation $B_{f,n,n,n}$ is specified by n^3 sample points, whereby $B_{f,n,n,n}$ does not run through the sample points, but each of them affects the approximated function. The sample points are also referred to as control points, since they enforce the progression of the

multivariate function. A critical issue is that the calculation of the Bernstein approximation requires a reasonable information in all sample points. In order to fulfill this requirement, the concentration value of a cell which contains no doping information (empty cell) is determined by averaging over the values of non-empty neighboring cells. Due to the fact that the evaluation of the Bernstein polynomial at an arbitrary point is computationally very expensive, the polynomial is only calculated for the middle point $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ of the domain $[0, 1]^3$. For that special point the Bernstein polynomial can be significantly simplified according to the formula given in (3.40) which enables a fast computation of the approximated value.

$$B_{f,n,n,n} \left(\frac{1}{2}, \frac{1}{2}, \frac{1}{2} \right) = \sum_{k_1=0}^n \sum_{k_2=0}^n \sum_{k_3=0}^n f_{k_1,k_2,k_3} \binom{n}{k_1} \binom{n}{k_2} \binom{n}{k_3} \left(\frac{1}{2} \right)^{3n}. \quad (3.40)$$

The drawback of this simplification method is that the obtained approximated value is independent of the given point position somewhere in the cell. This drawback is eliminated by also calculating the derivative of the Bernstein polynomial at the center of the cell and modifying the approximated value according to this local gradient as shown in Fig. 3.17. Therefore, the concentration difference $\Delta B_{f,n,n,n}$ between the new point and the cell middle point is calculated by the system of equations (3.41), (3.42) and (3.43) and added to the approximated value $B_{f,n,n,n}$ at the cell middle point. Equation (3.43) points out that it is possible to calculate the required three partial derivatives in a fast way too.

$$\Delta B_{f,n,n,n} = \nabla B_{f,n,n,n} \cdot \mathbf{d}, \quad (3.41)$$

$$\nabla B_{f,n,n,n} = \frac{\partial}{\partial x_1} B_{f,n,n,n} \mathbf{e}_1 + \frac{\partial}{\partial x_2} B_{f,n,n,n} \mathbf{e}_2 + \frac{\partial}{\partial x_3} B_{f,n,n,n} \mathbf{e}_3, \quad (3.42)$$

$$\left. \frac{\partial}{\partial x_i} B_{f,n,n,n} \right|_{(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})} = \sum_{k_1=0}^n \sum_{k_2=0}^n \sum_{k_3=0}^n f_{k_1,k_2,k_3} \binom{n}{k_1} \binom{n}{k_2} \binom{n}{k_3} \cdot \left(\frac{1}{2} \right)^{3n} (4k_i - 2n). \quad (3.43)$$

Analysis of the Smoothed Simulation Result

For the analysis of the implemented smoothing algorithm, numerical experiments were performed with the simulator MCIMPL-II on a three-dimensional structure equivalent to a one-dimensional problem. It is assumed that all simulated ions are statistically independent. Fig. 3.18 shows the three-dimensional phosphorus implantation result in a crystalline silicon substrate for $N = 4 \cdot 10^6$ simulated ions. The corresponding statistical fluctuation of the phosphorus concentration as a function of the penetration depth z is visualized in Fig. 3.19 for the unstructured grid. Each sample consists of the concentration values $C_1, C_2, \dots, C_n$ located in a horizontal plane $z = \text{const}$. The one-dimensional doping profile is derived by calculating the mean concentration value $\overline{C}(n)|_{z=\text{const}}$ for each sample. The standard deviation $S(n)$ of a sample defined by the values of n grid points in a plane $z = \text{const}$ is given by (3.44). The relative standard deviation σ of the dopant concentration in a horizontal plane according to (3.45) is a measure for the simulation error of three-dimensional results compared to one-dimensional results.

$$S(n)|_{z=\text{const}} = \sqrt{\frac{1}{n-1} \sum_{i=1}^n [C_i - \overline{C}(n)]^2}, \quad (3.44)$$

$$\sigma|_{z=\text{const}} = \frac{S(n)}{\overline{C}(n)}. \quad (3.45)$$

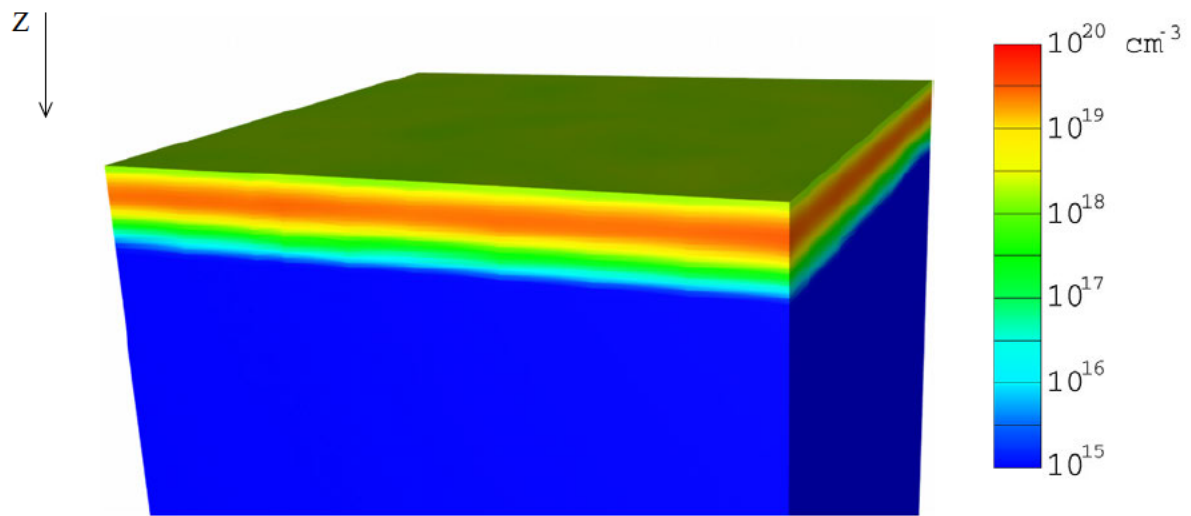


Figure 3.18: Smoothed result of a phosphorus Monte Carlo implantation in silicon, using $4 \cdot 10^6$ simulated ions, an energy of 25keV, and a dose of 10^{14} cm^{-2} .

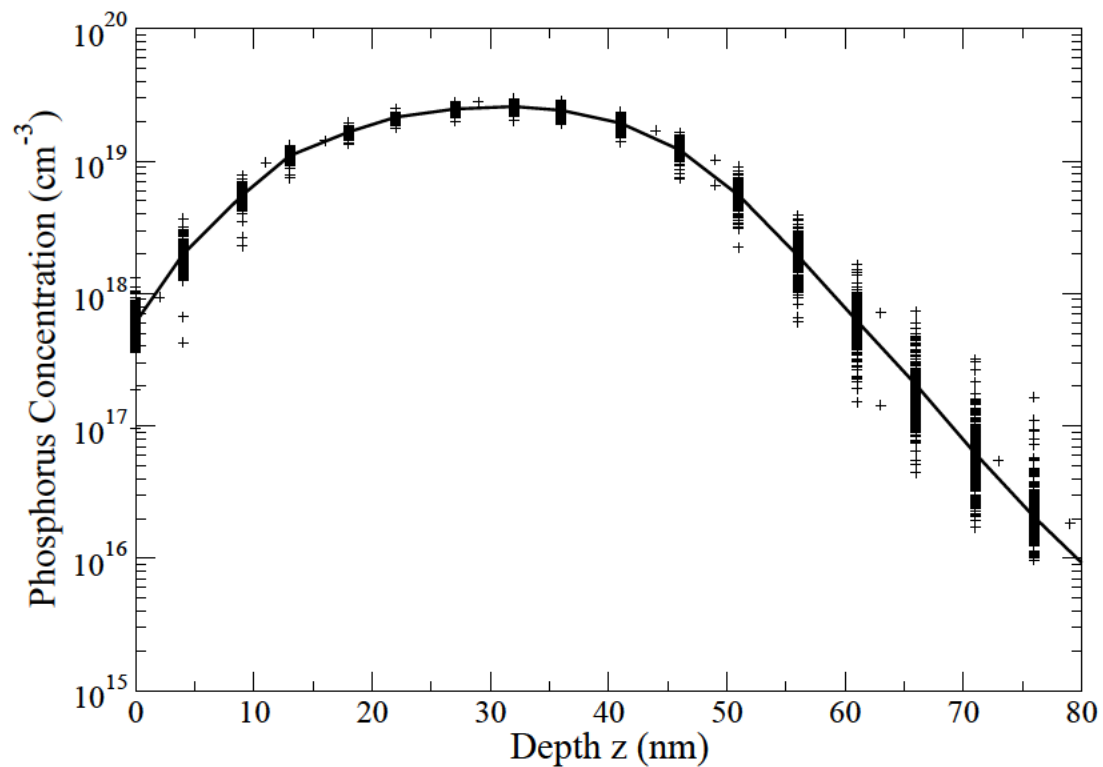


Figure 3.19: Fluctuation of the smoothed three-dimensional dopant distribution and the corresponding one-dimensional doping profile.

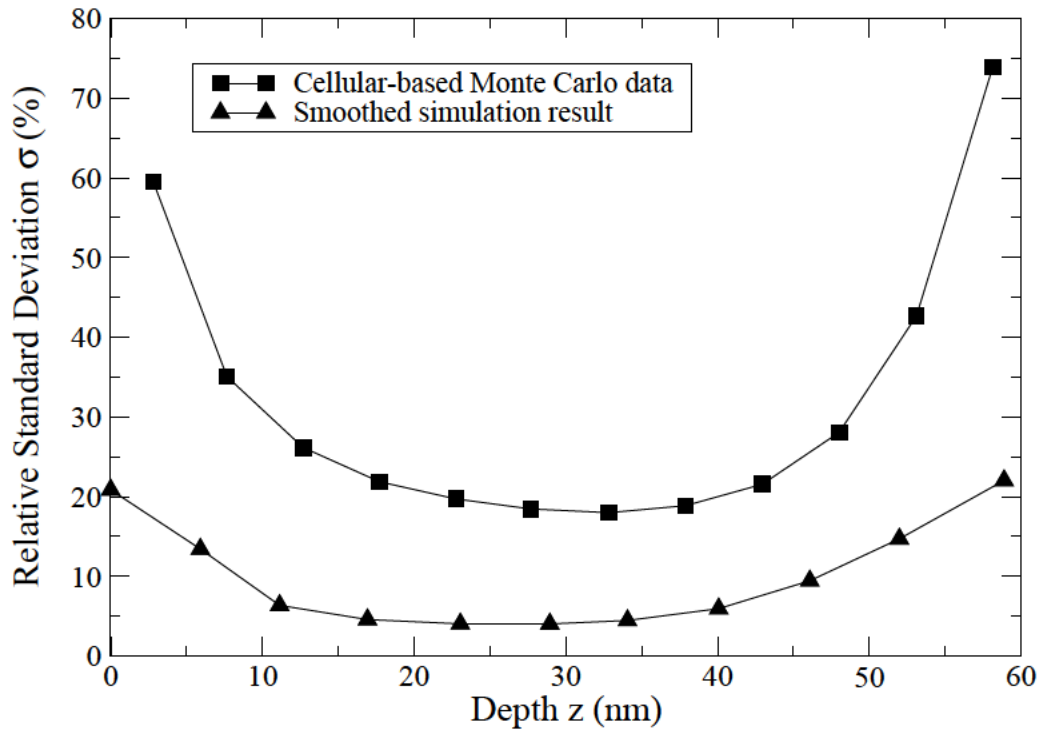


Figure 3.20: Improvement of the simulation accuracy by the smoothing procedure.

Fig. 3.19 depicts that the sample variance becomes minimal around the projected range R_p , since most of the ions come to rest there. For the evaluation of the postprocessing improvement the ratio of the maximal standard deviation $\sigma_{\max}$ within the range $2 \cdot \Delta R_p$ (twice the straggling at the mean projected range) of the doping profile, after and before smoothing, can be used. As shown in Fig. 3.20, $\sigma_{\max, \text{after}} / \sigma_{\max, \text{before}} \approx \frac{1}{4}$ within $2 \cdot \Delta R_p = 22\text{nm}$ at $R_p = 30\text{nm}$.

$$\sigma_{\max} \propto \frac{1}{\sqrt{N}}. \quad (3.46)$$

The theoretical simulation error $\sigma_{\max}$ of the Monte Carlo method follows from the Central Limit Theorem [59]. Equation (3.46) has been expectedly verified by simulation experiments with different N . In order to reduce $\sigma_{\max}$ by $\frac{1}{4}$, one has to increase N by a factor of 16. But as shown in Fig. 3.20, a significant improvement of the statistical accuracy can also be achieved by sophisticated postprocessing, in particular through the filtering effect of the Bernstein polynomials, which eliminates high-frequency fluctuations from the original Monte Carlo data.

The linear approximation of the delta concentration value $\Delta B_{f,n,n,n}$ between the grid point of the unstructured grid and the cell middle point reduces the effect of the cell discretization. The left diagram of Fig. 3.21 shows the smoothed doping profile generated by the Bernstein approximation without using the additional gradient-based approximation step. The internal cell dimension of 5nm produces equal concentration values for the first two samples. The right diagram shows the doping profile obtained by using the advanced smoothing technique. The advanced algorithm produces a smoother and therefore a more realistic doping profile. Longer simulation run times or worse statistics would arise, if the cell dimension of the simulator is further reduced to enhance the internal resolution. In contrast to that, the used smoothing

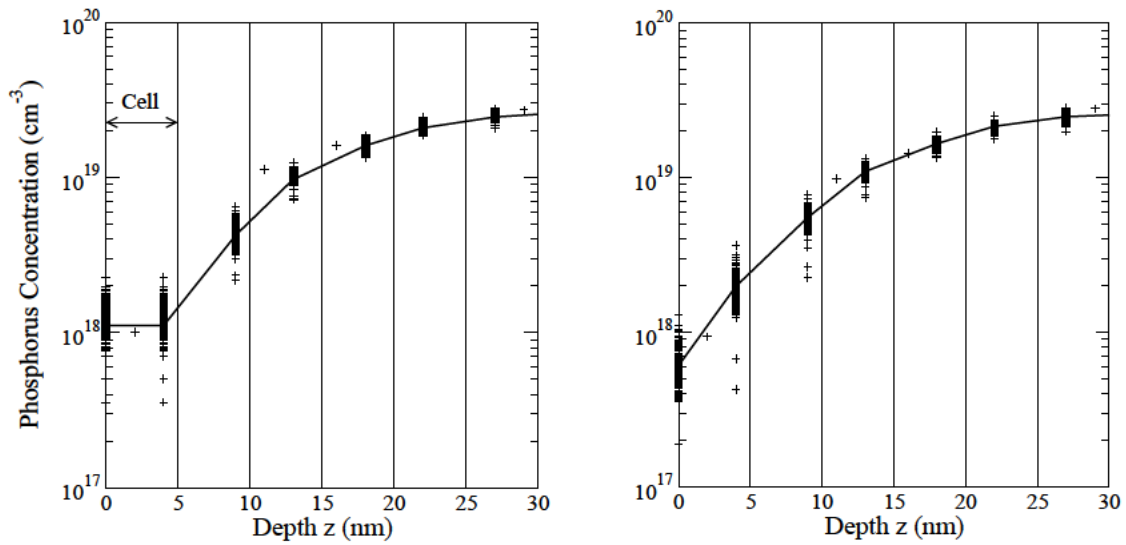


Figure 3.21: Smoothing without (left) and with (right) linear approximation step.

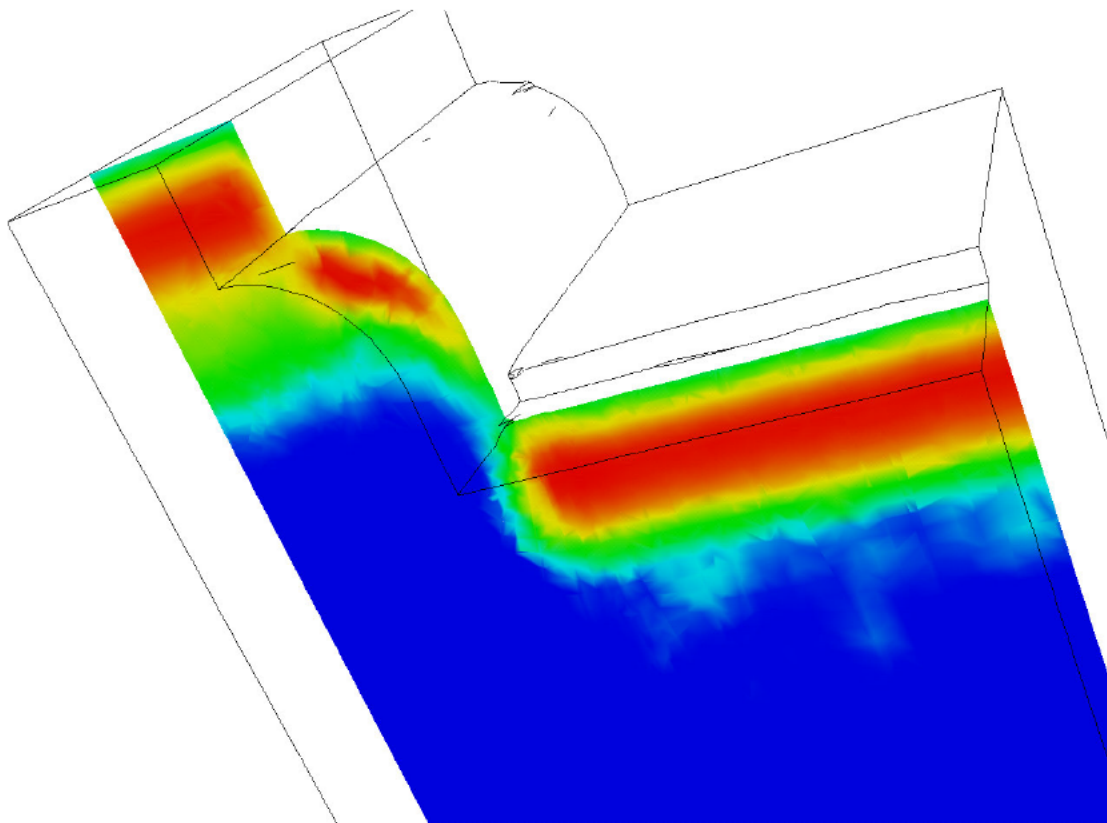


Figure 3.22: Implantation of arsenic ions into a complex device structure with an energy of 70keV and a dose of $3 \cdot 10^{15} \text{ cm}^{-2}$.

technique improves the accuracy of three-dimensional Monte Carlo implantation results in a computationally efficient way.

Being based on random numbers, the results obtained with the Monte Carlo technique are never exact, but rigorous in a statistical sense. Therefore, a confidence interval can be constructed for the one-dimensional doping profile shown in Fig. 3.19 in order to estimate the error of the mean in a plane $z = \text{const}$ [59]. The relationship (3.46) can also be used to estimate the number of initial ions N required to obtain a specific precision in a Monte Carlo simulation study. For the calculation of the required number N as a function of the desired maximum standard deviation $\sigma_{\max}$, a parameter γ is used which takes the dopant species and the implantation energy into account. The following formula can be used to estimate the number N for an implantation window size A and a desired precision $\sigma_{\max}$:

$$N = \gamma \frac{A}{A_0} \frac{1}{\sigma_{\max}^2}, \quad (3.47)$$

where $A_0 = 0.455 \mu\text{m}^2$ is the investigated top surface area of the simulation domain shown in Fig. 3.18, and the parameter $\gamma = 15992$ for a phosphorus implantation with an ion energy of 25keV [86]. Note that the computational effort of three-dimensional implantation applications grows proportionally to the implantation window size in order to maintain a certain statistical accuracy of the simulation results.

Fig. 3.22 shows the smoothed Monte Carlo implantation result. The arsenic source/drain implantation was performed with an energy of 70keV and a dose of $3 \cdot 10^{15} \text{cm}^{-2}$ into a modern MOS transistor structure. The simulation was carried out with 2000000 initial ions and the default split-depth of five to demonstrate the fluctuation of the resulting dopant distribution. It is recommended to use at least 2000000 ions/ μm^2 , otherwise the simulation result is inacceptably inaccurate due to statistical fluctuations.

3.2.5 Three-Dimensional Demonstration Example

The presented simulation example explains the accomplishment of three-dimensional implantation applications with the simulator MCIMPL-II in principle. For complex targets it is advantageous to add the desired unstructured output grid for the implantation result already to the input structure used for the ion implantation simulation rather than to generate the output grid on-the-fly as shown in Fig. 3.8. This approach allows to manually adjust the grid refinement for a specific application. A simulation application typically includes the following steps:

- Generation of the device geometry in the WSS format
- Addition of the unstructured grid to the geometry
- Simulation of the ion implantation step (with the option *reuse grid*)

Fig. 3.23 shows the non-planar oxide mask and the unstructured grid used in the implantation example. The two-segment geometry consisting of *silicon* and *oxide* was generated with the three-dimensional solid modeler LAYGRID [87]. LAYGRID reads its input from a text file which contains the geometric structure represented by layers and polygons, and some properties of the used materials. Each layer is defined by a two-dimensional mask and a layer thickness.

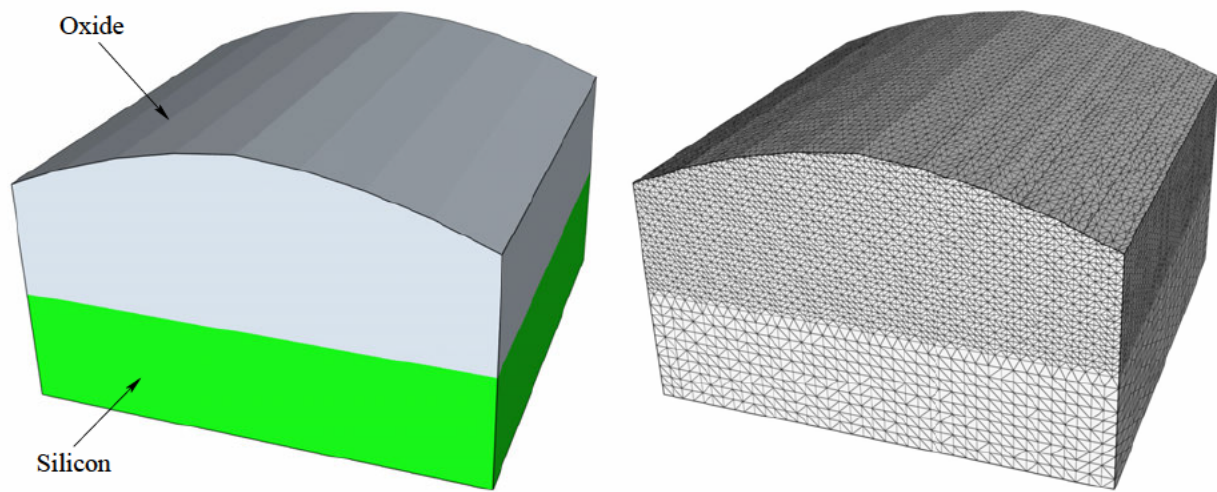


Figure 3.23: Non-planar two-segment structure (left) and unstructured grid (right).

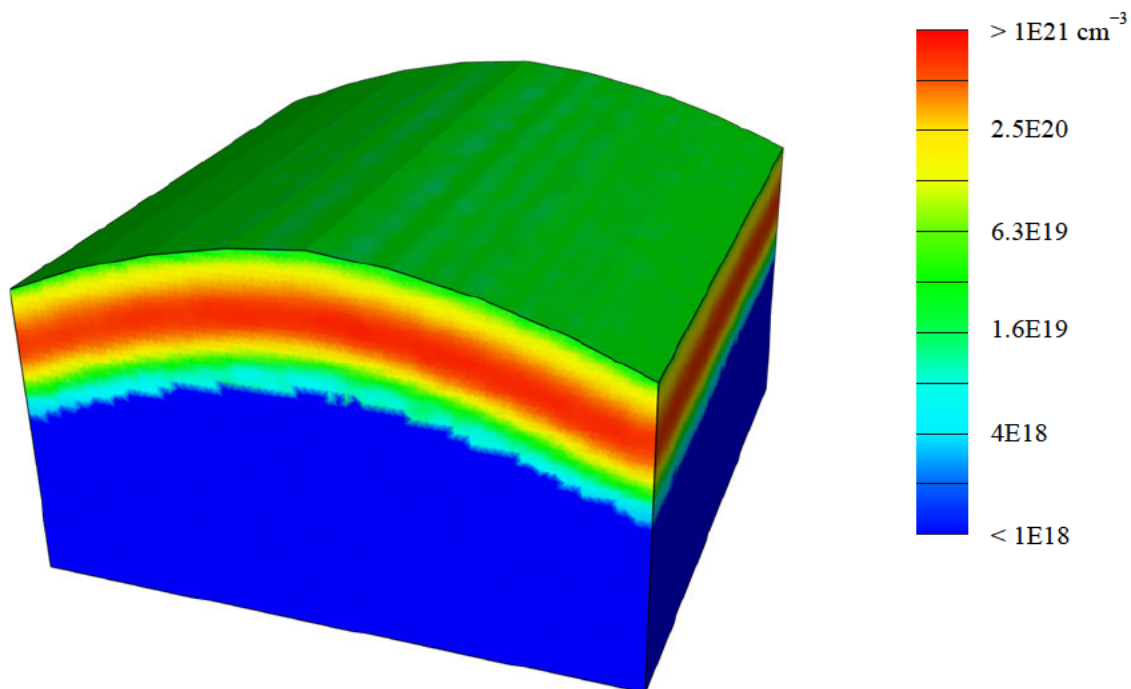


Figure 3.24: Boron implantation result in the non-planar oxide mask performed with an energy of 20keV and a dose of $5 \cdot 10^{15} \text{ cm}^{-2}$.

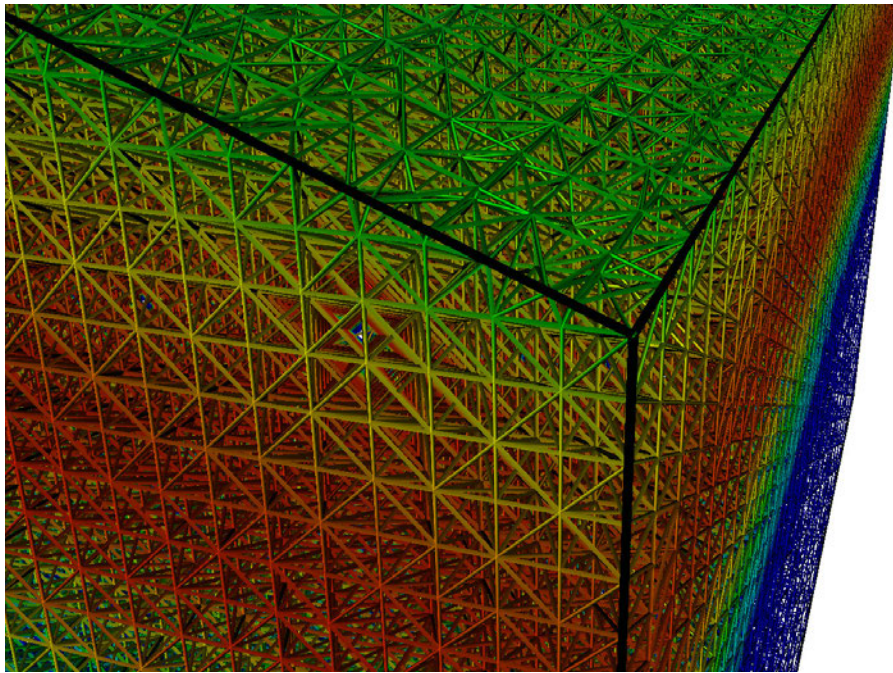


Figure 3.25: Visualization of the boron result and the grid lines in a geometry corner.

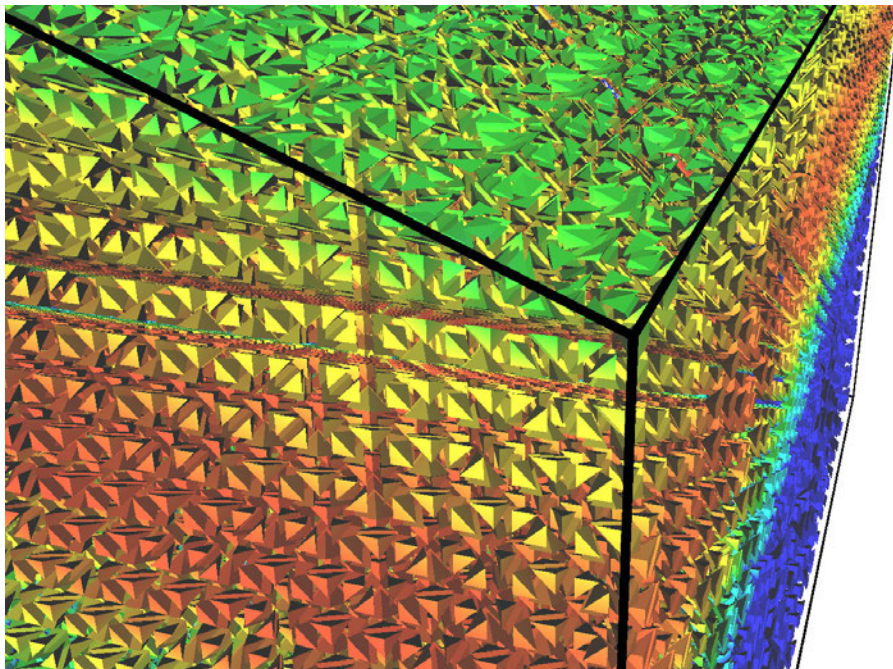


Figure 3.26: Visualization of the boron result and the tetrahedral elements which are shrunk to 40% of their original size.

The thickness is always constant for ideally planarized structures and for non-planar layers it is necessary to define a three-dimensional surface area. A layer mask definition contains the geometry information and material references of all included material segments. The resulting geometry is then written to a WSS file. The visualized grid in Fig. 3.23 has been added to the WSS file by the mesh generator DELINK with the *box refinement method*. This method allows to control approximately the distance of the grid points in the x , y , and z direction within a specified box-shaped container. A finer grid resolution is used up to the expected maximum penetration depth of the boron distribution. Fig. 3.24 shows the implanted boron distribution in the oxide mask which has been produced by 25 million simulated ions without using the splitting of trajectories. In this application, the implantation window of approximately $0.7\mu\text{m}^2$ is divided into 36 subwindows which requires to start 694445 ions per subwindow. An internal histogram resolution of 10nm was used to discretize a cuboid region (internal simulation domain) of the input geometry. The upper limit of the discretization cuboid is determined by the highest position of the oxide mask surface and the lower limit is derived by the estimated maximum penetration depth of 400nm from the lowest oxide mask surface position. Fig. 3.25 shows the grid lines and Fig. 3.26 the tetrahedral elements located in the zoomed-in right upper corner on the front side of the geomemtry. For the final boron result, 99754 grid points and 564887 tetrahedrons are used.

Chapter 4

Doping of Group-IV-Based Materials

While the first transistor was developed in 1947 by using germanium as the semiconductor material and GaAs devices have demonstrated high switching speed, it is silicon which completely dominates the present semiconductor market. This development has arisen due to the low cost of silicon CMOS technology. The fabrication processes and the device performance rely heavily on a number of natural properties of silicon, for instance, the availability of a good oxide. For alternative semiconductor materials much more expensive fabrication processes must be used, whereby the phenomenal yields achievable on a silicon CMOS line cannot be reached. One drawback of silicon is its relatively small carrier mobility. Since the device speed depends on how fast the carriers can be transported through the device channel under sustainable low operating voltages, silicon can be regarded as a relatively slow semiconductor. Today, it is commonly believed that a further improvement in the channel mobility beyond those that can be achieved with process-induced strain will be required in order to maintain continued commensurate device scaling. The higher carrier mobility offered by group-IV materials like SiGe compounds, germanium, and various heterostructures, for instance, biaxially strained silicon on relaxed SiGe, are required as new channel materials for bulk and on-insulator implementations [88–90].

While ion-implanted doping profiles are well studied in silicon for various dopant species and implantation conditions, such doping profiles are scarce in SiGe alloys as well as in pure Ge. An accurate and multi-dimensional simulation of ion implantation processes is required to optimize the doping profiles in these semiconductor materials for high-performance CMOS applications and optoelectronic devices. Since quantitatively predictive capabilities are a must for a Monte Carlo ion implantation simulator, the used models for implantations into silicon have been evaluated to extend the simulator to this wide class of materials on the basis of experimental results. For calibration purposes, a set of specifically selected experiments for arsenic and boron implantations into SiGe virtual substrates with different Ge content has been developed and carried out. Additional experimental results from other research groups obtained by arsenic and boron implantations into strained Si, relaxed SiGe layers with high Ge contents, and into Ge wafers have been included. The doping profiles in the investigated non-silicon materials are always compared to a reference doping profile in silicon, implanted under the same conditions. On the basis of these experiments various effects which influence the dopant distribution (e.g. Ge content in the alloy, damage accumulation, channeling effect) can be analyzed independently. The extended simulator is able to accurately predict the doping profiles in germanium and in SiGe alloys of arbitrary Ge content, and to estimate the produced point defects.

4.1 Silicon-Germanium Alloys

Silicon-germanium (SiGe) is a IV-IV compound semiconductor which offers enhanced carrier mobility and a higher dopant solubility compared to pure silicon. The remarkable potential of the SiGe material arises from the possibility to modify its properties by altering the composition. For instance, the band gap decreases from 1.12eV (pure silicon) to 0.66eV (pure germanium) at room temperature. The lattice parameter of the germanium crystal is 4.2% larger than that of silicon. Relaxed SiGe has a lattice parameter value which lies between those of the endpoint elements silicon and germanium depending on the Ge content in the alloy. Crystalline SiGe can be grouped into the two categories relaxed and strained. Strain engineering is used to enhance the carrier mobility for MOS transistors. By building different kinds of Si-SiGe heterostructures various properties for device design can be optimized. When silicon is epitaxially grown on SiGe, silicon forms a strained layer configuration up to a certain critical thickness. A strained SiGe layer can be grown on silicon in a similar way. A strained-Si/relaxed-SiGe structure produces tensile strain which primarily improves the electron mobility, while compressive strain obtained by a strained-SiGe/relaxed-Si structure boosts the hole mobility. Although the quality of SiGe virtual substrates or bulk wafers has steadily improved over the last years, the defect density is still too large to guarantee a reasonable yield in CMOS processing at present time [91].

4.1.1 Modeling of Ion Implantation in SiGe Alloys

The simulation of ion implantation in silicon with MCIMPL-II is based on general physical models which are explained in Section 3. Nevertheless, some of the models used for the trajectory calculation have to be extended or the change of an empirical parameter value is sometimes required in order to extend the simulation capabilities to SiGe alloys [92–94]. Precise material data and many SIMS profiles are used for the investigation of ion implantation.

Crystalline Partner Selection Model

Silicon and germanium, which both crystallize in the diamond lattice structure, are completely miscible forming $\text{Si}_{1-x}\text{Ge}_x$ solids with x ranging from 0 to 1. The most precise and comprehensive investigation of bulk lattice parameters and densities for $\text{Si}_{1-x}\text{Ge}_x$ alloys for x from 0 to 1 with Ge intervals of 5% has been carried out by Dismukes et al. [95]. We extended the target materials of the simulator MCIMPL-II from crystalline silicon to the class of $\text{Si}_{1-x}\text{Ge}_x$ alloys and germanium by adjusting the lattice parameter $a(x)$ of the crystalline model by

$$a(x) = 0.02733 x^2 + 0.1992 x + 5.431 \quad (\text{\AA}) \quad \text{for} \quad 0 \leq x \leq 1. \quad (4.1)$$

While Vegard's law determines the $\text{Si}_{1-x}\text{Ge}_x$ lattice parameter only by a linear interpolation between the lattice parameters of the endpoint elements silicon and germanium, equation (4.1) takes the small departure from Vegard's law into account [96]. The parabolic relation (4.1) for the lattice parameter as a function of the Ge content x is derived from measurement values in [95] and approximates the experimental data with a maximum deviation of about $10^{-3}\text{\AA}$. The deviation from Vegard's law has been confirmed in a recent study on SiGe epitaxial layers on (100) silicon substrates analyzed by X-ray diffraction and Rutherford backscattering [97].

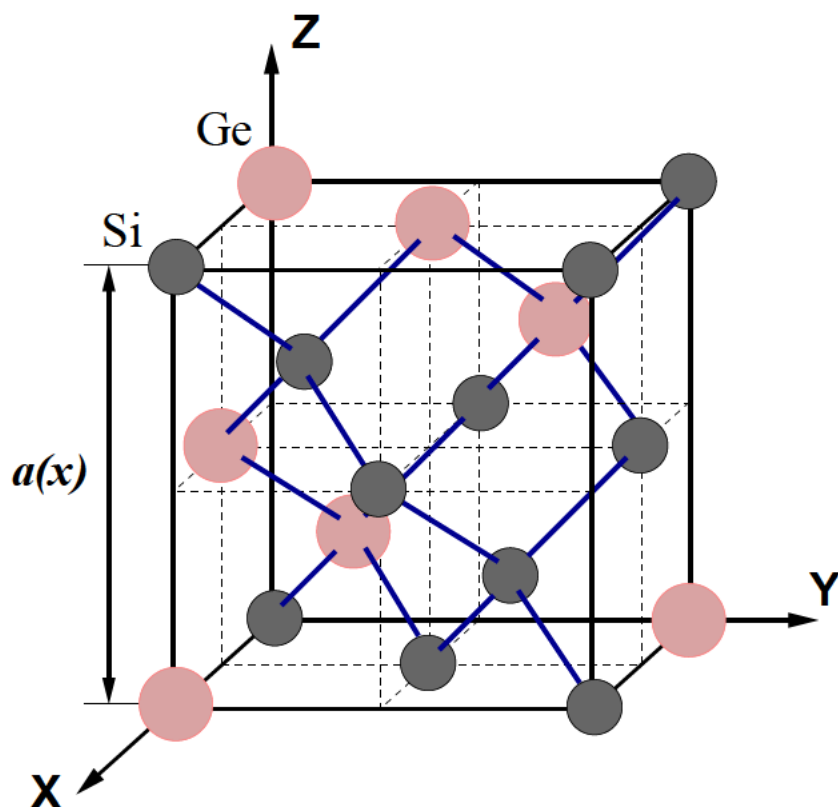


Figure 4.1: Local crystal model used for the simulation of ion implantation in Si, $\text{Si}_{1-x}\text{Ge}_x$ alloys of arbitrary Ge content, and pure Ge ($0 \leq x \leq 1$).

While the ion moves through the simulation domain, a local crystal model (as shown in Fig. 4.1) is built up around the actual ion position for searching the next collision partner. The selection of the target atom species for a collision event in $\text{Si}_{1-x}\text{Ge}_x$ targets is performed by probability x for germanium and $1 - x$ for silicon, respectively. This random choice of the atom species in the crystalline model is acceptable, because no ordering has been observed in bulk SiGe crystals and ordering mechanisms in epitaxial grown SiGe layers are still under investigation.

Table 4.1 summarizes some important physical properties relevant for ion implantation in silicon, germanium, and $\text{Si}_{1-x}\text{Ge}_x$ alloys with $x = 0.25$, $x = 0.5$, and $x = 0.75$. A linear interpolation between the endpoint elements silicon and germanium is used to derive the values for

Properties	Si	$\text{Si}_{0.75}\text{Ge}_{0.25}$	$\text{Si}_{0.5}\text{Ge}_{0.5}$	$\text{Si}_{0.25}\text{Ge}_{0.75}$	Ge
Mass (amu)	28.09	39.2175	50.345	61.4725	72.6
Atomic density (cm^{-3})	$5.02 \cdot 10^{22}$	$4.855 \cdot 10^{22}$	$4.712 \cdot 10^{22}$	$4.566 \cdot 10^{22}$	$4.418 \cdot 10^{22}$
Density (kg/m^3)	2329.11	3161.85	3939.23	4661.86	5326.69
Lattice constant ($\text{\AA}$)	5.431	5.4825	5.5374	5.5958	5.6575
Debye temperature (K)	640	573.5	507	440.5	374

Table 4.1: Approximation of SiGe material properties at 300K for ion implantation.

the average atomic mass and the Debye temperature in SiGe for different compositions. The values of the SiGe lattice parameter were calculated by using the quadratic approximation (4.1). The lattice parameter at a Ge concentration x , $a(x)$, determines the atomic density $N(x)$ for $\text{Si}_{1-x}\text{Ge}_x$ according to (4.2). Finally, the $\text{Si}_{1-x}\text{Ge}_x$ material density $\rho(x)$ is obtained by inserting equation (4.2) into equation (4.3) and by proportionately averaging over the atomic weights of silicon and germanium, M_{Si} and M_{Ge} .

For the simulation with MCIMPL-II the properties of an arbitrary SiGe material segment can be uniquely defined in the input WSS file by specifying the three quantities *molecular formula (composition)*, *material density*, and *crystal orientation*.

$$N(x) = \left(\frac{2}{a(x)} \right)^3 \cdot 10^{24} \quad (\text{Atoms/cm}^3), \quad (4.2)$$

$$\rho(x) = N(x) \left[(1-x) M_{\text{Si}} + x M_{\text{Ge}} \right] \cdot \text{amu} \cdot 10^6 \quad (\text{kg/m}^3). \quad (4.3)$$

Thermal lattice vibrations in silicon are considered in the crystalline partner selection model by using the Debye model with a Debye temperature value of 490K, as described in Section 3.1.2. Table 4.1 shows that germanium has a smaller Debye temperature value of 374K which corresponds to a smaller average vibration amplitude of the 2.6 times heavier germanium atom. We found by a comparison of simulated and measured implanted profiles that the model parameter value of 490K used for the simulation of silicon can also be applied for SiGe targets of arbitrary composition and pure germanium. Note that the used parameter value of 490K is close to the average value of the theoretical Debye temperatures in silicon and in germanium.

Nuclear and Electronic Stopping Power

The total stopping process of the ions in the target solid is modeled as a sequence of alternating nuclear and electronic stopping processes, as explained in Section 3.1.2 and in Section 3.1.3. The inverse transformation of the scattering integral (3.8) leads, amongst others, to (4.4) which determines the scattering angle ϑ of the ion in the laboratory system. The scattering angle ϑ depends on the scattering angle Θ in the center-of-mass coordinate system, on the mass M_1 of the ion, and on the mass M_2 of the involved atomic nucleus of the SiGe target.

$$\tan \vartheta = \frac{\sin \Theta}{\frac{M_1}{M_2} + \cos \Theta}. \quad (4.4)$$

From (4.4) it can be derived that if the ion is heavier than the target atom ($M_1 > M_2$), a maximal scattering angle $\vartheta_{\max} < 90^\circ$ exists according to

$$\sin \vartheta_{\max} = \frac{M_2}{M_1}. \quad (4.5)$$

For instance, if an arsenic ion hits a silicon atom then $\vartheta_{\max} = 22^\circ$, and if the arsenic ion hits the heavier germanium atom, a larger maximal scattering angle $\vartheta_{\max} = 69^\circ$ is possible. Due to the fact that the angles of subsequent collisions have to be added up for a turn around from the incident direction, the backscattering probability for dopant ions increases with the germanium content in the alloy.

The electronic stopping process is calculated with the empirical Hobler model. The only physical parameter required for this model is the impact parameter which is determined when selecting a collision partner. Due to the fact that the model implies a dependence on the charge and the mass of the atoms of the target material, the electronic stopping power is averaged in the case of a compound material like SiGe. The electronic stopping power of SiGe is larger compared with silicon, which is caused by the higher electron density due to the electron-rich germanium atom [98]. The calibration of the model for $\text{Si}_{1-x}\text{Ge}_x$ targets was performed by arranging the Lindhard correction parameter k_{corr} as a linearly rising function of the germanium fraction x . For the other three parameters of the model the values from crystalline silicon could be applied. We found the relations (4.6) and (4.7) by comparing simulated profiles with SIMS profiles, which determine the parameters $k_{\text{As}}(x)$ for arsenic and $k_{\text{B}}(x)$ for boron.

$$k_{\text{As}}(x) = 1.132 + 1.736 x, \quad (4.6)$$

$$k_{\text{B}}(x) = 1.75 + 0.375 x. \quad (4.7)$$

It is difficult to calibrate the electronic stopping model based on SIMS depth profiles for a couple of reasons. First of all, ion implantation experiments from different research groups exhibit a wide variation in results. Ziegler compared 48 papers on the range distributions of boron implantations in silicon and found a factor of about 2 for the variation in experimental results [17]. With sputter-profiling techniques, the first 10–20nm of the dopant concentration profile cannot be measured correctly due to transient sputtering effects such as preferential sputtering and implantation of the incident ions, which changes the total sputtering yield and distorts the profiles somewhat. Furthermore, it is fundamentally difficult to measure arsenic profiles in SiGe due to the presence of a severe mass interference at ^{75}As by ^{74}GeH [99]. Therefore, it is not possible to characterize arsenic profiles in SiGe by SIMS analysis with a resolution larger than about three orders-of-magnitudes below the maximum arsenic concentration.

4.1.2 Simulation Results and Discussion

We have studied the implantation of arsenic as an n-type and boron as a p-type dopant in crystalline SiGe layers with different germanium content. Fig. 4.2 shows simulated and measured arsenic implant profiles in $\text{Si}_{1-x}\text{Ge}_x$ layers with a thickness of 150nm on a silicon substrate. All implantations were performed with an energy of 60 keV, a dose of 10^{11} cm^{-2} , a tilt of 7° , and a twist of 15° . Two effects of the germanium content on the dopant profiles can be observed. Firstly, with increasing germanium fraction there is a shift towards shallower profiles. Secondly, the germanium content produces a stronger decline of the dopant concentration compared to silicon. It has been pointed out by interpretation of (4.5) that the heavier germanium atom produces an increased backscattering probability for the ions. The electronic stopping power of $\text{Si}_{1-x}\text{Ge}_x$ increases with the germanium fraction x and, therefore, causes a stronger decline of the concentration profiles. Fig. 4.3 demonstrates the successful calibration of the simulator for 38keV and 60keV arsenic implantations in $\text{Si}_{0.65}\text{Ge}_{0.35}$, using otherwise the same implantation conditions. The implanted boron profiles in SiGe layers with 53%, 63%, and 86% germanium content are very similar. Fig. 4.4 shows the simulated and measured result for a 20keV boron implantation into $\text{Si}_{0.47}\text{Ge}_{0.53}$. A native oxide of 1nm on the wafer surface was taken into account. Fig. 4.5 demonstrates again the effect of the germanium content on 5keV boron profiles. SiGe facilitates the forming of shallow junctions, but the trend to shallower profiles is non-linear.

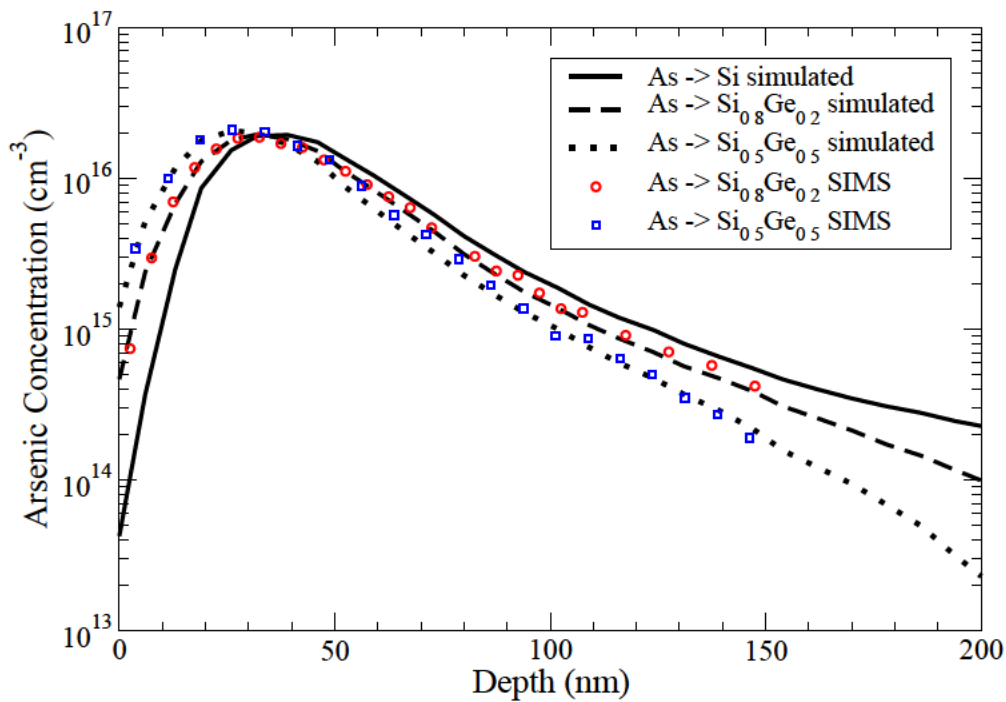


Figure 4.2: Simulated 60keV arsenic concentration profiles in (100) Si_{1-x}Ge_x layers with $x = 0, 20\%, 50\%$ compared to smoothed SIMS data.

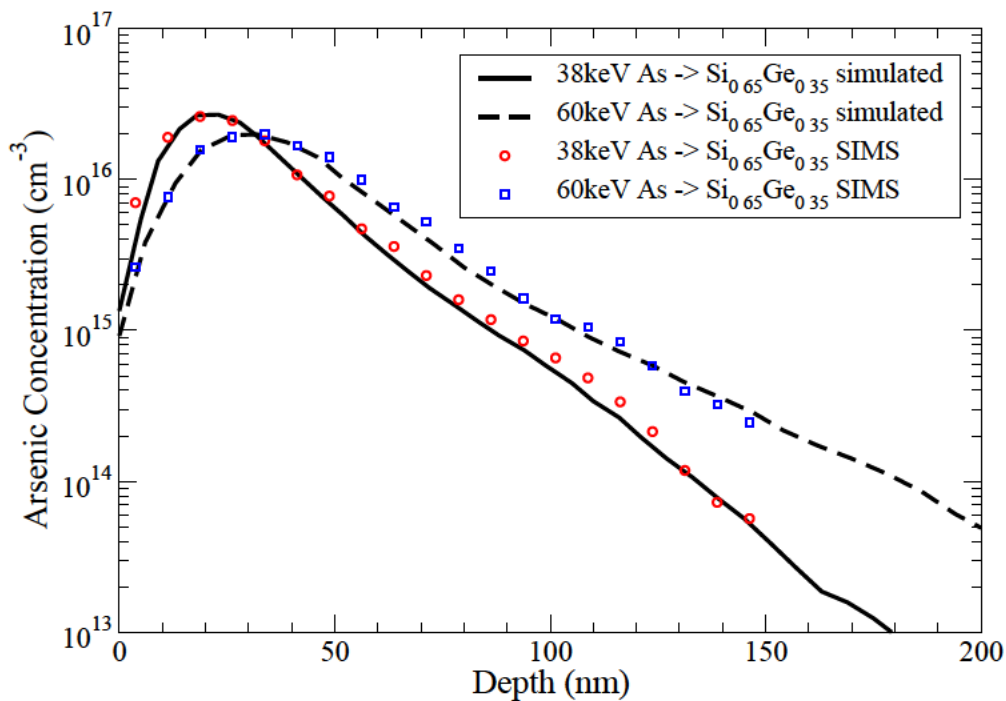


Figure 4.3: Simulated 38keV and 60keV arsenic profiles in (100) Si_{0.65}Ge_{0.35} layers compared to smoothed SIMS data.

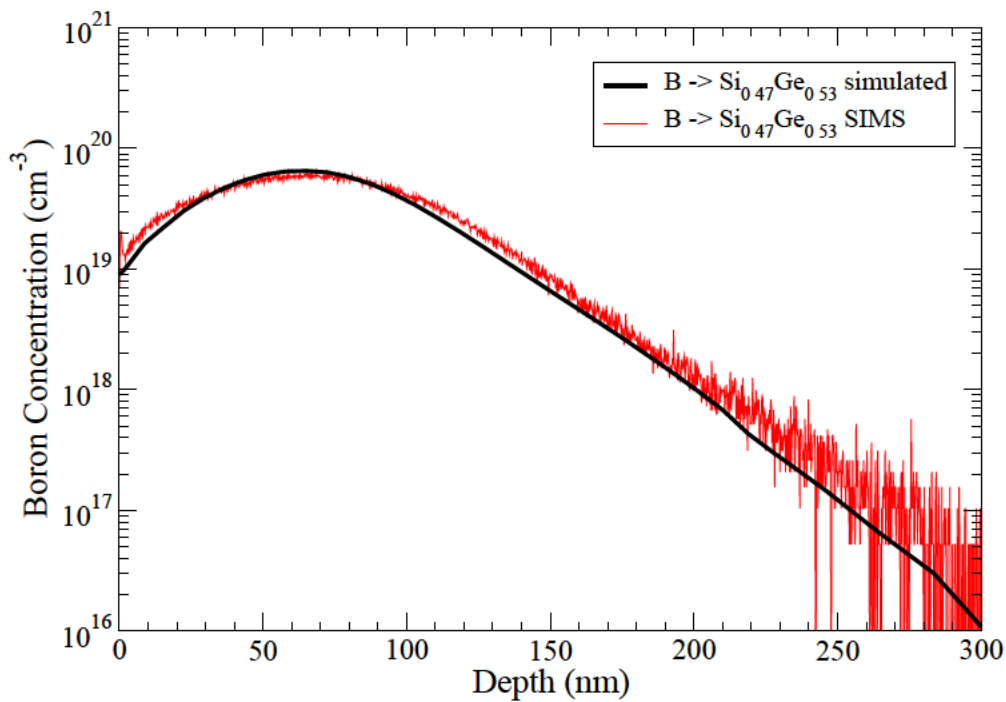


Figure 4.4: Simulated 20keV boron implant profile in (100) $\text{Si}_{0.47}\text{Ge}_{0.53}$ using a dose of $6 \cdot 10^{14} \text{cm}^{-2}$ and a tilt of 7° compared to SIMS.

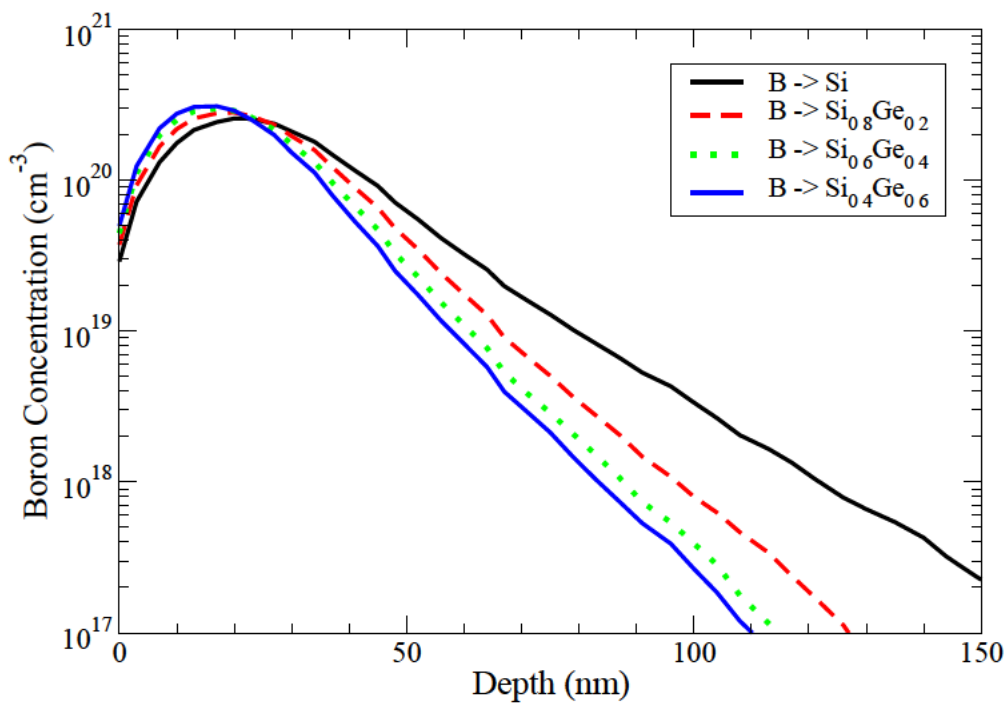


Figure 4.5: Simulated 5keV boron profiles in (100) $\text{Si}_{1-x}\text{Ge}_x$ with $x = 0, 20\%, 40\%, 60\%$ using a dose of 10^{15}cm^{-2} and a tilt of 7° .

4.2 Strained-Si/SiGe Heterostructure

Despite scaling the channel lengths into the sub-50nm regime, carrier mobility continues to be a critical parameter in scaled MOS devices and carrier transport remains far from ballistic [90]. This is partly because the mobility is degraded by increased channel doping (as predicted by the ITRS roadmap in Table 1.1 in Section 1.3). Strained silicon provides an attractive platform for building high-performance CMOS applications due to mobility enhancements compared to unstrained silicon. It turned out that strain-induced enhancements persist even at high channel doping levels, studied up to a dopant concentration of $6 \cdot 10^{18} \text{cm}^{-3}$ [100]. There are two dominant methods, global and local stress, for introducing strain in the silicon surface channel. Both methods produce changes in the silicon bandstructure due to breaking of the crystal symmetry, and hence alter carrier scattering and effective masses. Global stress techniques employ epitaxial technology to generate a thin layer of strained silicon on a thick relaxed $\text{Si}_{1-x}\text{Ge}_x$ layer. Local stress relies on process techniques such as modifications to shallow trench isolation, high-stress nitride-capping layers around the gate, and selective epitaxial $\text{Si}_{1-x}\text{Ge}_x$ in the sources/drain regions [101]. These techniques are effective in small device geometries where it is possible to induce uniaxial strain in the channel by stressing the regions around the channel. However, it turned out that the improvement in electron mobility using biaxially tensile strained silicon on relaxed $\text{Si}_{1-x}\text{Ge}_x$ is larger than that obtained for local stress techniques [88].

Fig. 4.6 shows the strained-Si/relaxed-SiGe heterostructure which is used to investigate the impact of strain on ion implantation. Relaxed SiGe layers are epitaxially grown on (100) silicon substrates using a grading technique to obtain the desired Ge composition. Next a constant composition layer is grown to spatially separate the subsequently grown strained silicon layer from the misfit dislocations contained in the graded SiGe layer. When silicon is grown on SiGe, the lattice mismatch between the two materials can be accommodated by uniform lattice strain

Strained Si
Relaxed $\text{Si}_{1-x}\text{Ge}_x$
Relaxed Graded $\text{Si}_{1-y}\text{Ge}_y$ $y = 0 \text{ to } x$
<100> Si Substrate

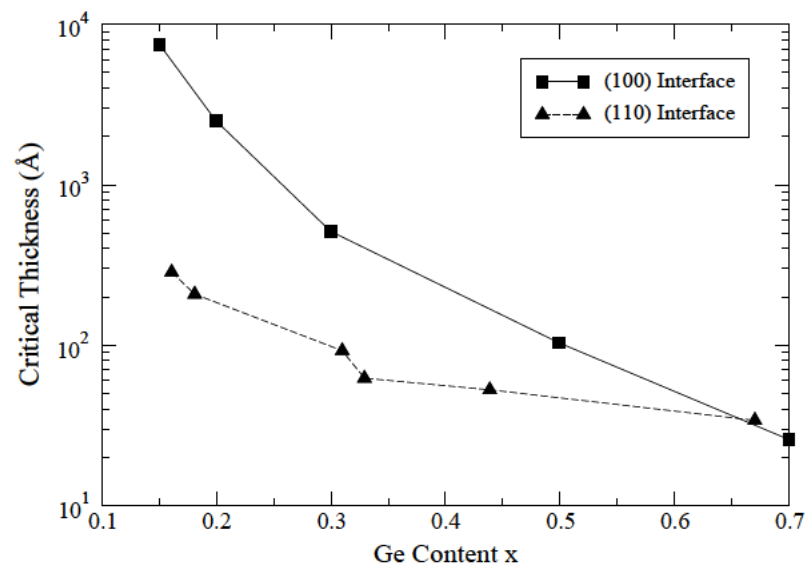


Figure 4.6: Schematic illustration of the strained Si/relaxed $\text{Si}_{1-x}\text{Ge}_x$ system (left) and experimental data for the critical thickness of strained silicon (right).

in sufficiently thin silicon layers [102]. If silicon is grown beyond its critical thickness, the strained crystal relaxes to its natural size and a high concentration of dislocations is introduced. Fig. 4.6 shows also typical experimental data for the critical layer thickness which depends on growth rates, growth temperature, SiGe surface orientation, and mostly on the Ge concentration [96].

4.2.1 Modeling of Biaxially Strained Silicon

A strained silicon channel is formed by a silicon layer with a thickness smaller than the critical thickness, epitaxially grown on the (100) surface of a relaxed $\text{Si}_{1-x}\text{Ge}_x$ buffer layer. The silicon layer is under biaxial tensile strain and the so-called *pseudomorphic interface* is characterized by an in-plane lattice constant $a_{\parallel}$ which remains the same throughout the heterostructure. By using the empirically determined parabolic relation (4.1) for the $\text{Si}_{1-x}\text{Ge}_x$ lattice parameter as a function of the Ge fraction x we obtain for strained silicon

$$a_{\parallel}(x) = 0.02733 x^2 + 0.1992 x + 5.431 \quad (\text{\AA}) . \quad (4.8)$$

The out-of-plane silicon lattice constant $a_{\perp}$, in the direction perpendicular to the interface plane, is reduced according to the continuum elastic theory [103],

$$a_{\perp}(x) = a_{\text{Si}} \left[1 - \frac{2C_{12}}{C_{11}} \left(\frac{a_{\parallel}(x)}{a_{\text{Si}}} - 1 \right) \right] \quad (\text{\AA}) , \quad (4.9)$$

where a_{Si} denotes the lattice constant of unstrained silicon, and C_{11} , C_{12} are the elastic constants of silicon ($C_{11} = 1.675$ Mbar, $C_{12} = 0.650$ Mbar at room temperature after [102]).

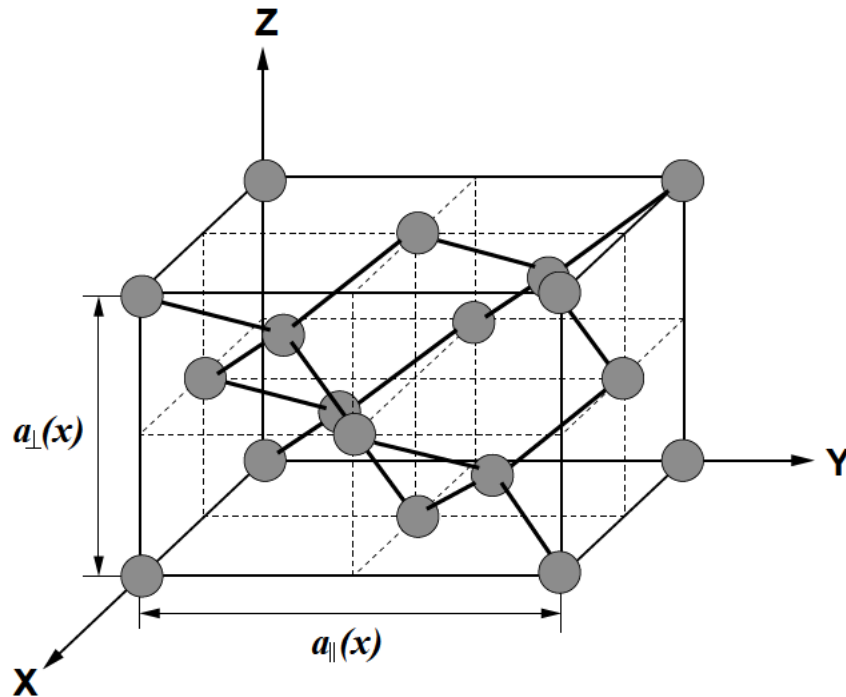


Figure 4.7: Crystal model for biaxially tensile strained silicon layers.

The constraints for the two lattice parameters in strained silicon are given by

$$a_{\perp}(x) < a_{\text{Si}} < a_{\parallel}(x) \quad \text{for} \quad 0 < x < 1. \quad (4.10)$$

The strain components parallel and perpendicular to the interface plane are then defined by

$$\varepsilon_{\parallel}(x) = \frac{a_{\parallel}(x) - a_{\text{Si}}}{a_{\text{Si}}} \quad \text{and} \quad \varepsilon_{\perp}(x) = \frac{a_{\perp}(x) - a_{\text{Si}}}{a_{\text{Si}}}. \quad (4.11)$$

Fig. 4.7 shows the strained unit cell with the edge lengths $a_{\parallel}$ and $a_{\perp}$, which can be used for the Monte Carlo simulation of ion implantation in strained silicon targets [104]. While the simulated ion moves through a strained silicon region, the strained crystal model from Fig. 4.7 is built up around the actual ion position for searching the next collision partner. The displacement energy of 15eV used for bulk silicon can be applied for strained silicon too. Due to the fact that the strained silicon lattice system is coherently aligned to the $\text{Si}_{1-x}\text{Ge}_x$ virtual substrate lattice, channeling ions can pass the interface between these two crystalline layers without being interrupted. While the implantation profiles in strained and unstrained silicon show only a very small difference at a given implantation energy, the penetration depth of ion-implanted dopants in relaxed $\text{Si}_{1-x}\text{Ge}_x$ is significantly reduced with increasing Ge fraction x , as demonstrated in Section 4.1. Thus the underlying $\text{Si}_{1-x}\text{Ge}_x$ layer helps to reduce the tail region of source/drain doping profiles in this heterostructure.

4.2.2 Ultra-Shallow Junction Formation

We study the implantation of boron as a p-type and arsenic as an n-type dopant in a silicon cap layer with a thickness of 12nm on a thick $\text{Si}_{0.8}\text{Ge}_{0.2}$ layer. Fig. 4.8 shows the simulated and experimental doping profile of a boron implantation with an energy of 400eV and a dose of 10^{15}cm^{-2} . Fig. 4.9 shows the arsenic implantation result, performed with an energy of 2keV and the same dose. The presented doping profiles demonstrate highly doped source/drain extension implants for a typical 65nm CMOS technology under the sidewall spacer, where lightly doped drain (LDD) structures used to be in previous technology generations.

Fig. 4.8 shows that the simulated boron profiles in strained and unstrained silicon are almost identically distributed, and the simulation result agrees well with the SIMS data. It is not possible to characterize arsenic concentration profiles in $\text{Si}_{1-x}\text{Ge}_x$ by SIMS analysis with a resolution larger than about three orders-of-magnitude due to similar atomic masses of arsenic and germanium [99]. As shown in Fig. 4.9 the Monte Carlo simulation can help to get a realistic continuation of the doping profile below the arsenic detection limit. The discrepancy between the predicted and measured doping profiles near the wafer surface may arise from a measurement error in this region. Feedback from industry revealed that this error can be eliminated by the deposition of amorphous silicon on the wafer before the SIMS measurement. Using this procedure, SIMS profiles show an increase in the near-surface region too. However, the simulation results in Fig. 4.9 demonstrate that the arsenic distribution in strained silicon has a slightly deeper penetration compared to unstrained silicon, which can be explained by a stress-induced volume dilation of the material. Strained silicon on $\text{Si}_{0.8}\text{Ge}_{0.2}$ has a strain $\varepsilon_{\parallel}(0.2) \approx 0.75\%$ and approximately 99% of the atomic density of unstrained silicon.

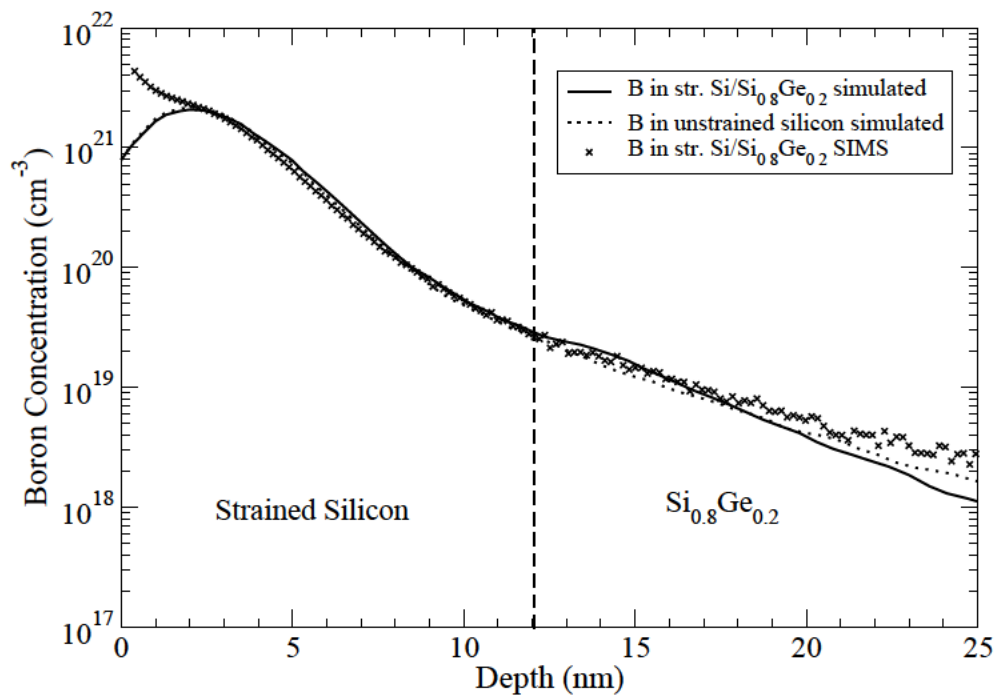


Figure 4.8: Simulated 400eV boron implant profile in a 12nm thick strained silicon layer compared to SIMS measurement.

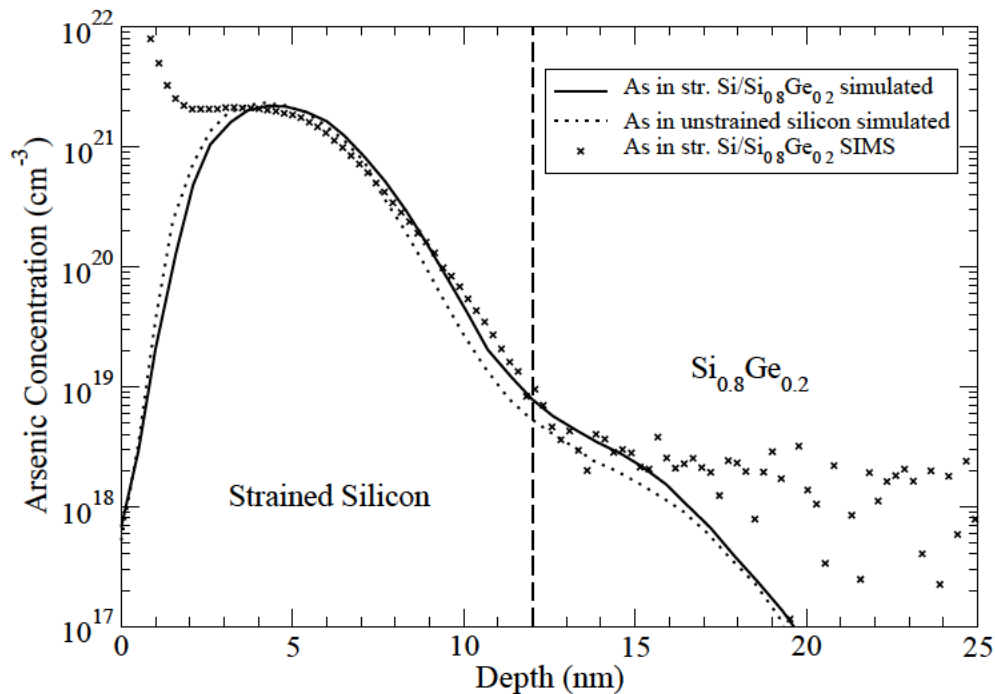


Figure 4.9: Simulated 2keV arsenic implant profile in strained silicon compared to SIMS data.

4.3 Germanium

Germanium has regained attention in the semiconductor industry for future silicon-compatible optoelectronic and advanced CMOS device applications. The carriers have lower effective masses and the intrinsic mobility is about two times higher for electrons and four times higher for holes in germanium compared to silicon, as shown in Table 4.2. Therefore, germanium offers the highest performance enhancement potential for channel engineering compared to bulk SiGe or strained silicon. On the one hand, the smaller band gap of germanium is advantageous to build photodetectors and, on the other hand, junctions made in a smaller band gap material will typically exhibit larger leakage currents.

In recent years, deep-submicron germanium MOS transistors have been processed in a silicon-like process flow by using either germanium oxynitride (GeO_xN_y) [105] or Hafnium oxide (HfO_2) based high-k dielectrics [106, 107] as the gate insulator. The diffusion of the p-type dopant boron is suppressed while the diffusion of the n-type dopants phosphorus, arsenic, and antimony is increased in SiGe and germanium compared with silicon [108]. Thus, the formation of ultra-shallow junctions in germanium is facilitated for p-MOS transistors, while it becomes more challenging for n-MOS devices. It was found in [107] that the junction leakage is about four decades higher for germanium at a chip temperature of 110°C compared with silicon. The reduction of the relatively large leakage current will be a key issue for Ge-CMOS technology to obtain devices with reasonably low I_{off} current. It is reported in [105], that the leakage current of boron implanted p^+/n junctions in germanium can be reduced down to the order of $10^{-4}\text{A}/\text{cm}^2$ with annealing at 400°C , which is considered acceptable for device operation. Ge-rich $\text{Si}_{1-x}\text{Ge}_x$ alloys ($x > 80\%$) and germanium have been recognized as promising materials for photodetectors in fibre-optical transmission systems due to the high optical absorption coefficient for an operation at a wavelength of $1.3\mu\text{m}$ in the near infrared (NIR) regime [109, 110]. The use of epitaxial Ge-on-Si technology allows the integration of germanium pin-photodiodes with CMOS circuits on a silicon chip to build optical communication receivers with low fabrication costs. Optical chip-to-chip communication solutions and even optical on-chip interconnects will be required to meet the challenges of differentiated, high-performance systems in the future.

Ion implantation is a crucial step for processing these device structures. An experimental and simulation study for introducing boron ions into (100) germanium wafers in the energy range from 5 to 40keV is presented in this section [112]. The successful calibration of the simulator MCIMPL-II for germanium is demonstrated by comparing the predicted boron profiles with SIMS data. A doping profile in germanium is shallower than in silicon for any given energy due to the larger nuclear and electronic stopping power. We found also that the produced crystal damage is significantly reduced in germanium, which is consistent with former experimental observations [113] indicating that boron-implanted germanium remains essentially crystalline.

Properties	Germanium	Silicon
Band gap (eV)	0.66	1.12
Electron mobility ($\text{cm}^2/\text{V-s}$)	3900	1500
Hole mobility ($\text{cm}^2/\text{V-s}$)	1900	450

Table 4.2: Important electronic properties of germanium vs. silicon at 300K [111].

4.3.1 Modeling of Ion Implantation in Germanium

The extended crystalline simulation model presented in Fig. 4.1 can be applied to germanium by using the maximum lattice parameter value $a(1) = 5.6575\text{\AA}$ and a probability of 100% for meeting a germanium atom at the next collision event. In a screened Coulomb collision the energy loss of the ion, ΔE , is equal to the transferred energy to the recoil atom,

$$\Delta E = \frac{4 M_1 M_2}{(M_1 + M_2)^2} \cdot \sin^2 \frac{\Theta}{2} \cdot E_0, \quad (4.12)$$

where M_1 and M_2 are the masses of ion and target atom, Θ is the transformed scattering angle in the center-of-mass coordinates, and E_0 is the kinetic energy of the ion before the collision event. From this equation it can be derived that a smaller energy loss ΔE occurs in nuclear collisions in germanium due to the different masses between ion and atom. The transferred energy ΔE from a boron ion to a germanium atom is approximately the half (0.568-fold) compared to ΔE in silicon at a given scattering angle. Note that the difference in masses between boron and germanium leads also to a strong backscattering effect for the light boron ions.

An advantage of the Monte Carlo simulation is that the used Kinchin-Pease model (as described in Section 3.1.4) allows to estimate the produced vacancies in the germanium crystal. Note that equal local concentrations of vacancies and interstitials are assumed, since the recoils themselves are not individually followed in our computationally fast simulation approach. However, a critical model parameter is the threshold displacement energy required for the ion to displace a target

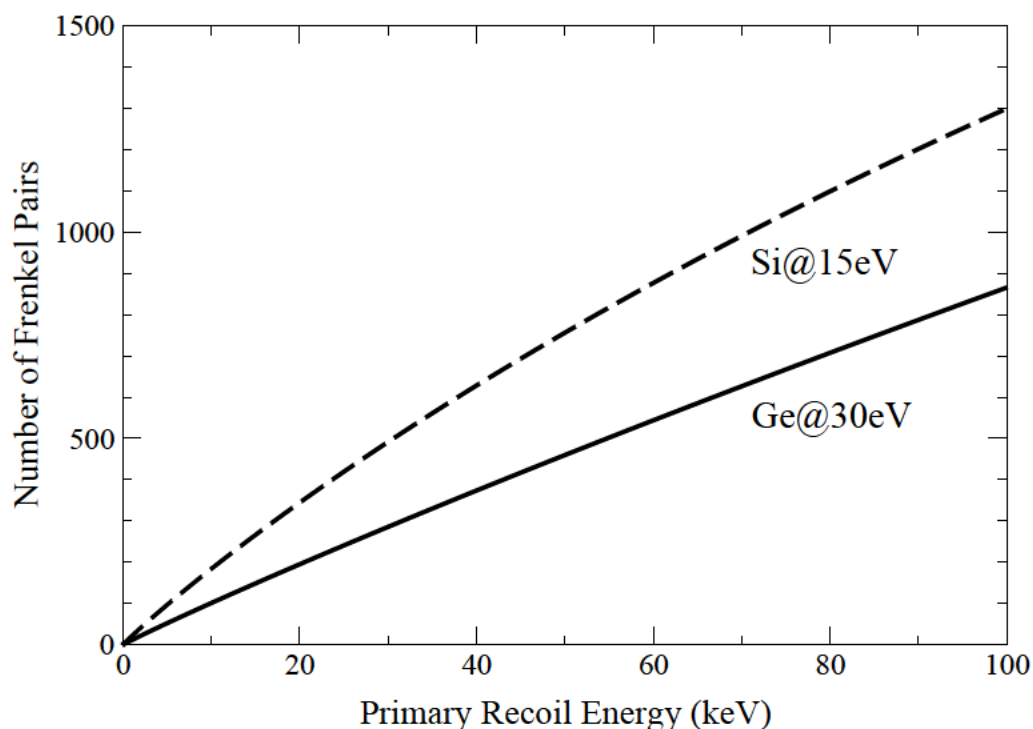


Figure 4.10: Number of Frenkel pairs generated by a primary knock-on atom in Si and in Ge, assuming a displacement energy of 15eV and 30eV.

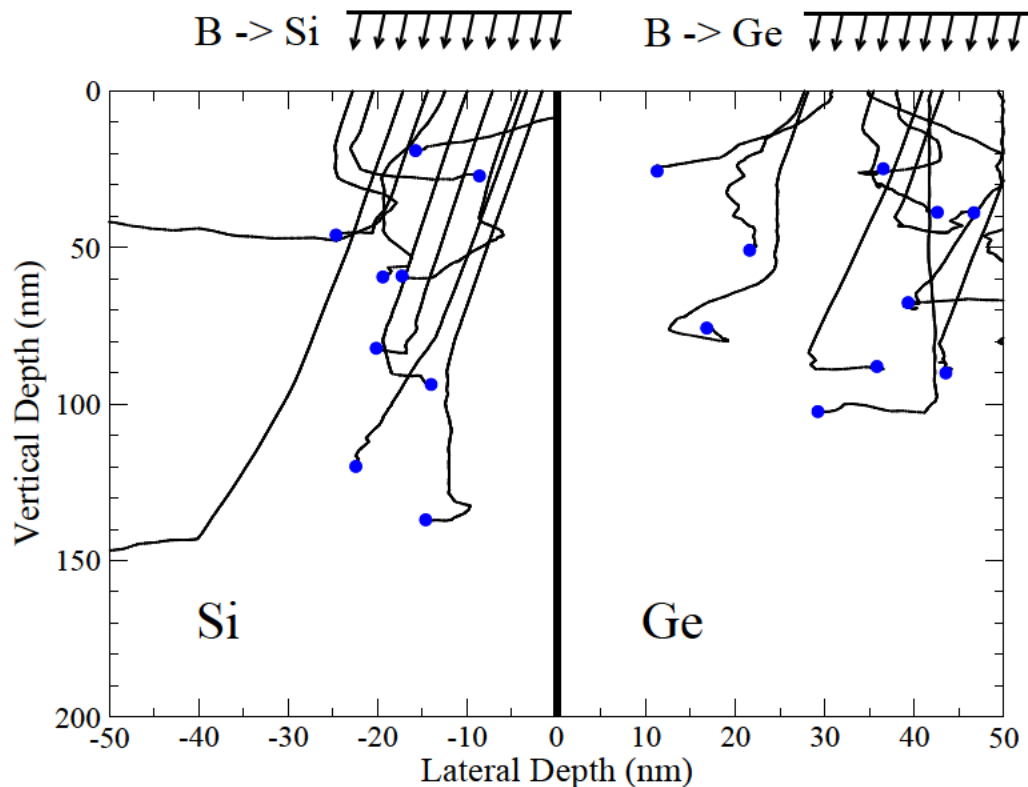


Figure 4.11: Comparison of the Monte Carlo simulation of ten boron trajectories in silicon and in germanium using an energy of 10keV and a tilt of 7° .

atom. A displacement energy E_d of 15eV has become widely accepted for silicon. We fitted a value of $E_d = 30\text{eV}$ for germanium by comparison of simulated boron profiles with SIMS measurements. Fig. 4.10 shows the number of produced point defects for a damage cascade, calculated with the modified Kinchin-Pease model. The used value for the displacement energy in germanium is in good agreement with $E_d = 31\text{eV}$ which was deduced by Mitchell in 1957 for germanium [114]. The larger E_d value is responsible for the generation of significantly fewer point defects by a boron ion in germanium compared with silicon for any amount of transferred energy ΔE to the primary knock-on atom of a cascade. The reduced damage production by ion implantation in crystalline germanium is consistent with former experimental observations [113].

The Lindhard correction parameter k_L of the empirical electronic stopping model, which is explained in Section 3.1.3, has been calibrated to adjust the strength of the electronic stopping power for boron ions in germanium. We increased the empirical parameter value from $k_L = 1.75$ for silicon to a value of 1.9 for germanium.

In the following simulation study, at least 10^6 trajectories were calculated for a one-dimensional boron profile. Fig. 4.11 shows the visualization of ten arbitrarily selected boron trajectories in silicon and in germanium. This comparison demonstrates that the larger nuclear and electronic stopping power of germanium, in particular the stronger backscattering of boron ions in germanium, typically reduces the trajectory length.

4.3.2 Simulation Results and Discussion

Germanium has a larger nuclear and electronic stopping power for incoming ions due to the heavier atomic mass and higher electron density. For this reason, an implanted dopant profile in germanium is significantly shallower than in silicon and SiGe for any given implantation energy. Fig. 4.12 shows that the calibrated simulator can accurately reproduce the measured 20keV boron concentration profiles implanted with a dose of $6 \cdot 10^{14} \text{cm}^{-2}$ in amorphous and in crystalline germanium targets. The amorphization of germanium was performed by the implantation of ^{72}Ge ions with an energy of 200keV and a dose of 10^{15}cm^{-2} . A channeling tail can be observed for the profile in crystalline germanium. Fig. 4.13 demonstrates a good agreement between the simulated and measured boron profiles implanted with a lower energy of 5keV and a lower dose of $3 \cdot 10^{13} \text{cm}^{-2}$. Fig. 4.14 compares simulated 20keV boron profiles in silicon and in germanium. We found the projected range R_p of the boron distribution in $\text{Si}_{0.5}\text{Ge}_{0.5}$ at a depth of 65nm, which lies well within the boundaries defined by the projected ranges in germanium at 55nm and in silicon at 80nm. Table 4.3 summarizes simulated and measured R_p and σ_p parameters for boron implants in crystalline silicon, $\text{Si}_{0.5}\text{Ge}_{0.5}$, and germanium targets. The projected range R_p is read off at the maximum concentration of a boron distribution and the provided straggling σ_p is the average value of the left and right straggling values which are determined by 60% of the maximum boron concentration. The results in the table were obtained with an implantation dose of 10^{14}cm^{-2} and a tilt of 7° .

Fig. 4.15 compares the simulated vacancy concentration profiles in silicon and in germanium associated with the 20keV boron implantations shown in Fig. 4.14. The vacancy maximum is not at the wafer surface, since the electronic stopping process dominates at high initial energies of the ions, when they enter the crystal. A boron ion enters most likely a channel at the surface and despite of the tilted incident direction it can stay at least a short distance inside a channel. The higher displacement energy of 30eV, the stronger backscattering of boron ions in germanium, and the smaller energy transfer ΔE from the ion to the primary recoil of a cascade are mainly responsible for the significantly smaller damage production in germanium. Previous experimental boron implantation results in germanium [113] performed up to a dose of 10^{14}cm^{-2} within the energy range of 25–150keV revealed that 100% of the boron ions are immediately active after implantation without thermal annealing since boron-implanted germanium remains crystalline. This is a unique phenomenon, since an annealing step is required for every other dopant species implanted in silicon or germanium in order to activate a significant amount of dopants. Finally, Fig. 4.16 illustrates the dose dependence of 40keV boron profiles in germanium, which were simulated with the Kinchin-Pease model. It is obvious that the shape of the profiles is influenced by the damage accumulation in the crystal.

Cryst. Material	Si	$\text{Si}_{0.5}\text{Ge}_{0.5}$	Ge	Si	$\text{Si}_{0.5}\text{Ge}_{0.5}$	Ge
Energy (keV)	5	5	5	20	20	20
R_p (nm)	18.91	15.44	14.32	79.52	65.32	55.27
σ_p (nm)	14.16	12.56	12.16	37.42	36.33	39.38
SIMS R_p (nm)	-	-	16.23	-	67.11	56.99
SIMS σ_p (nm)	-	-	11.23	-	40.58	34.91

Table 4.3: Projected range and straggling parameters for boron distributions.

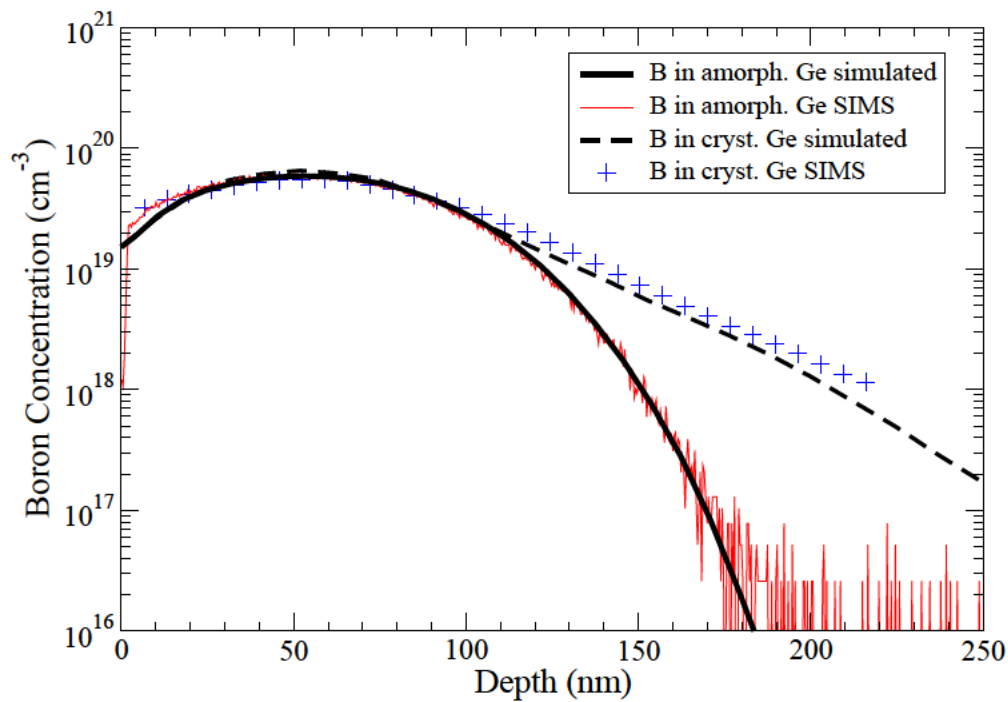


Figure 4.12: Simulated 20keV boron implantations in amorphous Ge and in (100) Ge using a dose of $6 \cdot 10^{14} \text{cm}^{-2}$ and a tilt of 7° compared to SIMS profiles.

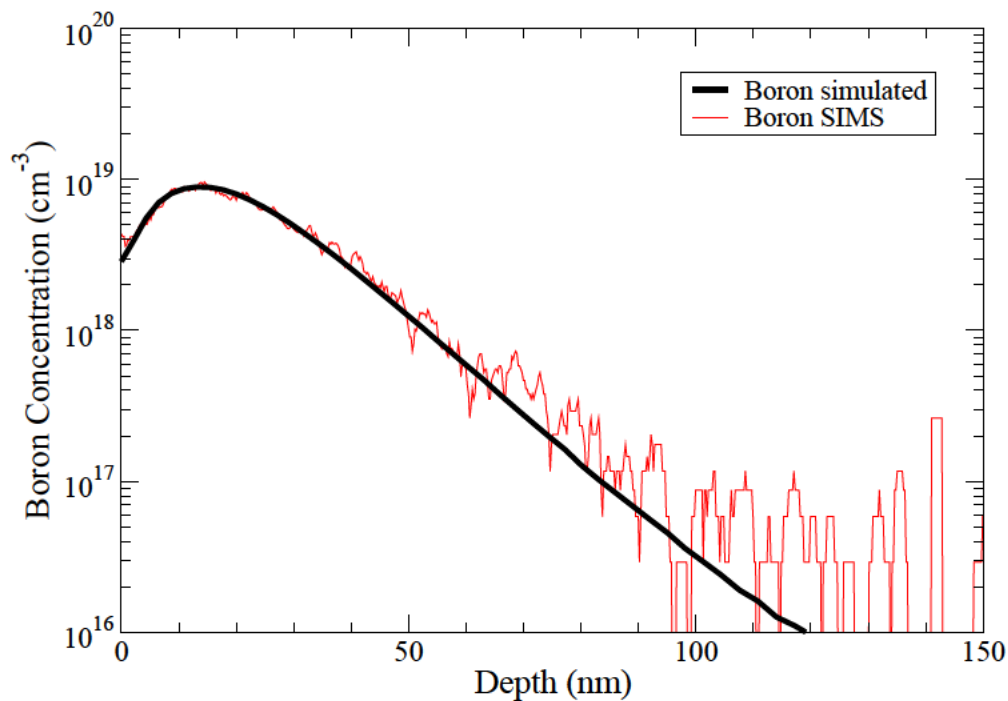


Figure 4.13: Simulated 5keV boron profile in (100) Ge using a dose of $3 \cdot 10^{13} \text{cm}^{-2}$ and a tilt of 7° compared to SIMS measurement.

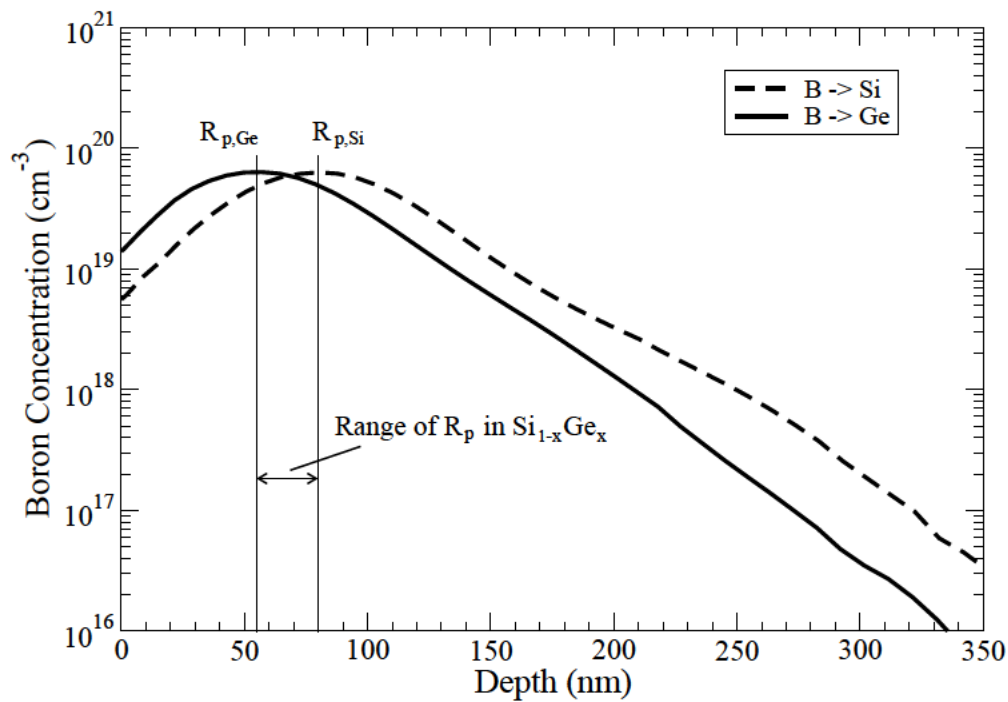


Figure 4.14: Comparison of simulated 20keV boron implant profiles in silicon and germanium using a dose of $6 \cdot 10^{14} \text{ cm}^{-2}$ and a tilt of 7° .

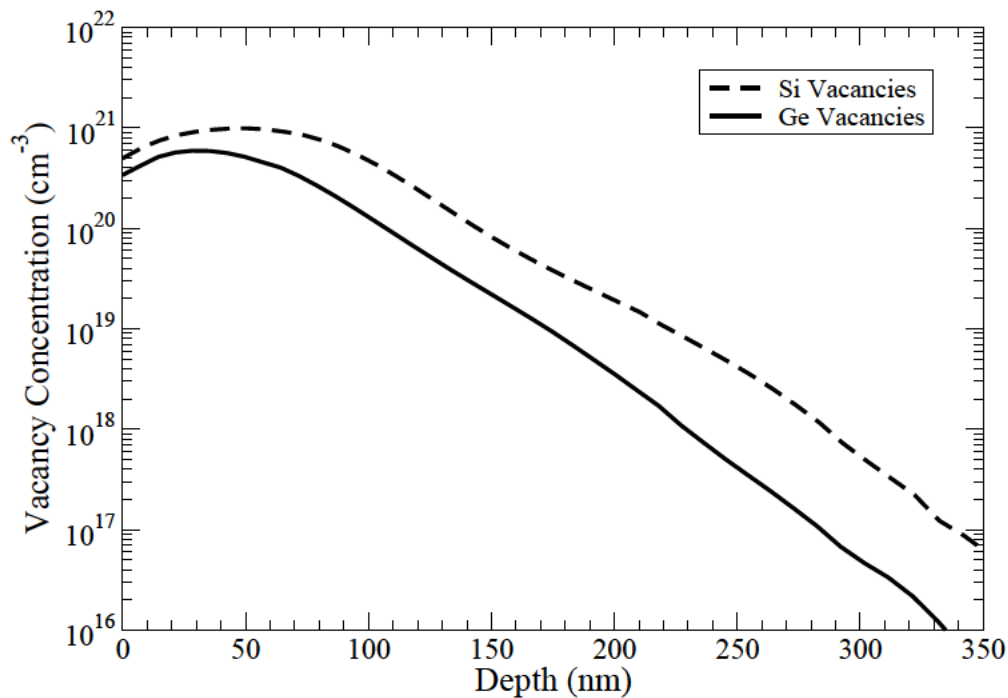


Figure 4.15: Comparison of produced vacancies for the 20keV boron implantations in silicon and germanium using a dose of $6 \cdot 10^{14} \text{ cm}^{-2}$ and a tilt of 7° .

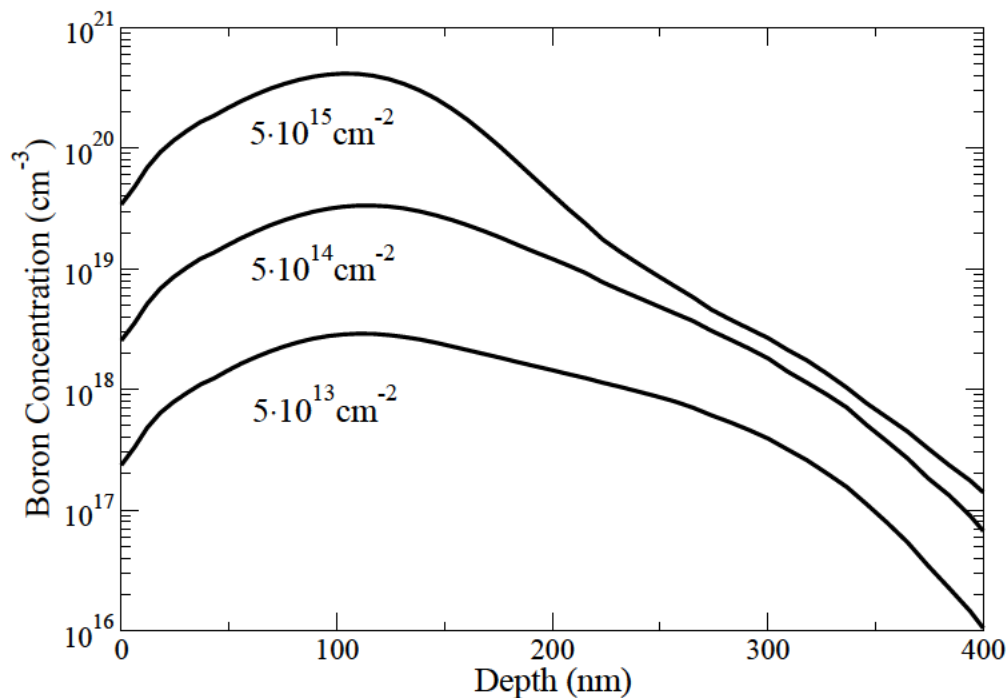


Figure 4.16: Simulated 40keV boron implants in (100) Ge at doses of $5 \cdot 10^{13}$, $5 \cdot 10^{14}$, and $5 \cdot 10^{15} \text{ cm}^{-2}$ using a tilt of 7° .

The simulated point responses in crystalline silicon and germanium are shown in Fig. 4.17 and Fig. 4.18 to study quantitatively the lateral and vertical penetration of boron ions. The used two-and-a-half dimensional input geometry has a depth dimension of 40nm, and the slot width of the implantation window in an impenetrable mask is 8nm. A high-resolution mesh which consists of 33181 grid points and 144159 tetrahedrons is added to the input structure to resolve the implanted boron distribution. Boron is implanted with an energy of 10keV, a dose of $5 \cdot 10^{15} \text{ cm}^{-2}$, and the ion beam is 7° tilted in such a way that the lateral component of the incident direction is parallel to the direction of view ($\langle 010 \rangle$ direction). Therefore, the presented point responses are symmetric. Approximately 420000 simulated boron ions of a total number of 50 million ions can enter the substrate at the mask opening and contribute to the Monte Carlo result represented by the internal histogram cells.

The visualization of single trajectories in silicon and in germanium (as shown in Fig. 4.11) and in particular the comparison of the point responses indicate that the boron distribution in germanium is significantly reduced in the vertical direction, while the lateral profile is quite similar in silicon and germanium. Additionally, it can be observed that the channeling tail is closely centered around the $\langle 100 \rangle$ axis in both cases. This demonstrates that in (100) silicon and in (100) germanium, axial channeling in the $\langle 100 \rangle$ direction dominates by far over channeling in other directions.

As demonstrated in this study, the used physics-based simulation approach in combination with experimental results allows to get a comprehensive understanding of implantation-related phenomena in germanium.

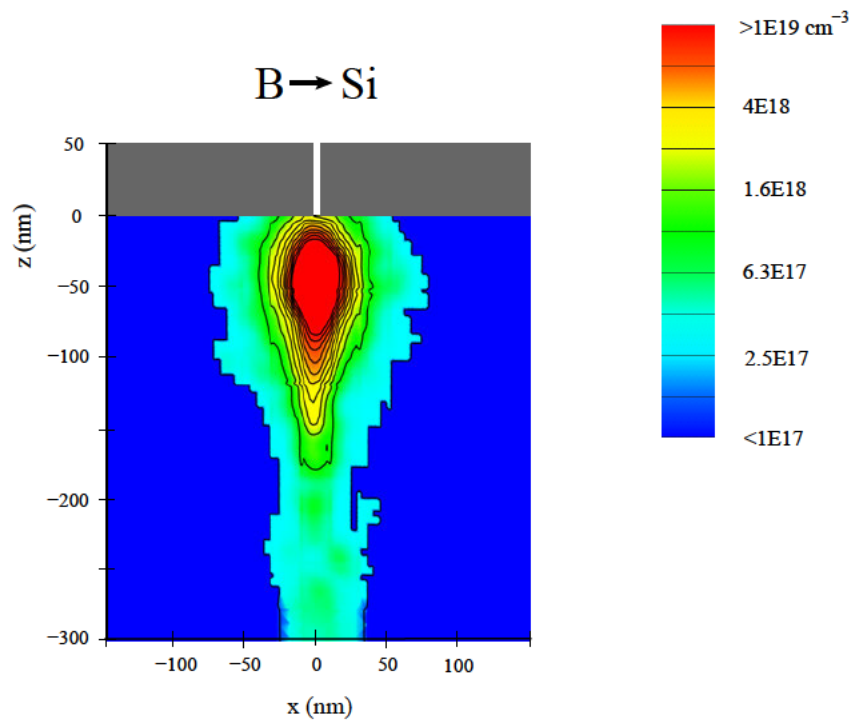


Figure 4.17: Simulated point response for a 10keV high-dose implantation of boron into crystalline silicon.

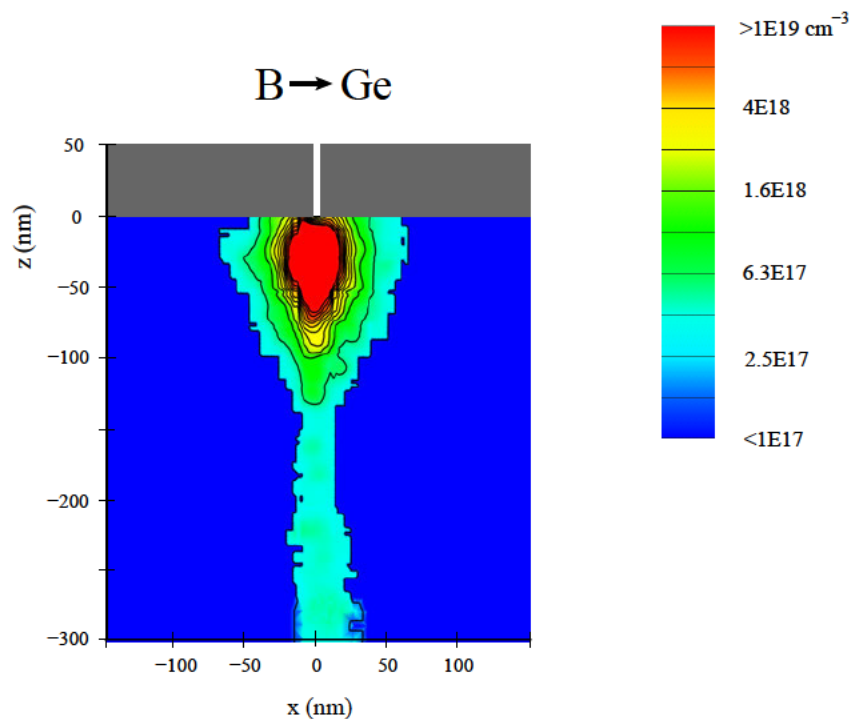


Figure 4.18: Simulated point response for a 10keV high-dose implantation of boron into crystalline germanium.

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